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SECTION OF

**CHEMICAL SCIENCES**



*President*  
**Prof. A. K. Bakhshi**



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OF THE  
NINETY NINTH SESSION OF THE  
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**PART II**

**SECTION OF  
CHEMICAL SCIENCES**

*President: Prof. A. K. Bakhshi*

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# **99<sup>th</sup> Indian Science Congress**

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## **I**

### **PRESIDENTIAL ADDRESS**

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# Theoretical Designing of Novel Low Band Gap Conducting Polymers

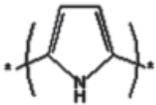
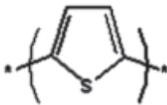
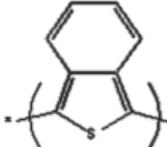
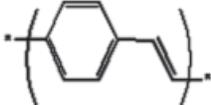
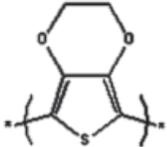
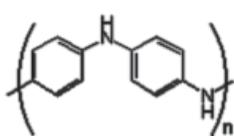
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## 1. Introduction

In the fascinating world of polymers, conducting polymers have always been the focus of attraction. The low electrical conductivity of polymers has been immensely used in the manufacture of insulators and dielectric substances. According to a report entitled “Conductive Polymers-Global Strategic Business Report”, published by Electronics.ca on March 23, 2011, **the US market for conductive polymers is forecast to reach 240.5 thousand tons by the year 2015**. Conductive polymers market is expected to grow at a healthy rate due to various advantages offered by these electricity-conducting plastics. Lightweight, easy fabrication, low cost and high resistance to heat is driving the growth of conductive polymers market in the United States. Rising demand for high performance and low cost materials for electrical and electronics product components and devices are likely to augment the conductive polymers utilization by the electronics industry.

Conductive polymers are organic polymers that conduct electricity. Such compounds may have metallic conductivity or can be semiconductors. The conductivity of such polymers is the result of several processes. Conducting polymers have backbones of continuous  $sp^2$  hybridized carbon centers. One valence electron on each center resides in a  $p_z$  orbital, which is orthogonal to the other three sigma-bonds. The electrons in these delocalized orbitals have high mobility when the material is “doped” by oxidation, which removes some of these delocalized electrons. Thus, the conjugated p-orbitals form a one-dimensional electronic band, and the electrons within this band become mobile when it is partially emptied. An increasing number of academic, governmental and industrial laboratories throughout the world are involved in basic research and assessment of possible applications of conducting polymers<sup>1-4</sup>. Figure 1 shows the chemical structures of most commonly studied conjugated polymers. These polymers have a wide range of conductivities despite having many structural similarities.

Polyacetylene (PA)		Polypyrrole (PPy)	
Polythiophene (PTP)		Polyparaphenylene (PPP)	
Polysothianaphthene (PITN)		Polyparaphenylene vinylene (PPV)	
Polyethylene dioxythiophene (PEDOT)		Polyaniline (PANI)	

**Fig. 1:- Chemical structures of monomers of most commonly studied conjugated polymers.**

Being semiconductors, CPs do not conduct unless free charge carriers are produced by excitation of electrons from the valence into the conduction band<sup>5</sup> or by chemical or electrochemical oxidation or reduction<sup>6</sup> referred to as p- and n-doping, respectively. The coupling between electronic and structural changes is known as electron-phonon coupling. The entity consisting of charge and associated geometry distortion is known as a “polaron”. Upon removal of a second electron either a second separate polaron may form or, a “bipolaron”, if the second electron is removed from the same site as the first<sup>7, 8</sup>.

The aim of theoretical investigation of conducting polymers (CPs) is, firstly, to understand electrical and optical properties and secondly, to design new systems with specifically tailored properties depending on molecular structure. Theoretical design of CP implies that their key properties i.e. structures in the neutral, doped, and excited states, IPs, EAs, band gaps, and band widths, can be predicted from theoretical calculations depending on their chemical structure. Band-gap of a polymer is a measure of

#### Section IV: Chemical Sciences

its ability to show intrinsic conductivity, while IP and EA values of a polymer determine its ability to form conducting polymers through oxidative and reductive doping respectively. The problems related to the industrial bulk applications of CPs namely low solubility and processibility explain the sudden emergence for the need of bandgap control. A key requirement for a polymer to become intrinsically electrically conducting is that there should be an overlap of molecular orbitals to allow the formation of delocalized molecular wave function. Reduction of the bandgap ( $E_g$ ) will enhance the thermal population of the conduction band and thus increase the number of intrinsic charge carriers. Besides this, molecular orbitals must be partially filled so that there is a free movement of electrons throughout the lattice. The decrease of  $E_g$  can also lead to true “organic metals” showing intrinsic electrical conductivity without resorting to oxidative or reductive doping. The lower oxidation potential associated with narrow gaps will result in a stabilization of the corresponding doped state.

From the moment polymers were found to be able to conduct electricity, upon appropriate doping, a number of technological applications have been implemented and a large number of other applications are envisioned. Applications of conducting polymers are driven by the unique combination of electronic, mechanical, as well as fabrication properties of this class of materials. The delocalized electronic structure enables high electrical conductivity which in conjunction with traditional properties of polymers (e.g., good mechanical properties, ease of fabrication, low cost, and low weight) enable conducting polymers to be commercially important. Li *et al*<sup>9</sup> have recently reported the synthesis and electrochemical applications of the composites of conducting polymers. These conducting organic molecular electronic materials have attracted much attention largely because of their many projected applications in solar cells, light weight batteries<sup>10</sup>, electrochromic devices, sensors and molecular electronic devices. Polymeric heterojunctions, solar cells have been fabricated by electrochemical deposition of PPY on n-silicon. Many conducting polymers such as polyacetylene, polythiophene, polyindole, polypyrrole, polyaniline etc. have been reported as electrode materials for rechargeable batteries<sup>11</sup>. It has been reported that the conducting polyheterocycles are good candidates for electrochromic displays and thermal smart windows<sup>12</sup>. The potential for conducting polymers in the area of electronics and photonics (nonlinear optics)<sup>13</sup> is enormous and has been used to fabricate diodes, capacitors, field-effect transistors (FET) and printed circuit boards.

## 2. Band gap engineering

Intensive research has been dedicated to synthesizing novel conjugated polymers with high conductivity upon doping. The process of doping of electrically conducting polymers is often the source of chemical instability in them. Another problem often associated with doped polymers is their poor processibility which is due to the insolubility and infusibility of these polymers. The possible elimination of doping in preparing conducting polymers while still achieving high conductivity is one of the original motivations for band gap engineering of polymers. Band gap engineering of conjugated polymers refers to the tuning of band gap to obtain desired properties or functionality. It includes band gap minimization and processibility improvement. Many researchers have focused on synthesizing conjugated polymers with small or even zero band gaps ( $E_g$ ) (figure 2) because of their expected good intrinsic electrical conductivity<sup>13</sup> and nonlinear optical properties<sup>14</sup>.

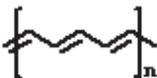
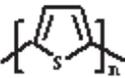
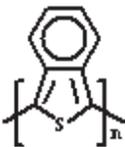
Name	Structure	Band gap (eV)
1. Trans-PA		
2. Polythiophene		2.1
3. Polyisothianaphthene		1.0
4. Polyisnaphthothiophene		1.4

Fig. 2:- Some low band gap conjugated polymers.

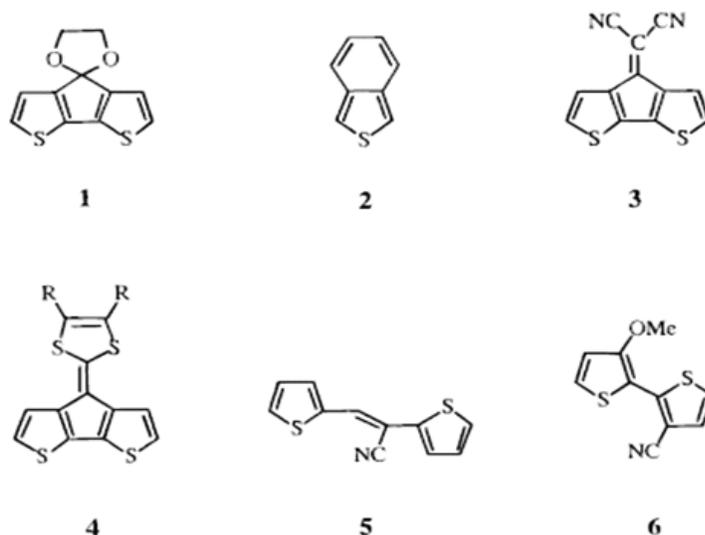
Still at the present moment, the development of stable, processable polymeric materials with a low band-gap is an important issue for further advancements in these fields. Thus, substantial efforts have been devoted to the design of conjugated organic

polymers with a small band-gap. Several parameters control the band gap of conducting polymers, including bond length alternation, inter-ring torsion angle, resonance energy, inter-chain effects and substituent effects<sup>15</sup>. Based on these parameters, several strategies for obtaining narrow-band gap systems have been suggested. These include:

## **2.1. Substitution/Fusion**

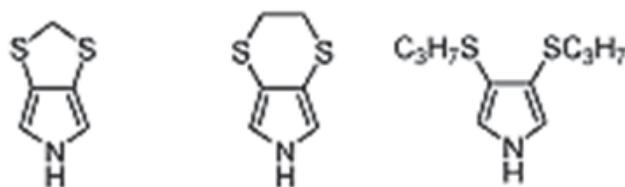
Various kinds of substituents are in use for improving solubility, decreasing band gaps, increasing polarizabilities, and optimizing luminescence efficiencies. Alkyl substituents on the backbone of polythiophene are often employed for increasing the solubility of polymer <sup>16</sup>, for example, polar substituents on polymer backbone increase hydrophilicity. Electropolymerization of **1** (figure 3) resulted in a polymer that is water-soluble and fully electroactive in aqueous solution <sup>17,18</sup>. The effect of substituents on band gap reduction, however, is not known very properly. In particular, dicyano <sup>19,20</sup> groups and dithia groups such as those in **3** and **4** were shown to reduce the band gap. In **3** the band gap reduction is mainly due to lowering of the LUMO level, while the effect on the HOMO was found to be moderate, while the origin of band gap reduction in case of dithia group is not well-understood. In contrast, introduction of a CN-substituted conjugated spacer group (cf. **5**) decreases the band gap by raising the HOMO level<sup>21,22</sup>. Alternating donor-acceptor units (**6**) are used to design polymers with low band gaps <sup>23,24</sup> and large polarizabilities. Rigidification of polymer precursors by employing fused ring systems was expected to reduce band gaps by increasing order. However, band gap reduction was not generally observed. Thermal stability of polymers due to azobenzene substituents in the main chain have been studied by Izumi et al. <sup>25</sup>. A series of cyano-substituted distyryl benzenes have also been synthesized <sup>26</sup> and it was observed that by properly adjusting copolymer compositions, combined properties of high electron affinity and transport were achieved. Recent studies on PA and polydifluoroacetylene (PDFA) <sup>27</sup> have shown that fluoro substitution of PA leads to narrower valence and wider conduction bands due to  $\sigma$ -donating ability of fluorine but no remarkable differences in the band gaps. PDFA was found to be an excellent candidate for n-type conductor.

Chart 1



**Fig 3:- Substituted polythiophenes**

Investigations of monomeric 3,4-disubstituted pyrroles <sup>28</sup> (figure 4) and corresponding polymers has suggested that the electron donating alkylthio substituents at the 3- and 4-positions of the pyrrole ring play an important role for the electrochemical properties of polymers.



**Fig 4:- Substituted pyrroles**

A series of novel low band gap polymers: poly(heteroarylene methines), soluble in common organic solvents were synthesized recently <sup>29</sup>. Electrochemical band gaps as low as 1.60, 1.68 and 1.76 eV were reported for the polymers PDTDOBQ-Me, PDTDOBQ-ORBr and PDTDOBQ-NO<sub>2</sub>, respectively.

Substitution also has some undesirable side effects. Bulky substituents induce deviations from planarity and decrease conjugation. Substituents such as the cyano group

that lower the HOMO level of the monomer increase the oxidation potential required for electrochemical polymerization. A substituent might change the structure and quality of the produced polymer to such an extent that analysis of intrinsic electronic effects of the substituent is difficult or impossible. Therefore, a detailed understanding of electronic effects is still lacking. Although in some cases, substitution may decrease the conductivity of the polymer but the resulting polymer has higher EA and therefore, can be used in LEDs.

Aniline oligomers substituted with electron-donor groups have been synthesized and their electronic properties calculated<sup>30</sup> through some semi-empirical quantum chemistry calculations. The studied substituents include methoxy, methyl, fluorine, nitro, and cyano groups, located at positions 2 or 3, in the benzenoid ring which have a large range of  $\sigma$ - $\delta$  electron donor-acceptor capability. The studies revealed that cyano and the nitro groups ( $\sigma$ - $\delta$  acceptor) induce an increasing of the ionization potential. Theoretical analysis of the orbital energies of molecules substituted with electron-acceptor groups shows a lowering of the LUMO energy values larger than those in the HOMOs cases. Thus, oligoanilines substituted with electron-acceptor groups (especially nitro groups) show the lowest energy. Conducting and highly stable alkoxy functionalized polythiophenes have been prepared<sup>31</sup> by Grignard Metathesis method<sup>32</sup>.

## **2.2. Ladder Polymerization**

Another way of canceling the bond-length alternation is reducing or eliminating the structural deformations that lead to the localization of alternating double and single bonds along the conjugated main-chain. This can be done by the construction of ladder polymers. Ladder structures are formed by joining simple polymers into symmetrical polymeric rings. The small energy-gap in ladder polymers is a consequence of the direct interplay of electron-lattice and lattice-lattice interactions in them<sup>33-35</sup>. This class of polymers, frequently referred to as one-dimensional graphite family, includes polyacene (PAC), polyacenacene (PACA), polyphenanthrene (PPh), polyphenanthro-phenanthrene (PPhP) and polyperinaphthalene (PPN). Polyacenes belong to a class of polycyclic aromatic hydrocarbons which are planar sets of linearly fused benzene rings with the general formula  $C_{4n+2}H_{2n+4}$ . Several molecules of this family are known to have interesting electronic and optical properties potentially applied to new materials<sup>36</sup>. Recently, four ladder type oligo-p-phenylene have been synthesized by Katz et al<sup>37</sup>. They have been used in copolymers to provide a deeper HOMO level for obtaining polymer solar cells with high open-circuit voltage.

In the case of fused ring polymers, the electronic properties are found to depend strongly on the particular way the rings are fused and the recognition of this has led to the employment of topological methods based on the concept of topomers. It has been used to rationalize<sup>38</sup> the large differences in the electronic properties of fused ring polymers such as polyacene, polyphenanthrene and polybenzanthracene. Polyisophenanthrene is predicted to have a band-gap between polyacene and polybenzanthracene. Ladder polymer (polyindenoindenes) consisting of condensed succession of six and five membered conjugated carbon rings have been synthesized. Seven topological isomers of these polyindenoindenes are considered theoretically. Three of the isomers are expected to have a band-gap smaller than 0.2 eV<sup>39</sup>.

### **2.3. Copolymerization**

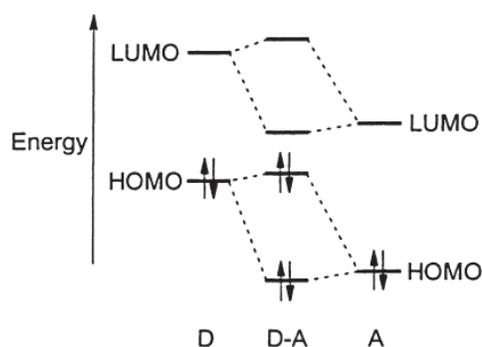
Copolymer synthesis offers the ability to alter the properties of a homopolymer in a desired direction by the introduction of an appropriately chosen second repeating unit. Several studies have been reported on conducting copolymers on their advantages over homopolymers for conductivity, stability and solubility<sup>40-45</sup>. These reports suggest that the copolymerization provides a convenient synthetic method to prepare conducting polymers with desired properties. The properties of copolymers can be modified by varying either the ratio of various constituents or the manner by which these are chemically attached.

Depending upon the band alignments of the two constituent polymers, copolymers like the inorganic superlattices may be divided into four types<sup>46,47</sup>. Type-I: - systems in which the energy gap of one component lies within the band-gap of the other component, Type-II Staggered:- Systems in which the top of the valence band of one component lies within the band-gap of the other and the bottom of the conduction band of the second lies in the band-gap of the first, Type-II Misaligned: - in these systems the conduction band minimum of one is below the valence band maximum of the second component, Type-III: - systems in which one of the components is semi-metallic while the other is a normal semiconductor.

Fluorene-acceptor alternating conjugated copolymers with varied bridged moieties have been engineered by Li et al<sup>48</sup> for photovoltaic applications<sup>49-51</sup>. Electrochromic and optical studies of fluorene based copolymers has been done recently<sup>52</sup>.

## 2.4. Donor-Acceptor Polymerization

Another important technique of obtaining low band gap polymers has been given by Havinga *et al*<sup>53,54</sup>. The technique is to **blend alternating donor–acceptor moieties** in a conjugated polymer chain resulting in eventual merging of the valence and conduction bands of the polymer material thus creating an intrinsically conducting organic “metal”. The built-in intra-molecular charge transfer in donor-acceptor architectures can facilitate ready manipulation of the electronic structure leading to low band-gaps<sup>55,56</sup>. The interaction between a strong electron-donor (D) and a strong electron-acceptor (A) may give rise to an increased double bond character between these units, since they can accommodate the charges that are associated with such a mesomerism ( $D-A \rightleftharpoons D^+ = A^-$ ). Hence, a conjugated polymer with an alternating sequence of the appropriate donor- and acceptor-units in the main-chain may show a decreased band gap. The band-gap is expected to be the lowest for a combination in which the electronegativity difference between donor and acceptor moieties is the highest. Calculations have shown that the hybridization of the energy levels of the donor and the acceptor, particularly the high-lying HOMO of the donor fragment and the low-lying LUMO of the acceptor fragment; yield a D – A monomer with an unusually small HOMO-LUMO separation<sup>57-59</sup> (figure 5).



**Fig. 5:- Hybridization of the energy levels of a donor (D) and acceptor (A) fragment leads to a D – A monomer with a narrow HOMO-LUMO energy separation.**

Various combinations of donors and acceptors have been used to tailor the polymer properties for applications in photovoltaics<sup>60</sup>, organic light emitting diodes<sup>61</sup>, electrochromics<sup>62</sup>. By combining strong donors with strong acceptors, it is possible to compress the band gap of the polymers<sup>63</sup>. Effect of donor-to acceptor ratio on the electronic properties thiadiazoloquinoxaline-based copolymers has been investigated<sup>64</sup>.

Numerous novel donor-acceptor polymers which differ in their electron donating and electron accepting moieties have been theoretically designed and investigated<sup>65-69</sup>. Polymers which have repeat units consisting of bicyclopenta-difluorodisilole bridged by electron accepting groups Y (Y= >C=CH<sub>2</sub> in PSIFCH, >C=O in PSIFCO, >C=CF<sub>2</sub> in PSIFCF and >C=C(CN)<sub>2</sub> in PSIFCN) have been studied<sup>70</sup>. Corresponding polymers based on the repeat units of bicyclopentadisilole (PSICH, PSICO, PSICF and PSICN) have also been studied<sup>71</sup>. Band gaps in all these polymers have been estimated to be about 1 eV and 2 eV.

The routes described above are followed to design conjugated polymers with tailor-made electronic properties using the existing knowledge of structure–property relationship of conducting polymers: the intra-molecular charge transfer, bridge length, and bond length alternation. However, sometimes the ultimate goal is not approaching zero band gaps but just tuning it according to the demands of the application. In that case also the above routes are helpful for obtaining well-engineered band gaps.

### **3. Methodology**

For a given purpose there may be thousands of polymers with unrelated optimal properties, out of which a few or none may be really effective. An economical and safe procedure is to calculate the electronic structure using a good quality Hartree Fock (HF) band structure calculation and then calculate the desired properties of a smaller pool of polymers. On the basis of the theoretical results one can predict which 15-20 polymers would have properties optimal for the given purpose. Though such calculations require very high computational time, they are certainly orders of magnitudes faster and cheaper than the conventional experimental approach.

Electronic band structures of homopolymers have been studied using ab initio Hartree Fock crystal orbital method<sup>72-74</sup>. The properties of a polymer can be obtained

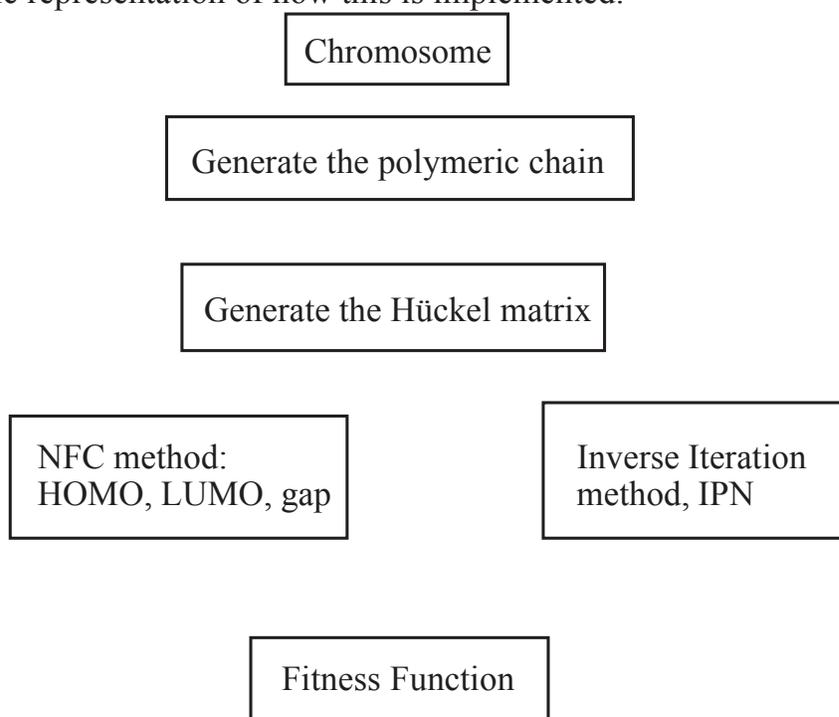
from the solution of the Schrödinger equation where the many electron wave function  $\emptyset$  for a polymer whose unit cell contains  $m$  electrons and  $Y$  atoms is approximated in the ground state as a Slater determinant of crystal orbitals  $f_i$  which are a linear combination of the basis functions  $\chi_v^j$  obtained on extending the LCAO approximation to the polymers. Due to very large size, extending the LCAO approximation to the polymers leads to an impractical situation of using an infinite basis set. This problem is overcome through the use of translational symmetry present in the polymer along with the Born-von-Karman boundary condition<sup>75-77</sup> to solve the one electron HF equation. This method is known as Hartree Fock Roothaan crystal orbital method. In the ab initio version of this method, all integrals are calculated numerically, while in the semi empirical techniques, some integrals are assigned zero values at the start and others approximated empirically. Some of the well known semi empirical formalisms are: CNDO (Complete Neglect of Differential overlap), INDO (Intermediate NDO), MINDO (Modified INDO), VEH (Valence Effective Hamiltonian) and DFT (Density Function Theory).

The copolymers and biopolymers (both periodic and aperiodic) have been studied using negative factor counting (NFC) method<sup>78,79</sup> based on Dean's negative eigenvalue theorem<sup>80-82</sup> in the tight binding approximation. The method can be extended to include multi neighbour interactions<sup>83</sup>. NFC basic idea is to obtain the eigenvalues of large matrices without direct diagonalization. With the eigenvalues, the eigenvectors of interest can be obtained (one by one) through the use of the inverse iteration method (IIM)<sup>84</sup>.

### **Genetic algorithm: towards optimum solution**

As discussed above, an exciting possibility in designing of novel low band gap polymers is the technique of copolymerization. It has been found that the electronic properties of the copolymers, though generally intermediate between those of its components, can be tuned by varying the percentage of components in the copolymer chain. Considering the large number of possible combinations of homopolymers, experimentally preparing copolymers becomes very expensive. Recently, many groups have attempted to use artificial intelligence or optimization methods to design new materials<sup>85,86</sup>. Genetic algorithm (GA) and Ant algorithm are such optimization techniques<sup>87, 88</sup>. These methods generate automatic solutions for the problem of determining the optimum relative concentration for binary, ternary, and quaternary copolymers presenting some pre-specified properties<sup>89-92</sup>. Genetic algorithms are implemented as a computer simulation in which a population of abstract

representations (called chromosomes or the genotype or the genome) of candidate solutions (called individuals, creatures, or phenotypes) to an optimization problem evolves toward better solutions. Traditionally, solutions are represented in binary as strings of 0s and 1s, but other encodings are also possible. The evolution usually starts from a population of randomly generated individuals and happens in generations. In each generation, the fitness of every individual in the population is evaluated, multiple individuals are stochastically selected from the current population (based on their fitness), and modified (recombined and possibly randomly mutated) to form a new population. The new population is then used in the next iteration of the algorithm. Commonly, the algorithm terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached for the population. If the algorithm has terminated due to a maximum number of generations, a satisfactory solution may or may not have been reached. In figure 6 we show a schematic representation of how this is implemented.



**Fig. 6: - Schematic representation of obtaining fitness function.**

### **Ant Algorithm**

The main sequence of steps in the ant algorithm has been described in a study by our group<sup>93,94</sup>. In ant algorithm, artificial ants (entities) cooperate to find a good path (solution). These ants communicate through chemical markers called pheromones. Ants

prefer paths with higher pheromone concentration. This gives rise to an autocatalytic process characterized by a positive feedback<sup>95,96</sup> which leads most ants to a good solution as per the optimization criterion. The algorithm starts with the random sorting of ants on the potential surface grid.  $P(x_i, y_i)$ . Each point in the grid represents a possible solution. To find the best possible solution, ants are moved over the 2-D grid. This movement is guided by the evaluation function<sup>97</sup>.

The above two algorithms have been combined with simple negative factor counting technique and inverse iteration method to solve the problem of designing conducting copolymers with pre-specified electronic properties. The combined use of NFC with IIM is a powerful tool in the study of disordered systems where we have to analyze many large structures.

#### **4. Some important results and their discussion**

##### **Polythiophene (PTP)**

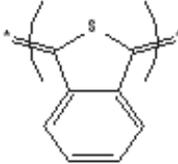
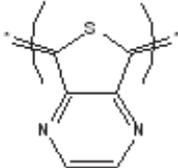
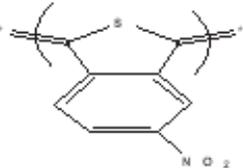
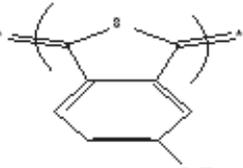
Polythiophene derivatives are currently among the most studied conducting polymers because of their relatively good conductivity, stability and potential industrial applications. Different oxy derivative polymers of thiophene (PTMO, PTDO)<sup>98</sup>, isothianaphthene derivatives (PITN)<sup>99</sup>, and various other donor acceptor copolymers containing polythiophene have been studied and compared with polythiophene through ab initio Hartree Fock Crystal Orbital method using double zeta basis set.

The effects of incorporation of varying percentages of vinylene units on the electronic structures and conduction properties of PTP have been investigated<sup>100</sup> using a negative-factor counting method in the tight-binding approximation. The results show that the incorporation of vinylene units makes the heterocyclic polymers better conductors of electricity both intrinsically as well as extrinsically and that the effects are more pronounced for the aperiodic distribution than for the periodic distribution.

##### **PITN Derivatives**

Among all the efforts toward the design of low band gap conducting polymers, poly(isothianaphthene) (PITN), whose band gap ( $E_g = 1.1$  eV) is about 1 eV lower than that of polythiophene (PT), was the first approach to the prototype of low band gap polymers. Both theoretical and experimental research showed that the reduced band gap of PITN is

caused by the intrinsic structure of the polymer backbone which tends to stabilize the electronic quinoid state <sup>101</sup>. Despite this, the practical use of poly(isothianaphthene) became limited due to its environmental instability. Since the first report of the small band gap conducting polymer, PITN <sup>102</sup>, many publications related to the modification of its chemical structure, as well as on other polymers representing structural variations on the isothianaphthene moiety, have appeared <sup>103,104</sup>. The motivation behind these efforts was to achieve further reduction of band gap and the development of soluble polymers. The band gaps achieved by these soluble polymers (figure 7) were in the range comparable with PITN (1.0-1.4 eV) and electrochemical properties of the polymers were found to depend on the substituents.

PITN derivative	Band gap/ eV	Colour
	1.1	blue / black
	1.0	black
	1.0	black
	0.9	black/ red tint

**Fig 7:- PITN derivatives with band gap and colour**

### **Poly(3,4-ethylenedioxythiophene) (PEDOT):**

At the beginning of the 90s, chemists at the Bayer company described a novel conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) which differs from polyisothianaphthene in the bridging group and contains heteroatoms and no double bonds. It has a unique combination of moderate band gap and low oxidation potential which confers an exceptional stability to the oxidized charged state. This exhibits high conductivity and good optical transparency in the visible spectral region. Based on these properties many applications of PEDOT have been rapidly developed including anti-static coatings, electrode material in supercapacitors or hole injection layer in OLEDs and solar cells<sup>105,106</sup>. The electronic structure and properties of 3,4-ethylenedioxythiophene (EDOT) based alternating donor–acceptor conjugated copolymers and their model compounds have been systematically studied<sup>107</sup> by DFT.

### **Bridged biheterocyclic systems**

HOMO and LUMO levels can be influenced by substitution of polymers, however, the possibility to decrease band gaps through simple substitution is limited. If symmetry can be employed to reduce the interaction of the substituent with one of the bands, the situation is different. In biheterocycles, the HOMO has a node through the center of the molecule. Therefore a bridging group that is positioned in this nodal plane influences the HOMO less strongly than the LUMO. This effect can be seen in polymers of 4-dicyanomethylene- *4H*-cyclopenta [2,1-*b*;3,4-*b'*]dithiophene (CDM)<sup>108</sup> and of *4H*-cyclopenta [2,1-*b*;3,4-*b'*]dithiophene-4-one (CDT) which have band gaps of 0.8 and 1.2 eV, respectively.

Bridged heterocyclic systems and copolymers have been studied by ab initio Hartree Fock method by our group<sup>109-111</sup>. These systems can be viewed as consisting of a backbone of sp<sup>2</sup> hybridized carbon atoms analogous to that of trans-cisoid polyacetylene stabilized by different bridging groups X (where X = S, O, NH, CH<sub>2</sub> etc.) and Y (where Y = >C=CH<sub>2</sub>, >C=O, >C=CF<sub>2</sub>, >C=C(CN)<sub>2</sub>) which are covalently bonded to neighbouring carbon atoms to form the heterocycles. Table 1 gives the band gap values for various donor acceptor polymers based on bridged heterocycles. Copolymers of silole and pyrrole<sup>112,113</sup>, PSICF and PSICN, PSIFCO and PSIFCN, PPDCO and PPDCN, PCDT and PCNTh, PPDCF and PPDCN, PSICO and PSICN, PPDCH and PPDCN have also been studied.

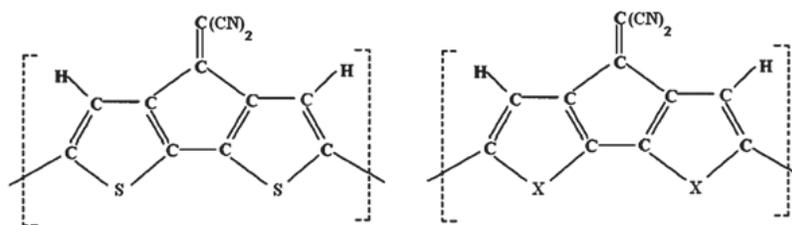
**Table 1: Band gap values for various donor acceptor polymers based on bridge heterocycles**

X \ Y	>C=CH <sub>2</sub>	>C=O	>C=CF <sub>2</sub>	>C=C(CN) <sub>2</sub>
CH <sub>2</sub> <sup>a</sup>	5.35	5.43	5.22	3.78
SiH <sub>2</sub> <sup>a</sup>	5.48	5.57	5.35	5.24
SiH <sub>2</sub> <sup>b</sup>	5.665	5.803	5.677	5.193
S <sup>a</sup>	5.81	5.85	5.76	5.69
S <sup>b</sup>	-	6.260	-	5.917
S <sup>c</sup>	6.238	-	6.257	5.927
O <sup>a</sup>	5.79	5.84	5.71	5.59
NH <sup>a</sup>	6.06	6.11	5.96	5.81
CF <sub>2</sub> <sup>a</sup>	5.38	5.46	5.20	3.88
SiF <sub>2</sub> <sup>a</sup>	5.54	5.62	5.38	3.53
SiF <sub>2</sub> <sup>b</sup>	5.665	5.763	5.620	5.145
GeF <sub>2</sub> <sup>a</sup>	5.49	5.68	5.44	3.43

All values in eV<sup>a</sup> MNDO- AM1 level of approximation. <sup>b</sup> Clementi's 7s/3p minimal basis set for the heavy atoms (C, N, O) and 9s/6p for S and four primitive Gaussian functions contracted to one s function for the hydrogen atoms.

### Novel binary copolymers based on donor-acceptor type polymers with dicyanomethylene linkages

In recent times our research group has been actively involved in designing novel binary<sup>114</sup> and ternary copolymers<sup>115</sup> using the GA. Some of our results are discussed here. We have investigated four novel binary copolymers. The basic structures of the unit cell of the various homopolymers investigated are shown in figure 8.



**Fig. 8:- Structures of the unit cells of the two D-A homopolymers A (PCNTh) and B (X=CF<sub>2</sub>)/ C (X=O)/ D (X=SiH<sub>2</sub>)/ E (X=CH<sub>2</sub>) constituting the copolymer.**

In all the four copolymers, one of the homopolymer components (A), polydicyanomethylene-cyclopentadithiophene (PCNTh) containing S as one moiety, is kept common, while the other has been varied by replacing the hetero atom S of the aromatic ring with group X which can be CF<sub>2</sub> (or B), O (or C), SiH<sub>2</sub> (or D) or CH<sub>2</sub> (or E) thereby forming copolymers of the type A<sub>x</sub>B<sub>y</sub>, A<sub>x</sub>C<sub>y</sub>, A<sub>x</sub>D<sub>y</sub>, or A<sub>x</sub>E<sub>y</sub> respectively. The >C=C(CN)<sub>2</sub> bridging groups help extend conjugation in the chain. The trends in electronic properties suggest that IP value is found to be the lowest when X=CH<sub>2</sub> (IP = 8.478 eV). As a result the copolymer containing PCNTh and X = CH<sub>2</sub> groups is expected to be the best possible candidate for p-doping since the electron can be easily knocked off from the top most energy level of HOMO. The copolymer comprising PCNTh and X = SiH<sub>2</sub> has maximum EA value of 8.303 eV and is hence expected to be a better candidate for n-type or reductive doping. The calculated band gap values of the four polymers increase in the order: CF<sub>2</sub> < O < CH<sub>2</sub> < SiH<sub>2</sub>, where S containing PCNTh is common to all copolymers. The copolymer containing X = CF<sub>2</sub> has the lowest E<sub>g</sub> value and is hence expected to show maximum intrinsic conductivity. The lowest gap value, 3.495 eV, also suggests that there is maximum difference in electronegativity of donor (X = S/CF<sub>2</sub>) and acceptor species (>C=C(CN)<sub>2</sub>) in this particular system.

**Table 2-Calculated electronic properties (IP, EA and E<sub>g</sub>) of the random binary Type-I copolymers along with their optimized percentage compositions as obtained from GA.<sup>a</sup>**

X	IP (eV)	EA (eV)	E <sub>g</sub> (eV)	Optimum solution
CF <sub>2</sub>	9.192	5.697	3.495	A <sub>3</sub> B <sub>97</sub>
O	8.996	4.172	4.824	A <sub>1</sub> C <sub>99</sub>
SiH <sub>2</sub>	8.996	3.803	5.194	A <sub>1</sub> D <sub>99</sub>
CH <sub>2</sub>	8.478	3.520	4.958	A <sub>1</sub> E <sub>99</sub>

<sup>a</sup>PCNTh (denoted by A) is common in all copolymers whereas different groups (X) of the second component are listed in the table.

The percentage compositions of the optimum solutions in all four cases suggest that PCNTh (denoted by A in Table 2) should be present in less amount and the other component having X = CF<sub>2</sub>/O/SiH<sub>2</sub>/CH<sub>2</sub> (denoted by B/C/D/E respectively in Table 2)

should be present in major amount in the copolymer in order to generate the optimum solution, i.e., copolymer possessing minimum band gap and maximum electron delocalization.

## **5. Conclusion**

Theoretical investigations are particularly useful for studying underlying causes of changes in properties upon chemical modification. Understanding these factors can lead to structure property relationships that are needed for “tailoring” new systems for specific applications. The ability to tailor polymers will be of great practical importance in different fields (computer technology, communications, non-linear optical devices, space research etc.).

The quantum chemical investigation of the electronic structure of polymers, which has been a challenging physical problem till a decade ago due to the complexity of these polymers, is now possible due to the new theoretical developments in the field of polymer science. A common feature of all these approaches has been to draw qualitative conclusions regarding conduction properties of various types of polymers on the basis of their electronic properties obtained from either their band structure calculations or their electronic DOS calculations. The results obtained through such calculations provide important guidelines for designing novel conducting polymers.

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# **99<sup>th</sup> Indian Science Congress**

3-7 January 2012, Bhubaneswar

**II**

**ABSTRACT**

**OF**

**PLATINUM JUBILEE LECTURE**



## Phosphorus-Supported Ligands: Versatile Coordination Platforms for the Assembly of Molecular Materials

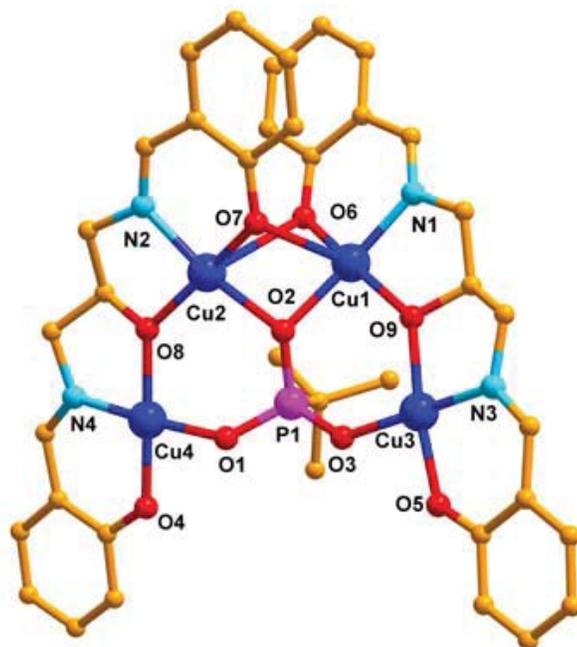
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Phosphorus-supported ligands such as phosphonates, phosphorus pyrazolides, -hydrazides and -hydrazones have been used in our lab for building multi-metallic assemblies (Figure). Some of these compounds are interesting magnetic materials or while some others possess third-order non-linear optical properties. This talk will summarize some of our recent efforts in this area.



**Figure: A tetranuclear Cu(II) cage containing a phosphonate ligand**



# **99<sup>th</sup> Indian Science Congress**

3-7 January 2012, Bhubaneswar

## **III**

### **ABSTRACTS OF AWARD LECTURES /**

### **YOUNG**

### **SCIENTIST AWARD LECTURE**



**DR. B.C. DEB MEMORIAL AWARD LECTURE**

**Conservation tillage and fertilization impacts  
on soil organic carbon pools in the Indian sub-  
Himalayas**

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**Key words:** Conventional tillage (CT); Carbon sequestration; Soil aggregation and carbon (C) pools; Labile C; Recalcitrant C.

The carbon sequestration potential of balanced fertilization, conservation tillage and organic farming practices was appraised in the north-western Himalayan soils. Rainfed and irrigated soybean-wheat systems have the potential to sequester about 20% of the added carbon, conservation tillage (zero and minimum tillage in the rainfed condition and zero tillage under irrigated conditions) had significant impacts on carbon retention in surface soils, annual farmyard manure (FYM) addition improved labile and long-lived (recalcitrant) carbon pools and annual application of FYM at 15 Mg ha<sup>-1</sup> is recommended for organic production of garden pea-french bean-babycorn/cauliflower in a sequence as crop productivity and soil organic carbon retention were significantly higher than plots with recommended NPK. Thus, the recommendations have tremendous potential for sustainable hill farming and could contribute to offset global warming.

## **PROF. R. C. SHAH MEMORIAL LECTURE**

# **Opportunity, Challenge and Scope of Click Reaction in Carbohydrate Chemistry: Triazole as rigid support in Intramolecular Glycosilation**

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Cu(I)-catalyzed Huisgen 1,3-dipolar cycloaddition (Click Chemistry) have extensively been used to achieve regioselective triazole and applied for the rapid construction of mechanically interlocked molecular-level architectures where their interest in various different branches of science is expanding exponentially. The protocol has several distinct advantages, most notably high chemoselectivity, excellent regioselectivity, tolerance to a variety of solvents and functional groups, mild and compatible reaction condition, efficient, reliability, very low background ligation rates, facile synthetic accessibility, straightforward way for making covalent connections between building blocks containing various functional groups, and moreover the high stability and widespread application of the resulting 1,2,3-triazole heterocycle in medicinal chemistry, tissue engineering scaffolds, dispersible nanomaterials, drug delivery agents, surface chemistry, material chemistry, polymer chemistry, macromolecules, dendrimers, glycobiology, and bioconjugation applications and also a promising catalyst in organic synthesis.

Carbohydrates are identified to play pivotal roles in various pathologically and physiologically important biological processes. The clear understanding of role of sugars in these important biological events has led to the increased demand for significant amounts of carbohydrate based molecules for their complete chemical, biological, medicinal, and pharmacological investigations. Therefore, tremendous efforts have been made to develop novel and facile procedures to achieve the desired sugar based molecules of great biological interest; where with an increasing focus on the glycoconjugates, click reaction of an azide and an alkyne has been increasingly used in the carbohydrate research field such as chemical labelling of biomolecules as well as preparation of oligosaccharide analogues,

#### *Section IV: Chemical Sciences*

glycodendrimers, scaffolds, micro-arrays, sialic acid, with their triazole based macrocycles using click chemistry of azido and alkyne groups present on sialic acid containing oligosaccharides.

I propose to highlights the rapidly increasing advantages of the click reaction that has extensively been used in carbohydrate chemistry, their widespread recent applications in ranging from bioactive ligands to new materials, triazole as rigid support in intramolecular glycosidation and macrocyclization along with their future potential scope in great detail.

**YOUNG SCIENTIST AWARD LECTURE**

**Designing Novel Nano Materials through Functionalization of Carbon Nanotubes with Supramolecules for the Application in Nuclear Waste Management**

**Mahesh Sundararajan**

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We have investigated the possible interaction between functionalized carbon nanotubes with uranyl using density functional theory. We have functionalised the carbon Nanotube with cucurbituril supermolecule. The oxidized carbon nanotube and hydroxylated cucurbituril interacts with each other via non-covalent interactions. Our calculations show that functionalized carbon nanotubes and cucurbituril can be used not only for improving the solubilities, but also for binding uranyl ion much more efficiently as compared to their unfunctionalised counterpart. These findings are new and can open up a new era for actinide speciation and separation chemistry using CNT.

# **99<sup>th</sup> Indian Science Congress**

3-7 January 2012, Bhubaneswar

## **IV**

### **ABSTRACTS OF**

### **SYMPOSIUM / INVITED LECTURES**

*Topic of Symposium*

**Tailoring of Novel Chemical  
Substances with Desired Properties**



## INVITED LECTURE

### 1. Novel Sugar-PEG Based Polymeric Architecture for Targeted Drug Delivery Applications

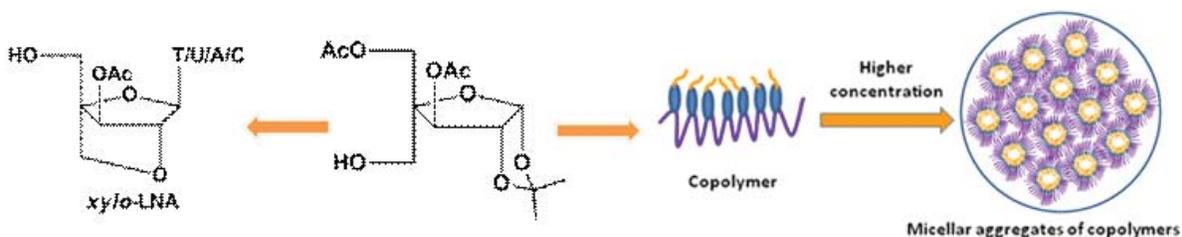
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The discovery of sugar modified nucleoside derivatives as potential antiviral agents and the emergence of antisense and antigene oligonucleotides as potential and selective inhibitors of gene expression have led to the considerable rise in the synthesis of modified nucleoside derivatives and nucleic acids involving them. Further, there has always been need to have biocompatible drug carriers capable of delivering water insoluble drugs with high transport and controlled release capacity.

We have developed an efficient biocatalytic methodology for the transformation of a trihydroxy sugar derivative derived from glucose into *xylo*-LNA, a monomer of antisense oligonucleotide and sugar-PEG co-polymer having application as drug carrier and its controlled release. Detailed results will be presented in the meeting.



## INVITED LECTURE

### 2. Contracted Porphyrinoids

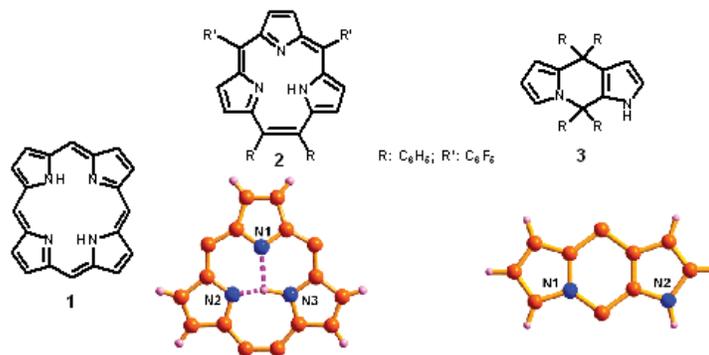
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Porphyrin (**1**) chemistry with various structural derivatives such as *normal*, *expanded*, and *contracted* porphyrinoids are found potential applications in the area of molecular recognition, catalysis, material science and medicine.<sup>1</sup> In particular, the *contracted* porphyrinoids have continued to gather much interest since the first synthesis of subphthalocyanines, the *contracted* homologues of phthalocyanines formed by three instead of four N-fused 1,3-diiminoisoindole units which represent fascinating example of nonplanar aromaticity with unique spectral and electronic features.<sup>2a</sup> Subsequently, series of *contracted* porphyrinoids such as, subporphyrazines<sup>2b</sup> and subporphyrin<sup>2c</sup> are reported recently. These set of compounds found to be an ideal candidates for the construction of supramolecular self-assemblies in spite of the increased ring strain. Very recently, our group reported *meso*-aryl[14]triphyrin(2.1.1) (**2**) which is the smallest congener of *meso*-aryl and  $\hat{\alpha}$ -unsubstituted porphyrin containing only pyrrole rings in its free-base form.<sup>2d</sup> On the other hand, calix[4]pyrrole is a class of fully *meso*-substituted porphyrinogen macrocycles and is known to be readily accessible hosts for fluoride and other anions both in solution and in the solid state.<sup>3</sup> However, the corresponding contracted calixpyrroles (**3**) are not known in the literature. In this lecture, we wish to address the synthesis, spectral and structural characterization of such *contracted* porphyrinoids.



## INVITED LECTURE

### 3. Theoretical evaluation of thermodynamic properties of multi component liquid mixtures: Graph theory

V. K. Sharma

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Randic et al.<sup>1-2</sup> have noted that while on the one hand hundreds of topological indices are known, on the other the interpretation of topological indices have received little attention. Basically topological index expresses in numerical form the topology of the chemical species it presents. Topological indices are designed by transforming a molecular graph into a number and possess a remarkable ability of being able to correlate and predict a very wide spectrum of properties for a vast range of molecular species. A very good correlation has been observed<sup>3-6</sup> between topological index of a molecule and its physico-chemical properties.

Since thermodynamic excess functions are a measure of solute solvent interactions and as (i+j) binary mixture may be assumed to have been formed by the replacement of like contacts in the pure (i) and (j) contacts by unlike (i-j) contacts in the mixture, it appear thermodynamic excess functions for binary mixtures of non-electrolytes could be utilized to see how like interactions in pure (say) (j) are influenced by the presence of pure (i) in the (i+j) mixture. Again, as the mathematical discipline of Graph theory has been utilized to determine the relationship between structure of a molecule and its physical and chemical properties. It was, therefore, felt that topology of a molecule constituting the mixtures can be utilized to predict thermodynamic properties like  $V^E$ ,  $H^E$ ,  $\kappa_S^E$  and  $G^E$  etc. These agreement form the base of an approach hence forth called Graph theory. The Graph theory (which in turns deals with the topology of a molecule) would be discussed in detail to predict  $V^E$ ,  $H^E$ , and  $G^E$  etc of binary and ternary mixtures (components differing in shape, size and polarity) along with nature extent of interactions and molecular entities existing in mixture.

## **INVITED LECTURE**

### **4. Challenges and application of functionalised layered double hydroxides**

#### **Kulamani Parida**

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Insertion of metals and organometallic species into inorganic layered solids offers an attractive route to nanohybrids in which complementary properties of the two components are expressed in a single material. Hydrotalcite of layered materials consist of a cationic brucite layers and anionic compounds in the interlayer. The properties of the layered double hydroxide can be altered by incorporating different anionic complexes and enzymes through electrostatic interaction. Herein, we describe a simple and efficient method for synthesizing various anions, Pd metal and transition metal complexes such as Ti, Fe, Ce intercalated Zn-Al/LDH by an ion exchange method. The anion/metal/complex intercalated LDHs were characterized by powder X-ray diffraction, FT-IR, UV-visible spectroscopy, N<sub>2</sub> adsorption desorption, Scanning electron microscopy, NMR and TGA techniques. All these spectroscopic studies confirm the successful intercalation of anions/metals/complex within the LDH structure. Molybdate intercalated Zn/Al LDH exhibits a higher photocatalytic activity for oxygen evolution. The carbonate intercalated Zn/Cr LDH are found to be an efficient photocatalyst for both dye degradation (99% for Xanthene group of dyes) and photodecomposition of water to hydrogen and oxygen. The visible light photocatalytic activity is ascribed to the charge transfer spectra of octahedral Cr ions. The well dispersed palladium nanoparticles (1-5 nm) on diamine functionalized LDH displayed unprecedented activity in Suzuki coupling reaction. The supported Ti-complex shows an excellent catalytic activity in cyclohexene epoxidation reaction using H<sub>2</sub>O<sub>2</sub> as oxidant in solvent free condition. Catalytic liquid phase oxidation of primary alcohols using molecular O<sub>2</sub> at room temperature is studied using Ce(III)-complex intercalated Zn/Al-LDH. These modified heterogeneous catalysts can be recovered easily and reused multiple times without significant loss in catalytic activity and selectivity, which is a better green alternative for practical applications.

## INVITED LECTURE

### 5. Physicochemical Investigations of Pyridinium Gemini Surfactants and Bile Salts with Phenothiazine Tranquilizer Drugs

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The utilization of micelles as drug carriers is considered to be beneficial due to their reduced toxicity, enhanced permeability, longer residence time in the system and appropriate sizes. Keeping this in view, the interactions of pyridinium gemini surfactants (PGS) with a phenothiazine tranquilizer drug, promethazine hydrochloride (PMT) have been investigated by conductivity, surface tension, fluorescence, UV-visible and  $^1\text{NMR}$  measurements. These studies can be further used to visualise the drug membrane interactions and understand the mechanism of drug action. PGS viz., 1,1'-(1,1'-(ethane-1,2-diylbis-(sulfanediyl))bis(alkane-2,1-diyl))dipyridinium bromide having alkyl chain length varying from 9, 11 or 13 i.e., [12-(S-2-S)-12], [14-(S-2-S)-14], [16-(S-2-S)-16] respectively, exhibit better DNA binding ability, lower cytotoxicity and critical micellar concentration (cmc) in comparison to the quarternary ammonium gemini surfactant 1,6-hexanediyl bis-(dimethyldodecylammonium)bromide. The mixed micellization studies of PGS with PMT have been investigated by conductivity, surface tension and steady state fluorescence measurements. The various physicochemical parameters for these binary mixtures have been evaluated. The interaction parameters in micelles ( $\hat{\alpha}^m$ ) as well as at the interface ( $\hat{\alpha}^0$ ) of drug-surfactant systems are negative, indicating synergistic interactions between them. The spectroscopic techniques such as fluorescence, UV-visible and  $^1\text{H NMR}$  have been employed to get the better insight of the nature of interactions between the PGS and PMT. In addition to this, the interactions of bile salts with phenothiazine tranquilizer drugs have been studied. The results of these physicochemical studies will be presented during the talk.

Mahajan et al, *Phys. Chem. Chem. Phys.*, (2011) DOI: 10.1039/c1cp22448d

## **INVITED LECTURE**

### **6. Supramolecular Chemistry of Trithiocyanuric Acid**

**V. R. Pedireddi**

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Aggregation behaviour of organic molecular entities has been exploited in the recent decades to understand the pivotal role of the intermolecular interactions such as hydrogen bonds in the self assembly process of small molecules towards the formation of supramolecular assemblies. Nature of the resultant supramolecular ensembles, in the solid state, generally, is being influenced by the donor-acceptor abilities of the constituents of the molecules. For example, while self assemblies of simple aliphatic hydrocarbons are mostly governed by the hydrophobic interactions, topologically similar molecules but with functional groups like –COOH group, the aggregation is predominantly, by the highly directional hydrogen bonds. In this regard, functional group approached synthesis of supramolecular assemblies is one of the challenging areas to realize the tailor-made assemblies for specific applications. In our endeavours, symmetrically substituted molecules have been found to be exotic supramolecular reagents to develop variety of assemblies, for example, trithiocyanuric acid. The landscape developed in this voyage would be discussed in the presentation.

## INVITED LECTURE

### 7. **Fulbright-Nehru Fellowships to the U.S. - Opportunities in the field of Chemistry**

**Dr. Sudarsan Dash**

*Senior Program Manager, United States-India Educational Foundation, Fulbright Commission in India, New Delhi*

Jointly funded by the Governments of India and the U.S., Fulbright-Nehru fellowships provide several opportunities for study, research, teaching and professional development in the United States of America. My presentation will focus on Fulbright-Nehru fellowship opportunities for Professors, Scientists, and Research Students in Chemistry. Academics and professionals in the field of Chemistry can explore possibilities to apply for one these fellowship programs:

**1. Fulbright-Nehru Doctoral and Professional Research Fellowships:** These pre-doctoral level research fellowships, for a maximum period of nine months, are designed for scholars who are registered for a Ph.D. at an Indian institution and also for professionals with significant work experience and accomplishments.

**2. Fulbright-Nehru Postdoctoral Research Fellowships:** These fellowships, for a maximum period of 12 months, are designed for Indian scholars and professionals who have a Ph.D. degree from an Indian institution within the past four years.

**3. Fulbright-Nehru Senior Research Fellowships:** For faculty, researchers and professionals from all disciplines who have a Ph.D. or equivalent published work. These fellowships, for a duration of up to eight months, aim to provide opportunity to do research on contemporary issues and concerns to contribute to the creation of knowledge.

**4. Fulbright-Nehru Visiting Lecturer Fellowships:** For faculty, researchers and professionals from all disciplines who have a Ph.D. or equivalent published work. These fellowships, four months, contribute to internationalization of the curriculum at the U.S. host institutions and understanding of recent developments in India.

**5. Fulbright-Nehru Environmental Leadership Program:** For mid-level Indian environment professionals in public/private sector or non-governmental organizations for

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up to four months in the fields of Environmental Information/Systems Reporting; Environmental Education; Environmental Policy, Regulations and Law; Environmental Sciences and Toxicology; and Environmental Management.

**6. Fulbright-Nehru International Education Administrators Seminar:** For mid- to senior-level Indian college and university administrators with at least two years of experience in international program development and management at their institutions. This two week seminar will enable participants to learn about various facets of U.S. higher education, including the types of institutions, accreditation, curriculum development, fund raising, student services and international education on U.S. campuses, as well as share knowledge on Indian higher education.

# **99<sup>th</sup> Indian Science Congress**

3-7 January 2012, Bhubaneswar

**V**

**ABSTRACTS OF**

**ORAL/POSTER**

**PRESENTATIONS**

**I. ORGANIC CHEMISTRY**



**1. Isolation and characterization of unusual glycolipid-ceramide molecule from extract of *Tinospora Cordifolia* (Guduchi) for exploration as a novel therapeutic agent**

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**Keywords:** - *Tinospora Cordifolia*, Guduchi, Isolation, Chromatography, Characterization, Glycolipid-Ceramide, Therapeutic agent.

Ceramide is a structural component of glycolipid. Ceramide derivatives have attracted attention as potential therapeutic agents for the treatment of cancer, ulcers and other diseases originating from cell regulation disorders. C-18 ceramides have reported to suppress tumour growth arresting properties in some carcinomas.

In the present studies in search of new bioactive entities from botanicals a molecule designated as IICT-HERB-2011 has been isolated by column chromatography fractionation of hypoglycemic ethyl acetate extract of *Tinospora cordifolia* and subsequently purification using preparative TLC procedure and it has been assigned chemical structure as an unusual C-17 glycolipid-ceramide molecule from an analysis of its UV, IR, ESI-MS and <sup>1</sup>H NMR spectral data.

This molecule will be explored further for its potential use as a novel therapeutic agent possibly a boon to human health.

**2. Synthesis and Antimicrobial Studies of Novel N-Glucosyl  
1, 3, 5-Triazin-2-one (hydrochlorides)**

**Sagar M. Jain\* and Shirish P. Deshmukh**

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**Keywords:-** Antimicrobial activity, Glucosyl-Isothiobiurets, Glucosyl- isocyanodichloride, Glucosyl 1,3,5-Triazin-2-one(hydrochlorides).

The 1, 3, 5-triazine heterocyclic system is today found in a number of bioactive molecules such as herbicides and pharmaceutical products. Various triazine substituted molecules exhibit diverse biological activities, thus it has been reported as potentially cardiogenic, anti-HIV, antitumor and anticancer agents. Some triazines have found clinical applications. Hexamethylmelamine (HMM) has for example been used as antitumor agents.

A series of novel N-glucosylated 1, 3, 5-triazin-2-one hydrochlorides possessing 1, 3, 5-triazine ring (substituted) were efficiently synthesized by oxidative cyclisation of perbenzoylated glucosyl-2-S-benzyl-2-isothiobiuretes with peracetylated glucosyl-isocyanodichloride. The identities of these newly synthesized compounds were established on the basis of usual chemical transformations and IR, <sup>1</sup>H NMR, and Mass spectral studies and evaluated for their in vitro antimicrobial activities using standard cup plate method against bacteria *E.coli*, *P. aeruginosa*, *P.vulgaris*, *B. cereus*, *S.aureus* and fungi *A.niger*, *C. albicans*.

### 3. Studies on Synthesis and Kinetic Hydrolysis of a Series of Chiral Organic phosphoramidates by Suitable Methods

**Soram Ibomcha Singh and Shashi Prabha**

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**Keywords:** Hydrolysis, physiological conditions, substituents, phosphoramidates

The study was focused on the nature of the substituents and their influence on the reactivity and the stability of the synthesized mixed chiral phosphoramidates. The ortho-chloro substituent has proved to be significant during hydrolysis resulting in maximum reactivity and also the presence of bulky groupings around the phosphorus atom hindered the approach of the nucleophile to a large extent, thereby resulting in the minimum rate of hydrolytic cleavage. DMF's presence has resulted in the deviation of the physiological conditions desired but no correlation could be tabled about its influence on the rate of hydrolysis.

### 4. New Potential Allelochemical From *Blumea Lacera* Dc.

**R.N.YADAVA\* and BHARTI BHARGAVA**

*Natural Products Laboratory, Department of Chemistry*

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**Keywords:** *Blumea lacera* DC. Compositae; Allelochemical; Seed.

*Blumea lacera* DC.<sup>1-3</sup> belongs to the Compositae family. It is commonly known as Janglimuli or Kakronda in Hindi. It is distributed throughout the plains of India. The plant is hot pungent, bitter and antipyretic. It cures bronchitis, blood diseases, fevers, burning sensation. It's root cures diseases of the mouth and mixed with black pepper is given in cholera. The juice of the leaves is used as an anthelmintic, febrifuge astringent, and diuretic.

The present paper deals with isolation and structure characterization of a new allelochemical (A) m.f. C<sub>32</sub>H<sub>38</sub>O<sub>19</sub>, m.p. 262-264°C, [M]<sup>+</sup> 726 (FABMS) along with a known compound myricetin (C) was isolated from the methanol soluble fraction of the defatted seeds of *Blumea lacera* (DC). A new compound (A) was characterized as 5,7,3',4'-tetrahydroxy-8-methoxy-flavone-7-O- $\alpha$ -L-rhamnopyranosyl-(1'!4)-O- $\alpha$ -L-arabinopyranosyl-4'-O- $\alpha$ -D-xylopyranoside (A) by several colour reactions, chemical degradations and spectral analysis.

**5. Determination of polyalcohols by Smith degradation technique from *Withania somnifera* Dunal (*Ashwagandha*) seeds oxo-polysaccharide**

**Dr. R. B. Singh**

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**Keywords:** Polyalcohols from *Withania somnifera* Dunal seeds oxo-polysaccharide by Smith degradation.

*Withania somnifera* Dunal is an important drug yielding plant in the ancient Ayurvedic literature and commonly known as *Ashwagandha*, and belongs to the family – Solanaceae. Plants occurs in India, Pakistan, Bangladesh, Sri Lanka, Thailand, Malaysia, Java, Israel, African & Asian Tropics. Roots and leaves are used in Tonic, Abortifacient, Astringent, Nervine, Aphrodisiacs, Mental problem, Depression, Infertility, Memory loss, Harmonal imbalance, Anti-oxidant, Anti-cancer, Leucoderma, etc. It is widely used in babies' tonic, reproductive function in men & women and in herbal drug industry. It is also recommended for spermatorrhoea infertility in women. Seeds and fruits are diuretic which can be used as a substitute for rennet to curdle milk. About a table spoon of seeds mixture is enough to coagulate a gallon of milk in a half an hour. Seeds powder yielded a water soluble polysaccharide as D-glucose and D-mannose in 1:3 molar ratio by GLC, column and paper chromatography. Present investigation mainly deals with periodate oxidized seeds polysaccharide was degraded by Smith degradation with sodium borohydride and sulphuric acid (1N) yielded glycerol and erythritol in 1.54 : 4.26 molar ratio with traces of thritol on Whatmann No. 3MM filter paper by paper chromatography. A large proportion of erythritol

released by acid hydrolysis (H<sub>2</sub>SO<sub>4</sub>) of polyalcohols which was obtained by reduction of sodium borohydride. Derivative of polyalcohols were produced as glycerol-tri-O-p-nitrobenzoate and tetra-O-tosyl-erythritol. Absorbances of polyalcohols were recorded on 540 mμ in photoelectrocolorimeter. The evidence of linkages in polysaccharide structure showed that the main polymer linkages are of (1'!4)-â-type and branching point with (1'!6)-á-type linkages. Ratio of erythritol to the amount of glycerol indicates a branching point on average of after every 8 hexose units. Above finding results indicates that the branching point on the average of 7 hexose units are in the backbone and 1 hexose in non-reducing end for the support of earlier proposed seeds polysaccharide structure of *Withania somnifera* Dunal plant.

## 6. Synthesis of Some Novel 2-*S*-tetra-*o*-benzoyl-D- glucopyranosyl-1 aryl-5-hepta-*o*-benzoly-â-D-lactosyl-2-isothiobiurets

**Kedar P. Pande<sup>1</sup> and Shirish P. Deshmukh<sup>2\*</sup>**

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**Keywords:** - Lactosyl isocyanate, glucopyranosyl isothiocarbamides, lactosyl isothiobiurets.

The study of *S*-and *N*-glycosides is important in carbohydrate chemistry Sugar isocyanate is good precursors and versatile intermediate for synthesis of *S*-and *N*-glycosides. Carbohydrates play an important role in the number of biological events and play an important role in their synthetic strategy as well. Similary the amino sugars are an important class of glycosidase inhibitors and are arousing great interest as potential therapeutic agents. Several 2-*S*-tetra-*o*-benzoyl-D-glucopyranosyl-1-aryl-5hepta-*o*-benzoyl- â-D-lactosyl-2-isothiobiurets have been synthesized for the first time by the interaction of hepta *o*-benzoyl-â-D-lactosyl isocyanate and *S*-tetra-*o*-benzoyl-D-glucopyranosyl-1-aryl isothiocarbamides. All the synthesized compounds were characterized on the basis of elemental analysis and IR, <sup>1</sup>HNMR and Mass spectral analysis. The polarimetric study of the compounds was carried out.

**7. Synthesis of New Class Of 3-Oxo-2-Hepta-O-Acetyl-b-D-Maltosyl-4-Aryl-5-Hepta-O-Acetyl-b-D-Lactosylimino-1,2,4-Thiadiazolidine (Hydrochlorides)**

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**Keywords:** Maltosyl aryl carbamides, *N*-hepta-*O*-acetyl-b-D-lactosyl-*S*-chloro isothiocarbamoyl chloride, lactosyl-1, 2, 4-thiadiazolidine (hydrochlorides)

Heterocycles and medicines are both interrelated because human are totally dependent on the drugs derived from heterocyclic rings. Heterocycles and their derivatives have attracted the attention of chemists mainly because of broad spectrum biological and pharmacological activities associated with this class of the compounds specially having *N*, *S* or both heteroatoms which exhibited marked chemotherapeutic activities. A series of novel 3-oxo-2-hepta-*O*-acetyl-b-D-maltosyl-4-aryl-5-hepta-*O*-acetyl-b-D-lactosylimino-1,2,4-thiadiazolidine (hydrochlorides) were synthesized by the interaction of *N*-hepta-*O*-acetyl-b-D-lactosyl-*S*-chloro isothiocarbamoyl chloride with various 1-hepta-*O*-acetyl-b-D-maltosyl-3-aryl carbamides. IR, <sup>1</sup>H NMR, Mass spectral studies and elemental analysis characterized the newly formed products.

**8. Synthesis of 4-aryl-5-hepta-O-acetyl-â-D-maltosylimino-3-thio-1,2,4-dithiazolidines (hydrochloride)**

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**Keywords:** *N*-maltosides, Isothiocarbamoyl chloride, Ammonium aryl dithiocarbamates.

Cyclization is one of the suitable methods for the synthesis of heterocyclic compounds. Heterocyclic derivatives of carbohydrates plays pivotal role in progressive findings about the synthesis, biological and pharmacological action. Sugar isothiocyanate is versatile reagent for the synthesis of sugar heterocycles. *N*-glycosylated-1, 2, 4-dithiazolidines and their derivatives shows antibacterial and antifungal activity.

In view of the applications of *N*-maltosides in medicinal chemistry and many other ways, it appeared interesting to synthesize some novel *N*-maltosylated dithiazolidines (hydrochloride). Here, we synthesized several 4-aryl-5-hepta-*O*-acetyl- $\alpha$ -D-maltosylimino-3-thio-1,2,4-dithiazolidines (hydrochloride) by the interaction of chloroformic mixture of *N*-hepta-*O*-acetyl- $\alpha$ -D-maltosyl-*S*-chloro isothiocarbamoyl chloride with ammonium aryl dithiocarbamates. The identities of these newly synthesized *N*-maltosides have been established on the basis of usual chemical transformations and IR, <sup>1</sup>H NMR and Mass spectral studies.

## 9. A facile and rapid one-step synthesis of 8-substituted xanthine derivatives via tandem ring closure of imidazole ring at room temperature

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**Keywords:** Xanthine; Adenosine receptor antagonists; *N*-Bromo succinimide (NBS); 2,2'-azoisobutyronitrile (AIBN); Asthma; COPD.

Poly-substituted xanthine derivatives are one of the most important chemical classes of adenosine receptor (AdoR) antagonists. A2B-AdoRs play an important role in causing asthma, chronic obstructive pulmonary disease (COPD) and fibrosis. Herein, we report for

the first time an easily accessible *N*-Bromo succinimide (NBS) promoted one-step synthesis of 8-substituted xanthine derivatives in presence of AIBN at room temperature. The present study was aimed at to develop a facile and rapid synthetic route for A2B-AdoR antagonists 8-substituted xanthines *via* tandem intramolecular ring closure of imidazole ring from 5,6-diamino-1,3-dimethyluracil by the rapid condensation of various aryl/ cycloaryl/heteroaryl aldehydes.

#### 10. New Allelochemical from *Artemisia vulgaris* Linn.

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**Key words:** *Artemisia vulgaris* Linn., Compositae, aerial part, Isoflavone glycoside.

A new isoflavone glycoside m.p. 242-244°C m.f. C<sub>34</sub>H<sub>43</sub>O<sub>19</sub> [M]<sup>+</sup> m/z 755 (FABMS), has been isolated from ethanolic extract of the aerial part of *Artemisia vulgaris* Linn., along with two known compounds as 3, 5, 7, 3', 4'-pentahydroxy-3-O- $\alpha$ -L-rhamnopyranoside and 5,4'-dihydroxy-3,7-dimethoxy flavone. A new compound was characterized as 5,7-dihydroxy-6,32,42-trimethoxy isoflavone-7-O- $\alpha$ -L-rhamnopyranosyl-(1'3)-O- $\beta$ -D-arabinopyranosyl-(1'4)-O- $\beta$ -D-xylopyranoside, by various chemical degradations, spectral analysis and color reactions.

#### 11. Synthetic potentiality of *N*-methyl isoxazolidines in the synthesis of 1, 3 amino alcohols under microwave irradiation

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**Keywords:** *N*-methyl isoxazolidines, 1, 3 amino alcohols, MWI

Microwave assisted N-O bond cleavage of some new *N*-methyl isoxazolidines under mild conditions have been studied. Owing to the labile nature of the N–O bond isoxazolidines provide easy access to a variety of fascinating 1,3-difunctional amino alcohols in a shorter reaction time with high yield and selectivity. The methodology may be considered as an important approach towards ‘Green Chemistry’ because of its eco-friendly nature.

**12. Synthesis, characterization and study of the antitumor activity of (*E*)-2-arylidene-1-indanones**

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**Keywords:** (*E*)-2-Arylidene-1-indanones; methodology; antitumor activity, trifluoroacetic anhydride; MFC-7 cells

Novel substituted (*E*)-2- benzylidene-1-indanones have been synthesized and evaluated for their cytotoxicity. It was observed that 2-arylidene-4,7-diethyl indan-1-one inhibited significantly the growth of MFC-7 cells in a dose dependent manner, without producing any alteration to the HBL-100 cells.

**13. Vapour phase transformation of o-toluidine in a fixed bed reactor: Activation energy and thermodynamic properties of zeolite catalysts.**

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**Key words:** Toluidines, Zeolites, Isomerisation, Disproportionation, Deactivation

The molecular sieve -zeolites are widely used in chemical industry as catalysts for

different hydrocarbon processes. The size and shape of the zeolites are responsible for shape selectivity in different reactions. Toluidines are important intermediates for the manufacture of dyestuffs and agrochemicals and are generally synthesized by electrophilic nitration of toluene followed by reduction of the intermediate nitrotoluenes. In the present work zeolite ZSM-5 (MFI), ferririte (FER) and faujasite Y type (FAU) are studied for isomerisation reaction at atmospheric pressure in the fixed bed reactor. Their activation energy, thermodynamic properties (enthalpy, entropy, and free energy) is calculated. The effect of process parameters (reaction temperature, contact time) on activity and product selectivity is studied. The nature of deactivation shows that rate of deactivation is faster over wide pore zeolite than that of medium pore zeolite.

**14. Di-n-butyltin (IV) complexes of 2-[(E)-4-hydroxy-3-[(E)-4-(aryl) imino-methyl] phenyldiazenyl] benzoic acids: Synthesis, characterization and *in vitro* cytotoxicity property**

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**Key words:** NMR, <sup>119</sup>Sn mossbauer, exocyclic, endocyclic, *in vitro* cytotoxicity.

Bis-n-Dibutyltin (IV) complexes of 2-[(E)-2-(3-formyl-4-hydroxyphenyl)-1-diazenyl] benzoic acid and 2-[(E)-4-hydroxy-3-[(E)-4-(aryl) iminomethyl] phenyldiazenyl] benzoic acids have been synthesized and characterized with the help of IR, NMR and <sup>119</sup>Sn Mossbauer spectroscopic techniques. The <sup>119</sup>Sn-NMR spectra of the compounds display a pair of resonances of equal intensities which confirms the presence of *endo* and *exo* cyclic tin atoms. The <sup>119</sup>Sn Mössbauer spectra of the di-n-butyltin(IV) complexes **1-5** show one well resolved single doublet which indicate that the four tin centres present in the molecule have a similar environment. The *in vitro* cytotoxic activity of {[<sup>n</sup>Bu<sub>2</sub>Sn(L<sup>2</sup>H)]<sub>2</sub>O}<sub>2</sub> (**2**) was tested across a panel of seven human cell lines and the cytotoxicity property of the compound has been investigated. It has been shown that compound **2** is more active *in vitro* than other two {[<sup>n</sup>Bu<sub>2</sub>Sn(LH)]<sub>2</sub>O}<sub>2</sub> compounds and most of the standard drugs against

all seven human cancer cell lines.

**15. A comparative study of conventional versus microwave synthesis and spectral characterization of some new biological active 1,3,4-thiadiazole, 2-oxo-azetidinone derivatives of 4-methyl-3-mercapto-1,2,4-triazole nucleus**

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**Keywords:** 1,2,4-triazole, thiadiazole, 2-oxoazetidine, conventional, microwave irradiation.

2-(2-Bromobenzylidenylamino)-5-[(4-methyl-3-mercapto-1,2,4-triazolo)methyl]-1,3,4-thiadiazoles (4a-i) and 1-[5'-{(4-methyl-3-mercapto-1,2,4-triazolo)methyl}-1',3',4'-thiadiazole-2-yl]-4-(2-bromophenyl)-3-chloro-2-oxo-azetidine (5a-i), were synthesized by conventional and microwave irradiation technique and characterized by different spectral aspects. The results suggest that a microwave activation technique is superior to conventional heating. It offers by far the shortest reaction time with better yield. These title compounds were synthesized in a simple and rapid microwave heating approach directly from easily available starting materials. All the synthesized products are evaluated for their antibacterial and antifungal activity against bacteria *Staphylococcus aureus* and *Bacillus subtilis* and fungi *Fusarium oxysporum* and *Aspergillus niger* when compared with standard drugs.

**16. Effect of Mordant on Linen Fabric Using *Mangifera indica* Leaves Dye Shambhavi Mishra\*, Dr. Ritu Pandey<sup>!</sup> and Dr. Rekha Dayal<sup>#</sup>**

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**Keywords:** Linen, *Mangifera indica* dye, Natural mordant

The present study was undertaken to judge the colourfastness properties of linen fabric dyed with *Mangifera indica* leaves, using natural mordants- *Terminalia chebula*, *Terminalia belerica* and *Phyllanthus emblica* by traditional method of dyeing. The dyeing process was carried out under the optimized conditions. The samples were evaluated for their colour fastness towards light, washing, rubbing and perspiration (acidic and alkaline), which were found overall satisfactory. A comparison of all three mordants showed that dyed fabric mordanted with *Terminalia belerica* exhibited good colour fastness in comparison to dyed fabric mordanted with *Terminalia chebula* and *Phyllanthus emblica*. The overall impact of mordant on colour strength and colour difference is better than the colour strength of unmordanted dyed samples.

## 17. A New Antiviral Allelochemical from *Lactuca sativa* (Linn.)

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*Lactuca sativa* (Linn.) belongs to the family Compositae. It is commonly known as “**Kahu**” in Hindi. It is found throughout in India. It is an erect, glabrous, herbaceous annual, 0.5-1.2m. high, widely grown for its crisp, edible, highly developed radical leaves, which appear before the flowering starts. Its leaves are used as cattle feed. It is used as hypnotic in bronchitis and asthma. The plant is sedative and the dried milk of the cultivated forms is used as a calmant. The seeds are emollient. The inspissated milky juice of the wild forms is used as a substitute for opium. The present paper deals with the isolation and characterisation of a new allelochemical m. p. 271-273 °C, m. f. C<sub>34</sub>H<sub>42</sub>O<sub>18</sub>, [M]<sup>+</sup> 738 (FABMS) along with two known compounds Luteolin (B) and Quercetin (C) from seeds of *Lactuca sativa* (Linn.). A new compound was characterized as 5-hydroxy-3, 6-dimethoxy flavone -5-O- $\alpha$ -L-rhamnopyranosyl -(13) -O- $\beta$ -D-gluco-pyranosyl-(13)-O- $\beta$ -D-xylopyranoside by various chemical degradations and spectral analysis.

## 18. Friedlander Synthesis Of Benzo[*h*] Naphthyridines From *O*-Aminoaldehyde

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**Keywords:** - Friedlander condensation, 4-amino-6-chloroquinoline-3-carbaldehyde, benzo[*h*][1,6] naphthyridines, Lewis acid.

Recently, we reported the use of 4-amino-6-chloroquinoline-3-carbaldehyde for the synthesis of various benzo [3,4-*h*][1,6]naphthyridine as a key intermediate derivatives.<sup>1</sup> The important of these derivatives and our interest in this area have led us to explore the synthesis of new polysubstitued benzo[*h*] [naphthyridine derivatives starting from 4-amino-6-chloroquinoline-3-carbaldehyde (*o*-aminoaldehyde).

Thus, reaction of 4-amino-6-chloroquinoline-3-carbaldehyde with CH acidic compounds such as ethyl cyanoacetate, acetylacetone and benzyl cyanide in DMF in presence of catalytic amount of HCl under reflux for 4-5 h afforded 9-chloro-1,2-dihydro-2-oxobenzo[*h*][1,6]naphthyridine-3-carbonitrile, 1-(9-chloromethylbenzo[*h*][1,6]naphthyridin-3-yl)-ethanone and 9-chloro-3-phenylbenzo[*h*][1,6]naphthyridin-2-amine, respectively, in moderate (55-59%) yields.

To improve the yield and to find more convenient methods for the Friedlander condensation of *o*-aminoaldehyde with various active methylenes, all above reactions were performed in basic medium to yields corresponding benzo[*h*]naphthyridine derivatives in excellent yields (86-93%).

Alternatively, all these reactions could be performed under neutral conditions. This was achieved by heating a mixture of *o*-aminoaldehyde and the active methylene compound at 160-180°C for 15-30 min without solvent and catalyst which afforded benzo[*h*]naphthyridines in moderate yields.

**19. Synthesis and Antimicrobial Activity of Some 2-[(4-Substituted-phenyl-3-chloro-azetidin-2-one)-5-(2'-methylamino-4-phenyl-1', 3' - thiazolyl)-1, 3, 4- thiadiazoles**

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**Keywords:** 2-amino-4-phenyl-1,3-thiazole; Thiadiazole; Arylidene; 2-Azetidinone; Antimicrobial activity.

A new 2-[(4- substituted-phenyl-3-chloro-azetidin-2-one)-5-(2'-methyl-amino 4-phenyl-1', 3' - thiazolyl)-1,3,4-thiadiazoles, 5(a-n) were synthesized from 2-substituted-benzylideneamino-5-[2'- methyl – amino 4'phenyl-1',3'-thiazolyl]-1,3,4-thiadiazole, 4(a-n) using 2-amino-4-phenyl-1, 3-thiazole as a starting material. The synthesized compounds have been screened in vitro for their antimicrobial activity against bacillus subtilis, Escherichia coli. Klebsiella pneumoniae and Streptococcus aureus bacteria and Aspergillus niger, Aspergillus flavus, Fusarium oxisporium and Trichoderma viride fungi respectively. Some of the compounds displayed pronounced biological activity.

**20. Conventional and Greener Approach for the Synthesis of Some Novel Substituted -4- Oxothiazolidine and Their 5-Arylidene Derivatives of 2-Methylbenzimidazole: Antimicrobial Activities**

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**Keywords:** 2- Methylbenzimidazole, Thiadiazole, Aryledene, 4-Oxothiazolidine Antimicrobial activity.

The aim of this work was to investigate the efficiency of N<sup>1</sup> –(2-Benzylidene-imino-5'-methylene)-1',3',4'-thiadiazole]-2- methylbenzimidazoles, **4(a-n)**; N<sup>1</sup> -[2'-{2-Substituted-

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Phenyl-1, 3-thiazolidin-4-one}5'-methylene-1', 3', 4'- thiadiazole]-2 methylbenzimidazoles, **5(a-n)** and N<sup>1</sup>-[2'-{2-Substituted- Phenyl-1-5 substituted- benzylidene-1,3- thiazolidine-4-one}-5 methylene 1',3',4' thiadiazole]-2 methylbenzimidazoles, **6(a-n)** for the synthesis by conventional and greener approach methods in terms of yield and reaction time along with antimicrobial activity against *Bacillus subtilis*, *Escherichia coli* *khebsiella pneumonia* and *Streptococcus aureus* bacteria and *Aspergillus niger*, *Aspergillus flavus*, *Fusarium oxisporium* and *Trichoderma viride* fungi *in vitro* at 50 and 100 ppm concentrations. Some of the compounds displayed pronounced biological activity. The structures of all the new compounds were established on the basis of elemental analysis and spectral data (IR, <sup>1</sup>H NMR and mass).

**21. Organophorus Derivatives Containing 1, 4-Phthalazine Bis (Hydrazones) as Chemotherapeutants against Fungal Pathogens of Sugarcane  
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**Keywords:** Phosphorus, Hydrazones, IR <sup>1</sup>H NMR, Fungitoxicity, Sugarcane pathogens.

The reactions of o,o-diethylchlorophosphate or diethylchlorothiophosphate with 1,4-phthalazine-bis(hydrazones), derived by the condensation of 1,4- dihydrazinophthalazine dihydrochloride monohydrate and 2-hydroxy benzaldehyde /4-hydroxy benzaldehyde/2-hydroxyacetophenone/4-hydroxyacetophenone. Have been studied and a variety of organophosphorus derivatives have been obtained. The derivatives have been characterized on the basis of analyses and spectral (IR, <sup>1</sup>H NMR) data and tested for their antifungal efficacy against *colletotrichum falcatum* , *Fusarium oxysporum* and *Curvularia pallescens* (all sugarcane pathogens). These compounds show promising results in inhibiting the mycelial growth of all the test fungi at 1000 ppm. Out of these, the most active compound is o,o-diethylchlorophosphate derivative containing 1,4-phthalazine-bis(hydroxyacetophenone), hydrazone (VIII), which shows activity of 70.2% at 1000 ppm concentration against C. Pallescence.

**22. Use of Agrochemicals & its Biological impact: An insight into prospects & concern**

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Eversince the advent of “**Green Revolution**” of the sixties during the last century, a lot of remarkable developments in the field of agricultural science & technology have taken place which brought about drastic changes in our life-style. There has been a great deal of improvement in the socio-economic scenario of agrarian India. The green revolution has been able to do away with hunger to a larger extent. Growth and development of agricultural science and technology gave birth to high yielding Varieties of crops which dramatically improved grain production level. The unprecedented large scale production of food grains acclaimed international recognition as for instance the wheat production in India during the mid-sixties exceeds that of the preceding four thousand years. Nevertheless the agriculture sector should pay attention to increasing food production, its protection and preservation by using ecologically sustainable methods. Although the urgent need is to enlarge the base of food security by revitalizing the earlier (traditional) cultivation methods of a wide range of food crops in order to produce a variety of staple foods to meet the requirement of a reasonably malnourished society, the hope of providing people with a better diet is still far away due to overwhelming population growth and excessive use of chemical fertilizers & pesticides. This affects the basic health and hygiene and poses grave threat to the ecological system. It is high time for agricultural scientists and chemists to work together in quest of effective & everlasting eco-friendly measures to get rid of such an ominous disaster in the days ahead.

**23. SYNTHESIS AND ANTIMICROBIL ACTIVITY OF 6-PHEYL AZO COUMARIN-3-CARBOXY PHENYL AMIDES**

**Rashmi Sinha**

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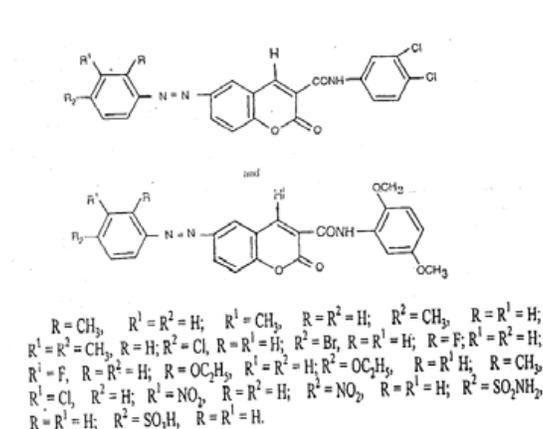
**Keywords:** IR/coumarin derivatives/antimicrobial activity/N-(2, 5-dimethoxy) phenyl

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malonamic acid/N-(3,4-dichlorophenyl malonamic acid)

Coumarin and its derivatives have been found to possess antibacterial<sup>1-5</sup>, antifungal<sup>6,7</sup> and anticoagulant activities.<sup>8</sup> Densal<sup>9</sup> has observed that some coumarin possessed antibacterial activity against *S. aureus* and *B. subtilis* and antifungal activity against *A. niger* and *T. mentagrophytes*.

The present work deals with the conversion of N-(2, 5-dimethoxy) phenyl malonamic acid and N-(3,4-dichloro) phenyl malonamic acid with some azo salicylaldehydes to form new coumarins bearing azo groups at position 6.



## 24. Characterization and Pharmaceutical Evaluation of Secondary metabolites from Aerial Part of *Cassia tora* Linn.

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**Key words:** *Cassia tora*, Pharmaceutical Evaluation, Secondary metabolite, Aerial Part.

Plants have played a significant role in maintaining human health and improving the quality of human life for thousands of years and have served humans well as valuable components of medicines, seasonings, beverages, cosmetics and dyes. The research on

plant derived products is playing a significant role in the drug delivery process of the pharmaceutical industry. Resistance to antimicrobial agents has become an increasingly important and pressing global problem. The search for new potential therapeutic compounds from plants and evaluation of their Pharmaceutical electrochemical analysis is necessary. Therefore, author took the challenging task of phytochemical and electroanalytical evaluation of Phytochemical Constituents of *Cassia tora* plant. It belongs to family Leguminosae and commonly known as 'Chakunda' or 'Pamad' in Hindi and distributed throughout in India and most tropical countries. This paper deals with the isolation and structural elucidation of a new bioactive compound 3, 5, 7, 4'-tetrahydroxy flavone-5-O- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)-O- $\alpha$ -L-rhamnopyranosyl-O- $\beta$ -D-xylopyranoside (01), along with two known compounds, Quercetin-3-O- $\beta$ -D-glucopyranoside (02) and Kaempferol-3-O- $\beta$ -D-glucopyranoside (03) were isolated from the stems of *Cassia tora* Linn. These compounds showed good antimicrobial activity against various microorganisms and all compounds also exhibited potential antioxidant activity. Ascorbic acid was used as a positive control. The petroleum ether soluble fraction of compound 01 showed strong antioxidant activity (IC<sub>50</sub>: 59.28  $\mu$ g/ml). The chloroform soluble fraction of compound 02 and compound 03 scavenged 50% DPPH free radical at the lowest inhibitory concentration (IC<sub>50</sub>: 57.82  $\mu$ g/ml) and (IC<sub>50</sub>: 55.38  $\mu$ g/ml) respectively.

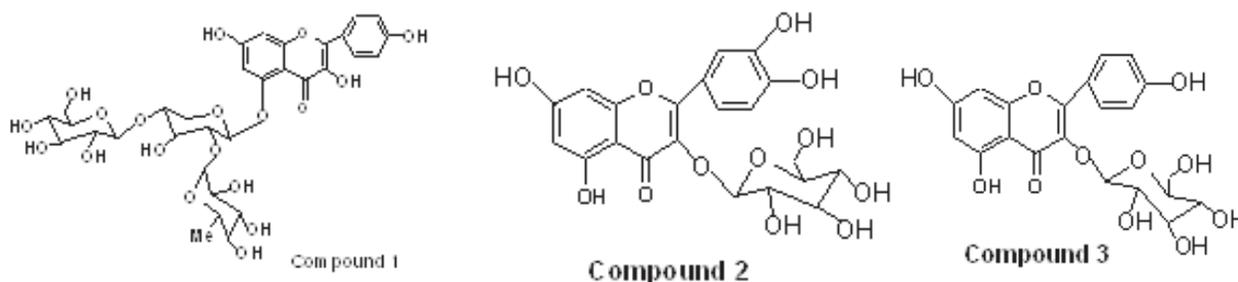


Figure: Structures of secondary metabolites isolated from *Cassia tora* Linn.

**25. Nitration of C<sub>13</sub>, and C<sub>23</sub>, Carbazole Alkaloids using Ceric Ammonium Nitrate**

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**Keywords:** *Murraya koenigii*, carbazole alkaloids, nitration, ceric ammonium nitrate.

In Course of our study of the nitration of carbazole alkaloids isolated from *Murraya koenigii*, we have observed the there is no report of the nitration of pyranocarbazole alkaloids with ceric ammonium nitrate in the literature. So we were interested to study the nitration of pyranocarbazole alkaloids girinimbine, koenidine, koenimbine and mahanimbine isolated from *M.koenigii*. Interstingly selective mononitration occurred in girinimbine and koenidine, whereas koenimbine and mahanimbine afforded dinitro derivatives as major products. Nitration of glycozolidine with ceric ammonium nitrate on the other hand furnished a dimeric dinitro compound. The preparation and structure elucidation of these new nitrocarbazole alkaloids will be discussed.

**26. A New Kinetic- spectrophotometric method for microgram determination of o- Toluidine in aqueous/mixed media**

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**Keywords:** Microgram Estimation of o-toluidine, Mn catalysed, periodate oxidation

The Mn (II) catalysed periodate oxidation of o-toluidine in acetone-water medium is first order with respect to catalyst, substrate and oxidant each. The progress of reaction was followed by monitoring the increase in the absorbance of reaction intermediate. The main reaction product characterized on the basis of melting point and spectroscopic studies, is methyl-1,4-benzoquinone. The effect of Ph, dielectric dielectric constant of medium, ionic strength and free radical scavengers was studied to develop the conditions for microgram determination of o-toluidine in the range 21.43 – 492.94 µg/ml. The characteristics of various calibration curves, Sendell's sensitivity, Molar absorptivity, percentage recovery, effect of interferrants and correlation coefficient have been evaluated. An attempt has been made for proposing a suitable mechanism for the reaction studied. Thermodynamic parameters are also reported.

**27. Synthesis of 1-Substituted-2-thio-(1H)-4-(3-phenylthiocarbamido-1-yl) - 6-(1-substitutedguanidino-3yl)-1, 2-dihydro-S-triazine.**

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**Keywords:** N-phenylformamidinoformamidinothiocarbaimde, 1, 3, 5- thiadiazines, S-triazines, synthesis.

Novel series of 1-substituted-2-thio-(1H)-4-(3-phenylthiocarbamido-1-yl)-6-(1-substituted- guanidine-3yl)-1,2- dihydro-s-triazine [4a(i) to 4f(ii)] has been obtained by the

isomerisation of 2-(1- substitutedguanidino -3-yl)-4-(3-phenylthiocarbamido-1-yl)-6-substitutedimino-1,3,3-thiadiazine [3a(i) to 3f(ii)] in presence of ethanolic sodium bicarbonate solution, which have been obtained by basification of their hydrochlorides [2a(i) to 2f(ii)] which are synthesized by the interaction of 1-Formamidino- (N- substitutedthioamido)-5-phenyl-2-thio 4-iminobiured (1a-f) and N-aryl/alkylisocyanodichlorides. The latter were prepared initially by the condensation of N-aryl/alkylisothiocyanate with N-phenylformamidinoformamidinothiocarbamide. The structure of all these compounds was established on the basis of elemental analysis, IR and PMR spectral data.

## 28. QSAR studies on the indolinones Derivatives as Kinase Inhibitors Activity

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**Keyword:** QSAR, FGFR, Indolinones Derivative (IDL<sub>S</sub>), Topological indices, Regression Analysis.

Quantitative structure activity relationship (QSAR) Studies on a series of indolinones derivative have been investigated as a potential inhibitor of protein tyrosine kinase of fibroblast growth factor receptor (FGFR) which is used as a major emerging strategy in cancer therapy. The significant correlation of activity pIC<sub>50</sub> were observed by using structural parameters like Balaban type Index and different molecular connectivity indices such as  $^0X^V$ ,  $^1X^V$ ,  $^2X^V$ , and  $^3X^V$ , which show vital role in Regression analysis and modeling of these indolinones derivatives.

**29. Iodobenzene diacetate Mediated Mild and Effective Synthesis of 1-Aryl/heteroaryl-[1, 2, 4]-triazolo [4, 3-a] quinoxalin-4(5H)-ones**

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**Keywords:-**Triazolo [4, 3-a] quinoxalin-4(5H)-ones, iodobenzene diacetate, oxidative cyclization, hydrazones

Triazoloquinoxalines exhibit a variety of pharmacological properties, including antitumor, antimicrobial and antidepressants besides being potent antagonists of several receptors such as adenosine and benzodiazepine. Conventional synthesis of [1,2,4]-triazolo[4,3-a]quinoxalin-4(5H)-ones involves thermal annelation of corresponding hydrazones in presence of ethylene glycol which is a high boiling solvent with long reaction time, cumbersome work-up and moderate yield. In the present protocol a mild, efficient and environmentally friendly synthesis of several 1-aryl/heteroaryl-[1,2,4]-triazolo[4,3-a]quinoxalin-4(5H)-ones (4) in high purity is described via iodobenzene diacetate mediated oxidative intramolecular cyclization of 3-(2-(aryl/hetroarylidenehydrazino)-quinoxalin-2(1H)-ones (3) and reaction times are considerably reduced. The title compounds are valuable precursors for the selective construction of highly functionalized organic molecules of synthetic and biological importance. The structural features of the new compounds have been determined from IR, <sup>1</sup>H NMR, mass spectral studies and elemental analysis.

**30. Synthesis and Biological Studies of Some 2, 3- Diphenylthiazolidin-4-ones and their Derivatives**

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**Keywords:** Diphenylthiazolidinones, bezylidenes, pyrazolines, biological activities,

antifungal, antimicrobial.

2, 3- Diphenylthiazolidin-4-one and its different benzylidenes have been used as the starting material in the present work. 4- Thiazolidinones are known to exhibit antitubercular, antibacterial, anticonvulsant, antifungal, antithyroid activities. These benzylidene derivatives possess unsaturated carbonyl groups which are further allowed to react with hydrazine hydrate and its phenyl derivatives to form different pyrazoline rings after cyclisation. Pyrazolines are found to be antipyretic, and show good antimicrobial and antifungal properties.

### **31. Synthesis, Antioxidant and Antimicrobial Activities Of Indolyl Opyrazoles**

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**Key words:** Indole, pyrazole, thiazole, antioxidant, antimicrobial activity.

A large number of synthetic drugs contains heterocyclic moieties and possess valuable properties as pharmacological agents. Amongst Nitrogen heterocycles, indole and its analogues occupied unique place in medicinal chemistry due to their wide range of pharmacological and biological activities. Therefore, it was considered worthwhile to synthesize a molecule encompassing both the above systems which may exhibit enhanced biological activities. Pyrazole moieties have bronchodilator, anti-inflammatory and oxidative hair-dye properties. 3-(2'-Phenyl-5'-substituted 1H-indol-3'-yl)-1phenylprop-2-

in-1-ones (1) on cyclodehydration with thiosemicarbazide gave 3-(2'-phenyl-5' substituted 1H-indol-3'-yl)5-phenyl-4,5-dihydro-1H-pyrazol-1-thiocarbamides (2). Compounds (2) on cyclocondensation with  $\alpha$ -bromoacetophenone yielded compounds (3). All the newly synthesized compounds were characterized by elemental analysis, IR, <sup>1</sup>H-NMR and mass spectroscopic studies. These compounds were screened for antioxidant activity and evaluated for antimicrobial activity against various organisms.

## **32. SYNTHESIS AND BIOLOGICAL ACTIVITIES OF THIAOLO [3, 2-A] PYRIMIDINE AND ITS DERIVATIVES LINKED TO INDOLE NUCLEUS**

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**Keywords :** Indole, thiazole, pyrimido[5,4-e]thiazolo[3,2-a]pyrimidine, antimicrobial, antioxidant activities.

Heterocyclic compounds have captured our attention for many reasons, chief among them are biological activities. A wide variety of indole derivatives have been described for their biological importance. Indole derivatives are found to be present in number of drug molecules e.g., indomethacin, hetroauxin, etc. Thiazolopyrimidines as antagonists are known to have potential biological importance. Therefore, it was considered worthwhile to synthesize a molecule encompassing both the above systems which may exhibit enhanced biological activities.

The key intermediate 5-amino-3-(4-aryl)7-(5'-substituted 2'-phenyl-1H-indol-3'-yl)-thiazolo[3,2-a]pyrimidin-6-carbonitriles (3a-i) were prepared by cyclocondensation of 2-amino-4-(4-aryl)thiazoles (1a-c) and the (5'-substituted 2'-phenyl-1H-indol-3'-yl)methylene carbonitriles (2a-c) in ethanol using catalytic amount of triethylamine under reflux condition. Compounds (3a-i) when subjected to heteroannulation with formamide, carbon disulfide and formic acid afforded the title compounds (4a-i), (5a-i) and (6a-i), respectively. The structures of all these previously unknown compounds were established

on the basis of their spectral and analytical data. These compounds have been screened for their antimicrobial and antioxidant activities. Most of the tested compounds exhibited mild to moderate antimicrobial activity against test microorganisms. Compound 4a was found to possess significant antifungal activity when compared to the standard drug fluconazole. Compounds 4g, 4h, 5e, 5h, 6b, 6f and 6h exhibited promising radical scavenging activity as compared to the standards. The results will be presented.

### **33. SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF SOME NOVEL COUMARIN BEARING PYRAZOLES**

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**Key words:** Coumarin, pyrazoles and antimicrobial activity.

Heterocyclic compounds are acquiring more importance in recent years due to the diverse pharmacological activities. Specifically, nitrogen, sulphur, oxygen containing five/six member heterocyclic compounds has occupied enormous significance in the field of medicinal chemistry. In addition, coumarin and pyrazoles were known for their potent biological activities such as antimicrobial, anti-inflammatory, anticancer and antiviral. In continuation of our research towards the synthesis and evaluation of various heterocycles, we present here the synthesis of coumarin analogs bearing pyrazole moiety. The synthon, 3-acetyl-2H-chromon-2-one on reaction with 3-substituted aryl-1-phenylpyrazol carboxaldehyde gave intermediate compounds –(E)-(3-substituted aryl-1-phenylpyrazol-4-yl)acryloyl)2H-chromen-2-ones. These chalcones upon cyclization with hydrazine hydrate yielded desired compounds in good yield. The characterization of all the synthesized compounds by spectral data such as IR, <sup>1</sup>H NMR and mass spectra and antimicrobial activities will be presented.

**34. New alginate stabilized silver nanoparticles beads for efficient removal of brilliant green dye**

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**Key words:** Silver nanoparticles; alginate beads; adsorption; brilliant Green

Silver nanoparticles have been grown on alginate gel using a green approach. The nanoparticles were characterized using scanning electron microscope (SEM) and UV-visible spectroscopy. Batch adsorption studies have shown that removal of brilliant green is dependent upon process parameters like contact time, initial concentration and pH. The adsorption data obtained from batch studies at optimized conditions have been subjected to Freundlich and Langmuir adsorption isotherm studies. The pseudo first and second order kinetic models were also applied to the experimental data. The silver nanoparticles beads were found to be an excellent adsorbent for adsorption of brilliant green from aqueous solutions.

**35. Novel citral and limonene based 2,5-disubstituted-1,3,4-oxadiazoles: A natural product coupled approach to semicarbazones for antiepileptic activity**

**Harish Rajak\*, Bhupendra Singh Thakur, Avineesh Singh,  
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**Key words:** 1, 3, 4-Oxadiazoles, semicarbazones, citral, limonene, anticonvulsants.

#### *Section IV: Chemical Sciences*

A series of novel series of citral and limonene based 2,5-disubstituted-1,3,4-oxadiazole were designed and synthesized for anticonvulsant activity. The chemical structures of the compounds were elucidated by elemental and spectral (IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and MS) analysis. The anticonvulsant activities of the compounds were investigated using maximal electroshock seizure (MES), subcutaneous pentylentetrazole (scPTZ) and subcutaneous strychnine (scSTY) models. Some of the selected active compounds were subjected to GABA assay to confirm their mode of action. The outcome of the present investigations proved that the four binding sites pharmacophore model is vital for anticonvulsant activity. The efforts were also made to establish structure-activity relationships among test compounds.

### **36. Synthesis and Evaluation of Some New Quinazolinone Derivatives for Their Anti Microbial Activity**

**Kumari Sujata & A.K. Kanth**

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**Key words**-Anti-microbial activity, Quinazolinones, CHN analysis.

The present work is a bonafide and novel for the synthesis of N<sup>1</sup>-3-(5-substituted-1,3,4-thiadiazol-2-yl)-(2-amino methyl) quinazolin-4(3H)-one derivatives. Around 30 new derivatives were synthesized, with the standard chemicals and well established procedures. The synthesized compounds were tested for their preliminary tests, physical constants, TLC, solubility, etc. The structures of the final compounds were confirmed by IR,  $^1\text{H}$ -NMR Spectra and CHN analysis. The proposed compounds were screened for their antimicrobial, antifungal, antitubercular and anti-inflammatory activities with the standard drugs in the well equipped microbiology and pharmacology lab by using standard methods.

**37. Microwave induced synthesis and 1, 3-dipolar cycloaddition reactions of novel dihydropyran derived nitron and their antibacterial activity.**

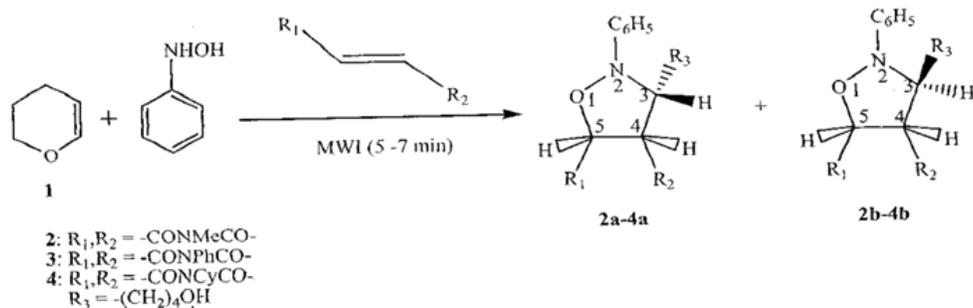
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**Keywords:** Solid phase cycloaddition reaction, novel isoxazolidines, amino alcohols, antibacterial activity.

Microwave induced 1,3-Dipolar cycloaddition reactions of novel dihydropyran derived nitron with various dipolarophiles have been studied in situ under solvent free conditions and found to afford novel isoxazolidine derivatives with high selectivity. Synthetic potential of the novel isoxazolidine derivatives are tremendous as they could be converted into acyclic chiral 1,3 difunctional amino alcohols by the reductive cleavage of the N-O bond when treated with zinc powder in dil acetic acid under microwave irradiation. All the synthesized compounds were screened for antibacterial and found to be very active.



**38. THIOISATIN-A MOIETY FOR HETEROCYCLIC INTEGRITY**

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**Keywords:** Thioisatin, photocycloaddition reaction, 1,3- dipolar cycloaddition reaction, azabicycloadducts, spiroyrrene, spiroyrrolidines, spirothiols, chalcones

#### Section IV: Chemical Sciences

Over the years our research program has revolved around developing novel sulphur heterocycles and understanding their reactions. In this respect heterocyclic species derived from thioisatins present fascinating chemistry. Azabicycloadducts and spiropyrenes by photochemical [4+2] - , spiropyrrolidines by 1, 3-dipolar-cycloaddition, spirothiol and chalcones by condensation reactions with aromatic amines and ketones present useful pathways for preparing a range of spiro and fused heterocyclic rings. An exclusive disulphide bond formation by dimerisation reaction has also been noted and characterized by X-ray analysis. The stereochemical course of the cycloaddition reactions has been investigated by spectral data and quantum mechanical studies. Details of our work during last one decade will be presented.

### 39. A [4+2] Photocycloaddition Pathway for Spiropyrene Derivatives

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**Keywords:** benzo [b] thiophene-2,3-dione; Friedal Craft's reaction; chalcones; photocycloaddition reactions; spiropyrenes

Over the years our research program has revolved around developing novel synthetic strategies based on thiophenic derivatives and understanding their photocycloaddition reactions. Consequently a series of chalcones have been synthesized by employing a facile synthetic pathway. These chalcones are precursors for spiropyrenes through which a variety of heterocycles which may act as building blocks for thiophenic drugs of industrial standpoint have been synthesised. A brief account of our recent efforts towards developing novel synthetic strategies for the synthesis of new sulphur heterocycles will be presented.

### 40. Potential Antioxidants from *Sesbania aculeata* Pers.

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**Key words:** Antioxidant and antibacterial Activity, *Sesbania aculeata*, Leguminosae.

Medicinal plants are relevant in both developing and developed nations of the

world as sources of drugs or herbal extracts for various chemotherapeutic purposes continue to play a dominant role in maintenance of human health since antiquities. Natural products play an important role in drug development programs of the pharmaceutical industry. Modern allopathic system of medicine is also based on plants and herbs. In the continuation of this strategy of new drug discovery we have studied only the stems of the *Sesbania aculeata* Pers plant for their antibacterial and antioxidant properties. *Sesbania aculeata* belongs to family Leguminosae and commonly known as 'Dhunchi' or 'Daincha' in Hindi. It is distributed throughout in plane India and most tropical countries. Its root is alexeteric, anthelmintic and diuretic. It is also useful in snake-bite and disease of eye. Its seeds are useful in ringworm and skin diseases. This paper deals with the significance and importance of medicinal plants. Potential antioxidant compound A (flavone glycoside), m.p. 222-224°C, m.f. C<sub>34</sub>H<sub>42</sub>O<sub>20</sub>, [M<sup>+</sup>] 770 (FABMS) has been isolated from the stems of *Sesbania aculeata* Pers. along with three known compounds Kaempferol 3-O-a-L-rhamnopyranosyl-(1®2)-b-D-glucopyranoside, (B) and Mearnsetin-3-O-a-L-rhamnopyranoside (C) Gehuain (isoflavone) (D). The compound A was characterized as 5, 7, 8-trihydroxy-6, 4'-dimethoxy flavone-7-O-a-L-rhamnopyranosyl-1®4)-O-b-D-xylopyranosyl-(1®4)--galactopyranoside by various chemical degradations and spectral analysis. Compounds A showed potent antioxidant activity, and antimicrobial activity. Antioxidant activity with the IC<sub>50</sub> value of 52.40 µg/ml and 60.15 µg/ml, respectively.

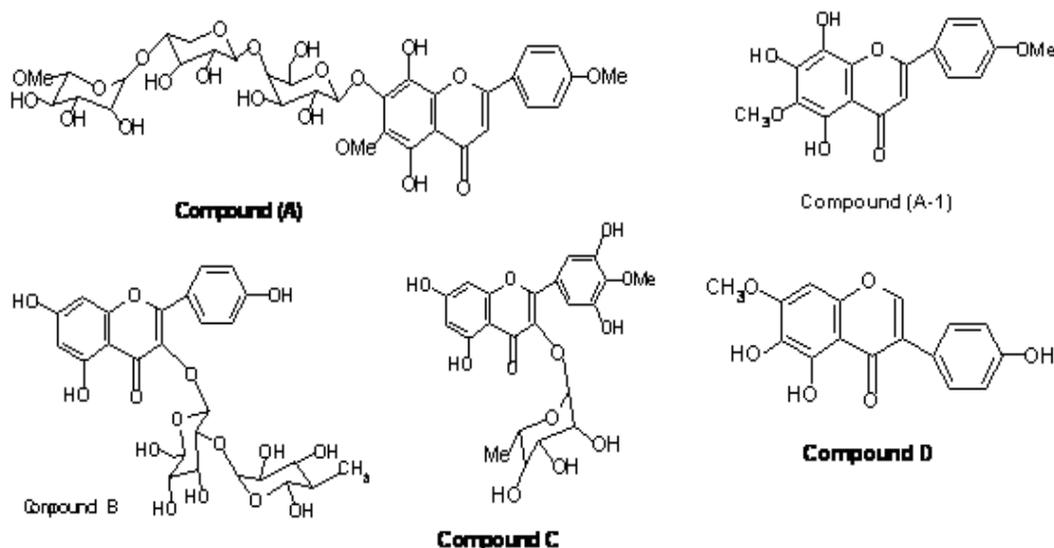


Fig: Potential Antioxidants isolated from *Sesbania aculeata* Pers.

**41. Solvent-Free Synthesis of Diethyl-1,4-Dihydro-2,6-Dimethyl-4-(1,3-Diaryl-1*H*-Pyrazole-4-yl)/Cycloalkyl Pyridine-3,5-Dicarboxylates as Potent Antimicrobial Agents**

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Multicomponent reactions have received considerable attention and emerged as one of the protocols in organic and medicinal chemistry. One such reaction that belongs to this class is Hantzsch synthesis. 1,4-Dihydropyridines are well known as calcium channel blockers and have emerged as one of the important classes of drugs for the treatment of hypertension. 1,4-Dihydropyridine ring is the common feature of various bioactive compounds such as vasodilator, antitumor, antidiabetic, antimicrobial, myocardial infarction, neuroprotectant peripheral vascular disorders, antitubercular, antiallergic, anti-inflammatory and platelet antiaggregatory activities. Dialkyl-1,4-dihydro-2,6-dimethyl pyridine-3,5-dicarboxylates have now been recognized as vital drugs in the treatment of angina and hypertension. In recent years, several synthetic procedures for the preparation of 1,4-dihydropyridines have been reported which includes microwave irradiation, use of reagents like TMSCl, catalysts like TBAHSO<sub>4</sub>, Yb(OTf)<sub>3</sub>, ionic liquids etc. Many of these protocols involve prolonged reaction times (classical Hantzsch reaction), expensive reagents and catalysts. Therefore, the development of an uncatalysed, nonconventional solvent-free method with less reaction time and high yields is imperative to extend the scope of the Hantzsch reaction. In recent years, solvent-free synthesis has become a hotspot of investigation, because it is a prominent green chemistry principle. As a continuation of our efforts on synthesizing heterocyclic compounds possessing significant biological activities with green and efficient method, we have taken up the synthesis of Diethyl-1,4-dihydro-2,6-dimethyl-4-(1,3-diaryl-1*H*-pyrazole-4-yl)/cycloalkyl pyridine-3,5-dicarboxylates through three component reactions of 1,3-diaryl-1*H*-pyrazole-4-carbaldehyde, ethylacetoacetate and ammonium acetate under solvent free conditions. It is an efficient, simple, uncatalysed and promising synthetic strategy to build 1,4-dihydropyridines. All the synthesized compounds were characterized by elemental analysis and spectral data such as IR, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR and Mass. Further, *in-vitro* antimicrobial activities of the compounds were screened against different pathogens.

**42. Reinvestigation on the Chemical Constituents of *Argemone mexicana* Linn. (Papaveraceae)**

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**Keywords:** *Argemone mexicana*; Papaveraceae; Hentriacontane-3,20-diol; Isorhamnetin 3-O- glucoside

*Argemone mexicana* Linn. (Papaveraceae) has long been used in Indian traditional system of medicine; flowers are found to be expectorant and have been used in the treatment of coughs as well. A number of pharmacological studies have showed that *A. mexicana* possesses various pharmacological properties including anti-inflammatory, antimicrobial, cytotoxicity and so on. In continuation of our works on the chemical screening of Indian medicinal plants, we herein wish to report our results from the reinvestigation of this plant. The dried flower petals yielded one aliphatic diol and one flavone glycoside characterized, respectively, as hentriacontane-3,20-diol and isorhamnetin 3-O-glucoside. The respective chemical structures were elucidated on the basis of detailed spectral studies including UV, FT-IR, NMR (<sup>1</sup>H & <sup>13</sup>C) and HR-MS as well as X-ray crystallographic studies.

**43.  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$  Catalyzed Solvent Free Multicomponent Synthesis of  $\alpha$ -Aminonitrile: A Novel and Efficient Protocol for Strecker Reaction at Room Temperature**

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**Keywords:**  $\alpha$ -aminonitriles; multi-component reaction;  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$ ; solvent-free; environmentally benign

Strecker reaction is one of the most important multicomponent reactions (MCRs) for straightforward synthesis of  $\alpha$ -amino nitriles that are useful intermediates for the synthesis of many natural and unnatural amino acids and nitrogen containing heterocycles such as thiadiazoles and imidazoles, *etc.* Literature survey revealed that trimethylsilyl cyanide (TMSCN) is very safe to handle and can act as an effective cyanide source. A number of strong and efficient Lewis acid catalysts have also been well documented earlier for this reaction; but most of these methods involve the use of organic solvents, and many of them suffer from waste disposal problem. Hence, a straightforward and novel method for the one-pot synthesis of  $\alpha$ -aminonitriles has been developed using  $\text{ZrOCl}_2 \cdot 8\text{H}_2\text{O}$  as catalyst at room temperature under solvent-free conditions. The process is very simple, cost-effective and environmentally benign.

**44. Novel Synthetic Strategies and Characterization for Spirothiazolidine Frameworks**

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**Keywords:** benzo[b]thiophene-2, 3-dione; Friedal Craft's reaction; imino compounds; thiazolidines; cyclisation reactions; spectral characteristics

Sulphur heterocycles are important class of chemical entities in medicine and food production. Over the years our research program has revolved around developing novel synthetic strategies based on thiophenic derivatives and understanding their cycloaddition reactions. Consequently a series of imino intermediates have been synthesized by employing a facile synthetic pathway. These intermediates are precursors for various heterocycles through which a variety of spirithiazolidines of medicinal relevance have been prepared by cyclisation reactions with mercaptoacetic acid. A brief account of our recent efforts towards developing novel synthetic strategies for the synthesis of new sulphur heterocycles will be presented.

**45. Synthesis, spectral characterization and biological evaluation of 8-chloro-5-methoxy-4H-1, 4-benzothiazines**

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**KEYWORDS:** 4H- Benzothiazines, antimicrobial activity and spectroscopic data.

Substituted 8-chloro-5-methoxy-4H-1, 4-Benzothiazines are synthesized by

condensation followed by oxidative cyclization of 2-amino-6-chloro-3-methoxybenzenethiols with *b*-diketones/*b*-ketoesters in presence of dimethylsulfoxide. The structures of the synthesized compounds have been established by elemental analysis and spectroscopic data. Their antimicrobial activity has also been carried out.

**46. Standardization of quality parameters of oil of Lemongrass (*Cymbopogon flexuosus*) grown in Orissa.**

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**Keywords:-**Cymbopogon flexuosus, essential oil composition, citral, geranial; netral;

Northern part of India is now immerging as the major essential oils producing area. A study was undertaken to evaluate the physico-chemical properties of lemongrass oil produced in Orissa. The oil collected for the study from the areas presently under extension of aromatic crops are Bandugaon block of Koraput, Bhanjanagar, of Ganjam\, Kandhamal, Rayagada & Balasore districts. Lemongras oils collected from these areas of Orissa and on analyzing it observed that lemongrass oil meets the BIS specifications and also have the higher Citral contents, which indicate good quality oil as the quality of lemongrass oil, decide mostly on the basis of citral contents.

**47. Assessment and Characterization of Physiochemical Parameters of Soil of Amanisghah-Nala of Jaipur City, Rajasthan (India) with reference to Agricultural and Irrigational Purposes**

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**Keywords:** Soil Pollution, Amanish-nala, Physical-chemical parameters, alkalinity, Micronutrients.

The aim of this study was to evaluate the levels of some physical and chemical soil parameters in Amanisha-nala of Jaipur city during post monsoon session 2010, to assess the quality of soil for determining its suitability for agricultural and irrigation purposes. Physico-chemical parameters of soil such as pH, EC, available organic-carbon, phosphate, potash and Micronutrients such as Zn, Fe, Cu and Mn were analyzed. The analysis of soil samples shows that there is a problem of alkalinity in soil nature regarding pH which is somewhat not permissible for irrigation and agricultural purposes. The percentage analysis of organic carbon shows low level in the entire soil samples. The mean concentration of Micronutrients is in order of Fe>Mn>Cu>Zn. (in ppm).

**48. Synthesis, structural characterization, anti-microbial and DNA cleavage studies of new binuclear metal complexes derived from o-hydroxyacetophenone**

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**Keywords:** Schiff base, binuclear, o-hydroxyacetophenone, anti-microbial, DNA studies

A new tetradentate ligand [H<sub>2</sub>L] has been synthesized by the condensation between

3, 3' diaminobenzidine with o-hydroxy acetophenone in the molar ratio 1:4. The reaction of ligand with metal chelation leads to bimolecular complexes of general formula  $[M-2(L)X_4]$ . The ligand and metal complexes have been characterized by elemental analysis, UV, IR,  $^1H$  NMR,  $^{13}C$  NMR, conductivity measurements, EPR and magnetic studies. In conductivity experiments all metal chelates were showed non-electrolytic in nature. The bonding sites are the nitrogen atoms of the azomethine and the oxygen atoms of the phenolic groups. All metal complexes exhibit octahedral in structure. The anti-microbial activities were screened against one gram positive bacteria (*S.aureus*) and one gram-negative bacterium (*E.coli*). The anti-fungal activity was screened against *asperigillus flavus*. All complexes were showed significant anti-bacterial and anti-fungal activities. The DNA cleavage studies of these complexes were investigated by gel electrophoresis method in presence of peroxide. All complexes cleaved efficiently.

#### **49. Synthesis of 3-Halo Flavones from 2-Hydroxy-3,-5-Disubstituted Acetophenone**

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**Keywords:** Flvones, Diketones, Dibenzoyl methane, Synthesis

Substituted acetophenone was reacted with substituted benzoic acid in pyridine medium as base in presence of phosphoryl chloride for five hours and the thick mass was decomposed by 1:1 HCl to get substituted benzoyloxy substituted acetophenone. This product was further subjected to BVT reaction to get substituted dibenzoyl methane. Substituted dibenzoyl methane is treated with pure bromine in DMF medium gives 3-halo flavones. B- Diketone is useful starting compounds for synthesis of various important

compounds viz. hormones<sup>1</sup>, oxygen and nitrogen containing heterocycles, pyrazoles<sup>2,3</sup>, isooxazoles<sup>4</sup>, 3-bromo flavone<sup>5,6</sup>, 3-chloro flavones<sup>7</sup>. Propane 1-3-dione reacts with dibromide to give 3-bromoflavone<sup>7</sup>;  $\beta$ -dicarbonyl compounds have been effectively chlorinated using sulphuryl chloride to form 3-chloro flavones. Acetyl acetone has been chlorinated with sulphuryl chloride in acetic acid<sup>8</sup>. Dibenzoyl methane gives "3-chloro dibenzoyl methane with sulphuryl chloride in Dioxane medium<sup>9</sup>. 3-chloro flavones were prepared by action of thionyl chloride or sulphuryl chloride with flavones<sup>10-12</sup>. Various 3-halo flavones were prepared by reaction of corresponding flavones derivatives with  $R_4NBr / Ph / (OAc)_2$  system under mild reaction conditions<sup>13</sup>. 1,3-diketones were transformed into 7-hydroxy-6-nitro flavone<sup>14</sup>. Dibenzoyl methane reacts in DMF medium or with bromine in DMF to give 3-halo flavones<sup>15</sup>.

## **50. Recent Trends in MAOS: A Review**

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The recent publication of several major reviews[1], [2] on microwave-assisted organic synthesis notwithstanding, plethora of very recent articles describing a variety of new chemical synthesis performed with microwave irradiation have appeared. This review will document many [3], [4] of these synthetic applications. The utilization of high intensity ultrasound in chemical processes is referred to as sonochemistry. It is well known [5], [6] that ultrasound irradiation provides a powerful technique for establishing unique chemical and physical conditions, such as a local increase in temperature of several thousands of Kelvins.

**51. Eco-friendly three-component regioselective synthesis of some pyrazolo [3, 4-*b*] pyridines under solvent-free condition**

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**Keywords:** Phenyl hydrazine;  $\alpha$ -Cyanoacetophenones;  $\beta$ -Diketones; Three-component; Solvent-free.

A solvent-free approach is described for the regioselective synthesis of some 3-aryl-1-phenyl-4,6-disubstituted-1*H*-pyrazolo[3,4-*b*]pyridines **5** via a three-component reaction between phenyl hydrazine **1**,  $\alpha$ -cyanoacetophenones **2** and  $\beta$ -diketones **4** in the presence of *p*-toluenesulphonic acid (PTSA). Initially, reaction was carried out by conventional stepwise methodology using solvents which afforded not only the inseparable regioisomeric mixture of (3-aryl-1-phenyl-6-aryl-4-methyl-1*H*-pyrazolo[3,4-*b*]pyridines **5**, its isomeric structure **6** (3-aryl-1-phenyl-4-aryl-6-methyl-1*H*-pyrazolo[3,4-*b*]pyridines but also an undesired product **7** (5-acetylamino-3-aryl-1-phenylpyrazoles). Three-component solvent-free synthesis has the advantages of easier workup, milder reaction conditions, environmentally benign procedure and high level of regioselectivity over the stepwise solvent-mediated reaction.

**52. Discovery of new 2-(4-cyanophenyl amino)-4-(quinoline-4-yloxy)-6-piperazinyl (piperidinyl)-1, 3, 5-Triazines acting as antimicrobial/antimycobacterial/anticancer agents**

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**Keywords:-** 2, 4, 6-Trichloro-1, 3, 5-triazin, 4-Hydroxyquinoline, Piperazine, Antimicrobial activity, Antimycobacterial activity

The pharmacological potency of novel 2-(4-cyanophenyl amino)-4-(quinoline-4-yloxy)-6-piperazinyl (piperidinyl)-1,3,5-triazines was determined against eight bacteria (*S. aureus*, *B. cereus*, *E. coli*, *P. aeruginosa*, *K. pneumoniae*, *S. typhi*, *P. vulgaris*, *S. flexneria*), four fungi (*A. niger*, *A. fumigatus*, *A. clavatus*, *C. albicans*) and *Mycobacterium tuberculosis* H37Rv strain. Bioassay results revealed that compounds **5d**, **5n**, **5q**, **5r**, **5s**, **5t** and **5u** could be considered as possible potential agents with dual antimicrobial and antimycobacterial activities at the lowest MICs ranging from 6.25-50 µg/mL. The structures of the compounds were elucidated with the aid of FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, <sup>19</sup>F NMR and elemental analysis.

**53. Investigation of Oil Agglomeration Process for Beneficiation of Waste Fine Coal from deposits of Bikaner, Rajasthan, India**

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**Keywords:** - Oil agglomeration; Lignite; Beneficiation; Ash; Fixed carbon.

Oil agglomeration is an effective technique for beneficiation and reducing the ash of coal fines. The finely ground coal, dispersed in water, is contacted with oil by intensive mixing. The hydrophobic coal particles collect onto the oil droplets to form the agglomerates which are then separated from the aqueous phase by screening. The aim of this study was to determine the appropriate various oils for lignites at selective agglomeration. Kerosene, diesel oil, burn fuel oil, olive oil, and various surface active components were used. All experiments were performed at room temperature. The best results were obtained with olive oil. Experimental studies were conducted on the lignite sample with ash, sulphur, volatile matter and fixed carbon contents of 31.15%, 1.35%, 20.80%, and 6.05%, respectively.

**54. A facile synthesis of 2-((3H-imidazo [4, 5-b] pyridin-2-ylthio) methyl)-5-aryl-1, 3, 4-oxadiazoles**

**Dayakar G\* and Sujatha I**

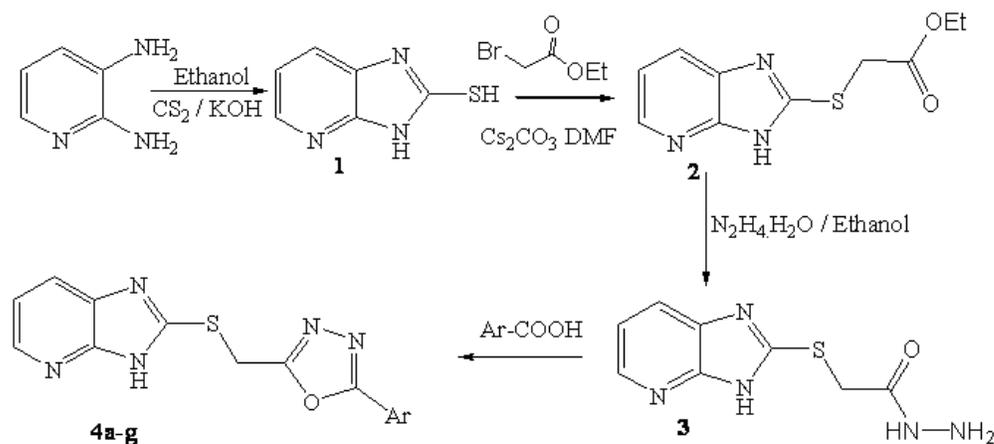
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**Key words:** Carbohydrazides, Oxadiazoles, antimicrobial activity, Imidazoles.

Hydrazides and related compounds have been described as useful building blocks for the assembly of various heterocyclic rings. Thus, different carbohydrazides were found

to be useful in chemical and pharma industry. The synthesis of compounds incorporating both 1,2,4-triazole, and 1,3,4-oxadiazole rings has been attracting widespread attention due to their diverse pharmacological proprieties such as antimicrobial, anti-inflammatory, analgesic and antitumor activities. Derivatives of 1,3,4-oxadiazole are also known to have a broad spectrum of biological activities. Hydrazides have been in general use as the starting materials in some 1,2,4-triazole and 1,3,4-oxadiazole syntheses. In continuation of our investigation on antimicrobial activities of heterocyclic compounds, we wish to report a common route to the synthesis of 2-((3H-imidazo[4,5-b]pyridin-2-ylthio)methyl)-5-aryl-1,3,4-oxadiazoles. 2-((3H-imidazo[4,5-b]pyridin-2-ylthio)methyl)-5-aryl-1,3,4-oxadiazole are synthesized by the reaction of 2-(3H-imidazo[4,5-b]pyridin-2-ylthio)acetohydrazide with benzoic acids and thionyl chloride. The structures of the products were established by spectral analysis like IR, <sup>1</sup>H NMR and Mass spectroscopy,



55. **Volumetric, acoustic and spectroscopic studies for binary mixtures of ionic liquid (1-butyl-3-methylimidazolium hexafluorophosphate) with alkoxyalkanols at T= (288.15 to 318.15) K**

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**Key words:** Ionic liquid; Alkoxyalkanols; Density; Speeds of sound; <sup>1</sup>H NMR

Densities and speeds of sound have been measured for the binary mixtures of ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate [bmim][PF<sub>6</sub>] with ethylene glycol monoethyl ether (EGMEE), diethylene glycol monoethyl ether (Di-EGMEE), triethylene glycol monoethyl ether (Tri-EGMEE) over the whole composition range at atmospheric pressure. Experimental densities have been used to estimate excess molar volumes, . Changes in isentropic compressibility have been estimated by using experimental speed of sound and density values. Excess properties were fitted to the Redlich-Kister polynomial equation to obtain the binary coefficients and the standard errors. The molecular scale interactions between ionic liquid and alkoxyalkanols have been investigated through <sup>1</sup>H NMR spectroscopy. NMR chemical shifts for hydroxyl group of alkoxyalkanols and their deviations show hydrogen bonding interactions of varying strengths between ionic liquid and alkoxyalkanol in their binary mixtures.

## 56. Correlation between hardness and basicity (pK<sub>a</sub>) of substituted anilines

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**Keywords:-**Aniline; HOMO-LUMO; Basicity; Hardness; Correlation coefficient.

In this work the correlation between hardness and basicity (pK<sub>a</sub>) of substituted and N-Alkylated anilines has been studied. The hardness values of aniline; ortho-; meta-; para-substituted amino-, methyl-, chloro-, nitroanilines and N-alkylated (N-methyl, N-ethyl, N-phenyl) anilines have been calculated using Koopmans' relation. The calculation of the energies of HOMO & LUMO of the above compounds has been done semi-empirical quantum mechanically (using AM1 & PM3 semi-empirical Hamiltonian) with the help of ArgusLab4.0 software. The high correlation between pK<sub>a</sub> values and hardness of substituted

and N-Alkylated anilines indicate the hardness bears direct relationship to the basicity of substituted anilines.

**57. Synthesis and characterization of complexes and their biological screening.**

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**Keywords:** - Macrocyclic complexes; infrared spectra; magnetic measurements, antibacterial activity.

A new series of complexes is synthesized by template condensation of oxalyldihydrazide and diacetyl in methanolic medium in the presence of trivalent salts forming complexes of the type:  $[M(C_{12}H_{16}N_8O_4)X]X_2$ ; where M = Cr (III), Fe (III) and X =  $Cl^{-1}$ ,  $NO_3^{-1}$ ,  $CH_3COO^{-1}$ . The complexes have been characterized with the help of elemental analyses, conductance measurements, and magnetic susceptibility measurements, electronic, infrared and far infrared spectral studies. On the basis of these studies, a five coordinate distorted square pyramidal geometry for these complexes has been proposed. The biological activities of the metal complexes have been tested *in vitro* against a number of pathogenic bacteria to assess their inhibiting potential. Some of the compounds have been found to exhibit remarkable antibacterial activities.

**58. Spectroscopic characterization of medicinally potent Schiff base derived from carbazole moiety**

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**Key words:** Spectroscopic, medicinally, potent, carbazole

Microwave-assisted synthesis and characterization of the tin (II) complexes are

reported. octahedral complexes of tin (II) have been synthesized by the reaction of (E)-N-(8,9-dihydropyrazolo[4,3-b] carbazol-6(1H,5H,7H)-ylidene)thiazole. The complexes so formed were characterized by various physicochemical studies i.e. elemental analysis, conductance measurements, molecular weight determinations. Bonding of complexes is discussed in terms of their IR, XRD, <sup>1</sup>H NMR studies. Ligands acts as bidentate towards metal ion via nitrogen donor sites. Elemental analysis and NMR spectral data of the ligands with their complexes agree with their proposed structures. The anti-microbial activities of the ligands and their corresponding tin (II) complexes have been screened against various strains of bacteria and fungi.

**59. Allylation of aldehyde with allyltributylstannane under solvent-free conditions**

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**Keywords:** Aldehyde, allyltributylstannane, homoallylic alcohol, solvent-free, silica

In recent years, homoallylic alcohols are finding various applications in the field of organic total synthesis and pharmaceutical research [1]. Many acid catalysts, BF<sub>3</sub>.Et<sub>2</sub>O, SnCl<sub>4</sub>, TiCl<sub>4</sub>, AgOTf, and ReBr (CO)<sub>5</sub>, Sc (OTf)<sub>3</sub>, palladium and platinum complexes are used to catalyze this transformation. But requirement strictly anhydrous conditions, hazardous solvent, long reaction time, expensive catalyst are some of drawbacks, besides being inconsistent in terms of reaction yields and require either high temperature. Here, we wish to report our finding on the utility of silica gel (60-120 mesh) as catalyst for the synthesis of homoallylic alcohols by grinding a mixture of aldehyde and allylstannanes in the absence of any solvent at ambient temperature.

**60. Synthesis, spectral, thermal, XRD and antimicrobial studies of some transition metal complexes involving 2-amino-6-nitrobenzothiazole moiety**

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**KEYWORDS:** Complexes, Spectral, Schiff-base, XRD, Thermal analysis, Antimicrobial

The coordination complexes of Co (II), Ni (II) and Cu (II) derived from 5-bromosalicylaldehyde / 2-hydroxy-3-methoxybenzaldehyde with 2-amino-6-nitrobenzothiazole have been synthesized and characterized by elemental analysis, FT-IR, FAB-mass, molar conductance, electronic spectra, <sup>1</sup>H-NMR, ESR, magnetic susceptibility, thermal and XRD analysis. The complexes are coloured and stable in air. Analytical data revealed that all the complexes exhibited 1:2 (metal: ligand) ratio with coordination number 4 or 6. IR data shows that the ligand coordinates with the metal ions in a bidentate manner through the phenolic oxygen and azomethine nitrogen. FAB-mass and thermal data show degradation pattern of the complexes. The thermal behavior of metal complexes shows that the hydrated complexes loses water molecules of hydration in the first step; followed by decomposition of ligand molecules in the subsequent steps. XRD patterns indicate crystalline nature for the complexes. The Schiff base and metal complexes show a good activity against the Gram-positive bacteria; *Staphylococcus aureus* and Gram-negative bacteria; *Escherichia coli* and fungi *Aspergillus niger* and *Candida albicans*. The antimicrobial results also indicate that the metal complexes are better antimicrobial agents as compared to the Schiff bases.

**61. Effect of Locked Nucleic Acid modification on Thermal Stability of Non-canonical DNA Structure**

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**Keywords:** LNA, Parallel and antiparallel duplexes, kinetics, thermodynamics

We studied the kinetic and thermodynamic effects of locked nucleic acid (LNA) modifications on parallel and antiparallel DNA duplexes. Kinetic parameters showed that association and dissociation rate constants for formation of LNA-modified parallel duplex at 25.0°C were 3 orders larger and 6 orders smaller, respectively, than the unmodified one. Thermodynamic parameters showed that extent of stabilization for parallel duplexes (3.6 kcal mol<sup>-1</sup> per modification) was more significant than antiparallel duplexes (1.6 kcal mol<sup>-1</sup>). This large stabilization was due to decrease in  $\Delta H^\circ$  which was greater than  $T\Delta S^\circ$ . These results demonstrated that LNA modification specifically stabilized the noncanonical parallel duplex.

**62. The effect of sodium dodecyl sulphate micelles on the kinetics of oxidation of L-cysteine by iron (iii)-1, 10-phenanthroline complex**

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**Keywords:** Kinetics and mechanism, L-cysteine, iron (iii)-1, 10-phenanthroline and sodium

dodecyl sulphate

The effect of sodium dodecyl sulphate micelles on the kinetics of oxidation of L-cysteine by iron (iii)-1, 10-phenanthroline complex in perchloric acid medium was studied at 30<sup>0</sup>C. The progress of the reaction is followed by measuring the absorbance of tris-phenanthroline iron(II) formed at 510 nm. The reaction showed first order dependence with respect to iron(III). The rate of the reaction increases with increase in phenanthroline concentration and [cysteine] as well and the order with respect to cysteine was found to be two. The rate of the reaction decreases with increase in [SDS] and [H<sup>+</sup>]. Stoichiometric study and product analysis confirmed that the product of oxidation of cysteine to be cystine. A suitable mechanism has been proposed to explain the observed kinetics involving the reaction between [Fe(phen)<sub>2</sub>RSH]<sup>3+</sup> and zwitterionic form of cysteine in rate-determining step. The activation parameters of the reaction were computed using linear least squares method and the values of E<sub>a</sub> and "S<sup>#</sup> were found to be 64.8 ± 1.1kJmol<sup>-1</sup> and -50.5 ± 3.5JK<sup>-1</sup>mol<sup>-1</sup> respectively.

**63. Optimization, Immobilization and Kinetic Parameters for the Production of Itaconic Acid by *Aspergillus terreus* MTCC 479**

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**Keywords:** Itaconic acid, *Aspergillus terreus*, Immobilization, Kinetic parameters

Itaconic acid is commercially produced by the cultivation of *Aspergillus terreus* with different carbon sources. Molasses is one of the best carbon sources among various carbohydrates, because it is pure, inexpensive and available in a mass supply. The reaction was carried out at various molasses concentrations, temperatures, incubation time intervals,

agitation speed and pH. The present study reveals that the maximum itaconic acid was produced at 35 °C, molasses concentration of 10%, agitation speed of 200 rpm, at 3.5 pH and incubation time of 120 hrs with a yield of 0.4976 g/l, specific growth rate of 0.04199 hr<sup>-1</sup> and minimum doubling time of 14.84 hrs. And also the maximum itaconic acid concentration was obtained for 0.5 cm cube and doubled the concentration after 14 days with immobilized mycelium than free mycelium.

#### **64. Convenient Methodologies for the Synthesis of Novel Benzodiazocine Derivatives**

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**Keywords:** benzo[b]thiophene-2, 3-dione; Friedal Craft's reaction; chalcones; benzodiazocine; Cyclisation reactions; Spectral characteristics

Synthesis of 6-(phenyl)-benzo[b]thiophen [2, 3-e][1,4] benzodiazocine derivatives have been achieved for the first time by reaction of chalcone with *o*-phenylene diamine. Over the years our research program has revolved around developing novel synthetic strategies based on thiophenic derivatives and understanding their reactions. Consequently a series of benzodiazocines have been synthesized by employing a facile synthetic pathway. Some of the benzodiazocine derivatives are used as antipsychotic and antiobesity agents. The structures are assigned with the help of analytical and spectral studies.

#### **65. Synthesis and Characterization of 4', 6'Bis-2(arylamine)-5-triazine derivatives of biological and PC model Computational studies**

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**Key words:** Atriazine, ametryn, herbicides S-Triazine metabolites analysis.

Triazine is the chemical species of six member heterocyclic ring compounds (1). With three nitrogen's replacing carbon hydrogen units in the benzene ring structure. The names of the three isomers indicate which of the carbon hydrogen units on the benzene ring position of the molecule have been replaced by nitrogen's called 1,2,3-triazine(2,3,4), 1,2,4-triazine, and 1,3,5-triazine respectively. Symmetrical 1, 3, 5-triazine is the common triazines are prepared from 2 azidocyclopropene through thermal rearrangement (1, 2, 3) triazine from 1,2, dicarbonyl compounds with amidrazon by condensation reaction (1,2,4-triazine) and from cyanuric acid amide by trimerization (1,3,5-triazine) pyridine is the aromatic nitrogen heterocycle compound having only one nitrogen and diazines are with 2 nitrogen atoms and tetrazines are with 4 nitrogen atoms on the benzene ring systems. Triazines are weak base. Triazines have much weakened resonance energy than benzene, so nucleophilic substitution is preferred that electrophilic substitution. Triazines are basic structure of herbicides simazine, trietazine (5, 6, 7,).

**66. DESIGNING OF A NOVEL BIOLOGICAL ACTIVE COMPOUND:  
AB-INITIO STUDIES OF S-BENZYL  $\hat{\alpha}$ -N-  
(FURYLMETHYLKETONE) DITHIOCARBAZATE**

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**Keywords:** S-methyldithiocarbazate, Furylmethylketone Schiff base, HF/STO-3G, HF/3-21G & HF/6-31G1 *ab-initio* methods, Correlation Coefficient (CC), HOMO-LUMO energy and Hardness-Softness.

The molecular geometry, net atomic charge and atom electron densities, HOMO-LUMO energy, Hardness-Softness, vibrational frequencies and thermodynamic parameters of the S-benzyl  $\hat{\alpha}$ -N-(furylmethyl ketone)dithiocarbazate, a novel biologically active

compound, are examined theoretically at the *ab-initio* HF/STO-3G, HF/3-21G & HF/6-31G levels. The correlation coefficients are reported for bond lengths, bond angles and vibrational frequencies at different levels of calculations. Net atomic charge and atom electron density data reveal the coordination sites in S-benzyl  $\hat{a}$ -N-(furylmethylketone) dithiocarbazate when it undergoes complexation with transition metal ions. Consequently, performance of *ab-initio* method at different levels of calculations has been tested to find the best auxiliary tool for the designing of a novel material.

## 67. “SYNTHESIS, CHARACTERIZATION AND FLUORIDE ADSORPTION BEHAVIOR OF MCM-41”

**Bodhaditya Das<sup>a,\*</sup>, Rashmi Rekha Devi<sup>a</sup>, Anup Kumar Talukdar<sup>b</sup>  
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**Keywords:** MCM-41, mesoporous silica, fluoride

Mesoporous MCM+41 was synthesised at room temperature using tetraethylorthosilicate (TEOS) with cetyltrimethylammonium bromide (CTAB) and employed as an effective adsorbent for the adsorption of fluoride from aqueous solution. The synthesised MCM+41 was calcined at 550<sup>0</sup>C and characterized by X-ray diffraction (XRD) pattern and Fourier Transformed Infrared (FTIR) spectroscopy. The adsorbent MCM+41 was found suitable for fluoride removal (85.5%) from 10mg/L with pH range 6.50-7.29 with adsorbent dose 0.5mg/L. The experimental results indicated that Langmuir isotherm model expressed the absorption isotherm better than Freundlich and Dubinin-Rudeshvich isotherm models and the mechanism of adsorption process was mainly due to physical adsorption.

**68. Estrogenic Pterocarponoids Extracted from Seeds of Plant *Crotalaria Mucronata***

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**Key words:** *Crotalaria Mucronata*, Pterocarponoids, Estrogenic Principles

*Crotalaria Mucronata*, commonly known as ‘san’, is a small sized plant belonging to family ‘Leguminosae’. Estrogenic properties of extracts isolated from seeds of plant *Crotalaria Mucronata* are being reported. The identification of the Estrogenic principles was carried out using color tests and separation techniques. The screening of various extracts prepared from seeds of the plant was carried out on female albino rats by uterine weight procedure. The substance was administered orally as well as intravaginally to the immature rats and the Estrogenic activity was evaluated on the basis of ‘uterine weight response’ and number of ‘vaginal openings’. It was found that out of various fractions attempted, Pterocarponoids present in ethyl acetate and acetone soluble fractions isolated from seeds of this plant showed adequate Estrogenic activity.

**69. Removal of Phenol from aqueous solution using Okra mucilage**

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**Key words-** Phenol, Flocculation, Okra Mucilage, Polysaccharide, Biodegradability.

The application of food grade polysaccharide namely *Hibiscus esculentus* (Okra) has been assessed for the removal of phenol from aqueous solution. Flocculation studies were carried out under varying experimental conditions of contact time, phenol concentration, flocculent dosages and pH. The maximum removal obtained was 67.39%

after 60 minutes and it was obtained at acidic pH(6.0) with optimum mucilage dose of 30ml/lit.

**70. Synthesis of Novel Thiazole Substituted Pyrazole Derivatives and Study of Their Antimicrobial activity.**

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**Keywords:** Thiazole, Pyrazole, Hantzsch reaction, Vilsmeier Haack reaction, Antimicrobial activity.

A series of new 1-[4-(2,3,4-Substituted -phenyl) thiazol-2-yl] -3-(2,3,4-substituted -phenyl)-1H-pyrazole-4-carbaldehyde (**4a-m**), 4-[4-(4-Substituted-phenyl) thiazol-2-yl]-3-(4-substituted-phenyl)-1-phenyl-1H-pyrazole (**7a-i**), 4-[4-(4-substituted phenyl)thiazol-2-yl]-1-phenyl-1H-pyrazol-3-amine (**10 a-g**) have been synthesized by using Vilsmeier Haack formylation and Hantzsch reaction in high yield. All the synthesized compounds were tested for antimicrobial activity, among the synthesized compounds most of the compounds showed potent antimicrobial effect against gram positive and gram negative bacteria as well as fungi species.

**71. SYNTHESIS OF NEW DERIVATIVES OF 4-AMINOTHIENO [2,3-*d*] PYRIMIDINE-6-CARBONITRILE BY CONVENTIONAL AND NONCONVENTIONAL GREEN METHODS**

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Temperature and time dependent regioselective reaction was studied on oxothieno [2, 3-*d*] pyrimidine-6-carboxamide **3** with POCl<sub>3</sub> and PCl<sub>5</sub>. At 25-50 °C, 1° amide rearranges to nitrile furnished compound **4** as major product, while at higher temperature 80-110 °C, with 1° amide, 2° amide also react with the reagent furnished fully aromatized 4-chlorothienopyrimidine-6-carbonitrile **5** in major amount. Time required for formation of product **4** and **5** decreases with temperature. The C4-*ipso* chloro displacement by amines in compound **5** yielded new 4-aminothieno [2, 3-*d*] pyrimidine-6-carbonitrile derivatives **8a-h** and **9a-e** both by conventional and non-conventional green methods.

**72. A STUDY ON ALTERING PHYSICO-CHEMICAL PROPERTIES OF BENGAL GRAM STARCH BY ESTRIFICATION (ACETYLATION) FOR VARIOUS FOOD APPLICATIONS**

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**Key words:** Acetylation; Native Starch; Bengal gram; pasting properties; swelling; solubility  
Retrogradation; Gelatinization;

#### *Section IV: Chemical Sciences*

Bengal gram starch was isolated using wet milling *modus operandi* and the native starch was chemically modified to have a substituted acetylated starch. Both the moieties were characterized and the comparative study was done. Native and the acetylated starch components were pure and composed of more than 98% carbohydrate fraction. Three levels of acetic anhydride *viz.* 6%, 8% and 10% were used for the reactive modification at 50°C keeping the reaction condition alkaline with 0.02M NaOH. The acetylated starch was found to have more amylose content to its native fraction. At 6%, 8% and 10% reactant level the percent acetyl content was 2.14%, 3.35%, 4.47% and DS 0.082, 0.130 and 0.176 respectively. Water absorption, oil absorption, solubility was higher but swelling power and percentage transmittance values on storage for the acetylated starch was lower than its native part. Pasting temperature ( $T_{0C}$ ) and pasting time ( $t_m$ ) was significantly lower for modified starch depicting that it requires lesser time and thermal energy for gelatinization hence while other preparative process as well. The stability of the formed gel was higher in terms of syneresis and the resulting starch gel confirmed lesser degree of retrogradation on DSC analysis. The FTIR spectra of the acetylated starch showed a specific peak at  $720.3\text{ cm}^{-1}$  depicting introduction of carbonyl stretch of acetyl group and this characteristic peak was absent in the native sample. Granule size and morphology of native and modified starch was similar with exceptional evidence of minute fissures.

### **73. Phase Transfer Catalyst Mediated Synthesis of Biologically Significant 9-(3, 5-Dinitrophenyl-4-yl) -8- (2-methylprop-1-en-1-yl) - 6- [(1E) -2-phenylprop -1- en-1-yl] -2-thiol-9H-purine as p38 MAP Kinase Inhibitor**

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**Keywords:** Docking, p38 MAP kinase inhibitor, Phase Transfer Catalysis, Purine

The paper accounts the synthesis of 9-(3,5-dinitrophenyl-4-yl)-8-(2-methylprop-1-en-1-yl)-6-[(1E)-2-phenylprop-1-en-1-yl]-2-thiol-9H-purine as p38 MAP

kinase inhibitor. The p38 MAP kinase is closely associated with cytokine-driven progressing of rheumatoid arthritis and related inflammatory diseases. The inhibition of p38 MAP kinase is an attractive approach for treatment of cytokine mediated diseases. Purine derivatives are found as effective inhibitor for p38 MAP kinase. Therefore, a novel route was designed to achieve the synthesis of 9-(3,5-dinitrophenyl-4-yl)-8-(2-methylprop-1-en-1-yl)-6-[(1E)-2-phenylprop-1-en-1-yl]-2-thiol-9H-purine compound. The compound was synthesized in excellent yield (65-75%) and the structure was characterized on the basis of consistent IR, <sup>1</sup>H NMR, FAB-Mass and elemental analyses data. The purity of the compound was ascertained by TLC. Moreover, newly designed inhibitor i.e. 9-(3,5-dinitrophenyl-4-yl)-8-(2-methylprop-1-en-1-yl)-6-[(1E)-2-phenylprop-1-en-1-yl]-2-thiol-9H-purine was tested for their ability to inhibit p38 MAP kinase which is closely associated with cytokine-driven progressing of rheumatoid arthritis and related inflammatory diseases. For the investigation of binding modes protein-ligand docking has been performed. The initially inhibitor model was prepared with ChemOffice and modified with ArgusLab package. Protein structure was prepared with inbuilt preparation tool of Molegro Virtual Docker (MVD). Docking studies have been performed using MolDock using default settings. The results obtained from docking studies were found in agreement with our experimental findings.

#### 74. Toxicity Studies of Quinolone derivatives on Biological systems

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**Keywords:** Quinolones, Cytotoxicity, Pollen tube germination, Root tip germination

In *vitro* cytotoxic assessment of new N-linked Quinolones are done in various concentrations ranging from 5 μg to 50 μg by using Trypan Blue dye exclusion assay and found to be nontoxic to viable mammalian cells. Further, N-linked Quinolones are tested for cytotoxicity on *Hibiscus* pollen tube and on *Allium cepa* (onion) root tip germination and found to be non-toxic on pollen tube and root tip germination. Moreover, cytotoxicity

testing is done on Guppy (*Poecilia reticulata*) fishes and found that N-linked quinolones is non-toxic. This study proves that, N-linked Quinolones are non-toxic to Biological systems and can be used for various applications especially for Medicinal purposes.

**75. Preparation of conductive hydrogel based on poly (acrylamide-co-acrylic acid) and polyaniline and their actuation behavior.**

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**Keywords:** Hydrogels, conducting polymers, electroactive behavior, crosslinker.

Electrically conducting composite hydrogels of poly (acrylamide-co-acrylic acid) and polyaniline were prepared by two- step synthesis process. The hydrogels were prepared by aqueous polymerization technique at room temperature by varying the amount of crosslinker. Then hydrogel film was immersed in oxidative media and subsequently in aniline solution. Aniline was absorbed on the surface of the film and polymerized. The structural confirmations were determined by FTIR, UV-visible analysis, XRD and SEM. The electrical conductivities were evaluated by Four-probe method. The electroactive behaviour of composite hydrogels was investigated by measuring effective bend angles at different applied voltages.

**76. Microwave-enhanced efficient synthesis of some polyfunctional pyridazines**

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**Key words:** microwave-enhanced synthesis, polyfunctional pyridazines, Ionic Liquids.

Microwave-enhanced highly efficient protocol for the synthesis of polyfunctional pyridazines beginning from 3,6-dichloropyridazine in environmentally, 3,6-diaminopyridazine and 3-chloro-6-methoxypyridazine. These derivatives were then be converted to a variety of polyfunctional pyridazine. The ionic liquids used were 1-n-butyl-3-methylimidazolium hydroxide/tetrafluoroborate/hexafluorophosphate and 1,3-di-n-butylimidazolium hydroxide. This powerful strategy is less time consuming green methodology. The ionic liquid employed may be recovered, recycled.

**77. Synthesis, antibacterial and antifungal activity of some pyridoquinazolines derivatives**

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**Keywords:** - "Arylaldehyde, urea, P Aminobenzoic acid, PPA, Benzoin, antibacterial, Antifungle."

Alkylidenoarylideno bis ureas were synthesized by ureido-alkylation in the

presence of alcohols, which on treatment with p-aminobenzoic acid results in 4-aryl-6-carboxylato, 1, 2, 3, 4-tetra hydro quinazolines. Reaction of (II) with benzoin in presence of polyphosphoric acid yields, 4-aryl 8, 9 diphenyl 2-oxo-1, 4 dihydro 3H, 7-oxo, 1,3 diazo, anthracene – 2, 6 dione, the new compounds (III) has been screened for their antibacterial, antifungal activity.

**78. A new route for Synthesis of o-Aminocarbonitrile pyrazole and synthesis of new Pyrazolo [3, 4-*d*] pyrimidines, Pyrazolo [3, 4-*d*] pyridazin-7-ones**

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**Keywords:** cynopyrazoles, pyrazolopyrimidines, pyrazolopyridazins

Synthesis of ethyl 5-amino-4-cyano-1-phenyl-1*H*-pyrazole-3-carboxylate **5** has been achieved via abnormal Beckmann rearrangement of *o*-chloroaldehyde **1**. Reaction of 5-amino-4-carbonitrile with Conc. H<sub>2</sub>SO<sub>4</sub> furnished expected 5-amino-4-carboxamide pyrazole. Key intermediates 5-amino-4-carbonitrile and 5-amino-4-carboxamides were used for the synthesis of bicyclic pyrazolo pyrimidine derivatives. The replacement of C-5 Cl of *o*-chlorocarbonitrile **3** with secondary amine furnish new synthon **8** which was further used for synthesis of pyrazolo [3, 4-*d*] pyridazin-7-one and 3-(hydrazinylcarbonyl)-pyrazole-4-carboxamide.

**79. Thermodynamics of binding phenazinium dyes with DNA and polynucleotides: A comparative study**

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**Key words:** phenosafranin, safranin O, thermodynamics, enthalpy, entropy

Natural and synthetic compounds that bind to deoxyribonucleic acid comprise an important class of ligands to study DNA interaction phenomena for potential use as therapeutic drugs. Such interaction studies remain incomplete without the proper understanding of the underlying forces and thermodynamic factors. Phenazinium dyes are an important class of molecules with such practical utility. The thermodynamics of the complexation of two phenazinium dyes phenosafranin [PSF] and safranin O [SO] (Fig.1) with natural DNAs, *Clostridium perfringens*, Calf thymus and *Micrococcus lysodeikticus*, and polynucleotides, poly(dG-dC).poly(dG-dC), poly(dG).poly(dC), poly(dA-dT).poly(dA-dT) and poly(dA).poly(dT)] have been elucidated by helix melting, differential scanning calorimetric and isothermal titration calorimetric techniques.

The binding phenomena were favoured by both negative enthalpy and positive entropy changes in each case although there were significant differences in the thermodynamic parameters depending on the nature and sequence of base pairs. The binding affinity values are of the order of  $10^5 \text{ M}^{-1}$  and the affinity was higher for the higher GC containing DNAs for both the dyes revealing GC specificity. Strong enthalpy-entropy compensation was also evident in the energetics of their interaction. The negative heat capacity values in all cases suggest sequence specific binding. The binding process was driven by both electrostatic as well as hydrophobic forces but overall hydrophobic forces had a major contribution. A higher preference of PSF over SO was observed in the results revealing the role of the bulkier substituents in intercalation interactions.

**80. Study of thermal stability and curing behavior of rice husk reinforced urea – formaldehyde resin prepared under isothermal condition.**

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**Keywords:** Green Composite, FTIR, TGA, XRD, Resin, Thermal stability.

Rice husk, a waste produced from cereal crop is reinforced into Urea- formaldehyde resin matrix to enhance its thermal stability. The successful incorporation of rice husk into polymer backbone through the formation of covalent and hydrogen bonding is shown from FTIR, <sup>13</sup>C NMR and XRD analysis. The curing behaviour of this green composite is shown by using various kinetic models and evaluation of the kinetic parameters shows the mechanism of thermal degradation. TG and DTG analysis shows the decomposition pattern and explains the barrier effect caused due to silica present in rice husk. XRD technique provides crystal dimension and lattice pattern. Particle size has been calculated. The reinforcement of RH into resin matrix is proved to be effective (i) by decreasing the molar ratio of formaldehyde to urea which reduces the emission of toxic formaldehyde and (ii) by enhancing polymeric properties including thermal stability and (iii) by producing a cost effective material from a agricultural waste.

**81. SYNTHESIS, SPECTRAL CHARACTERIZATION AND ANTIOXIDANT EVALUATION OF 10H-PHENOTHIAZINES**

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Jaipur-302004, India*

**Keywords:** 10H-Phenothiazine, antioxidant activity and spectroscopic data.

10H-substituted phenothiazines is prepared by Smiles rearrangement. These synthesized compounds have been screened for their antioxidant activity. These heterocyclic compounds act as a base for their ribofuranosides preparation by treating them with sugar. The structure of 10H-Phenothiazines has been established by elemental analysis, IR, <sup>1</sup>H NMR spectral data.

**82. Synthesis and biological evaluation of some novel pyrazolo [3, 4-b] pyridines bearing benzenesulfonamide and trifluoromethyl moieties as antimicrobial agents**

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**Keywords:** Pyrazolo [3, 4-b] pyridines, benzenesulfonamide, trifluoromethyl-?-diketones, antibacterial activity, antifungal activity.

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The synthesis and biological evaluation of a library of thirty differently substituted pyrazolo[3,4-b]pyridines bearing benzenesulfonamide moiety at position-1 and trifluoromethyl group at position-6 are reported. The heterocyclic system present in the target compounds (**5a-j**, **6a-j** and **7a-j**) was constructed in good yields by refluxing various 5-aminopyrazoles (**3a-c**) with differently substituted trifluoromethyl-?-diketones (**4a-j**) in glacial acetic acid. All the target compounds (**5**, **6** & **7**) were evaluated for their *in vitro* antibacterial activity against four pathogenic bacterial strains namely, *Staphylococcus aureus*, *Bacillus subtilis* (Gram-positive), *Escherichia coli*, *Pseudomonas aeruginosa* (Gram-negative) and *in vitro* antifungal activity against two pathogenic fungal yeasts namely, *Saccharomyces cerevisiae* and *Candida albicans*. Compound **5b** exhibited moderate antibacterial activity against Gram-positive bacteria and two compounds namely, **5c** against *Saccharomyces cerevisiae* and **6i** against *Candida albicans* exhibited moderate antifungal activity. However, none of the compounds showed any activity against Gram-negative bacteria.

### **83. Chitosan: An Efficient, Recyclable Green and Biodegradable Catalyst for the Synthesis of triheterocyclic 4H-pyrimido [2, 1-b] benzothiazole derivatives in Aqueous Media**

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An efficient method has been developed for the preparation of 4H-pyrimido [2, 1-b] benzothiazole derivatives by the condensation of aldehydes,  $\alpha$ -ketoester and 2-aminobenzothiazole in aqueous media using chitosan catalyst. The reaction uses benzothiazole as a new component and good yield is obtained at 60 °C in aqueous media. Atom economies, good yield, environmentally benign, recyclability, biodegradability of catalyst and easy to work up are some of the important features of this protocol.

## 84. Starch sulfuric acid (SSA): A Renewable Catalyst to Promote One Pot Synthesis of Acridinediones

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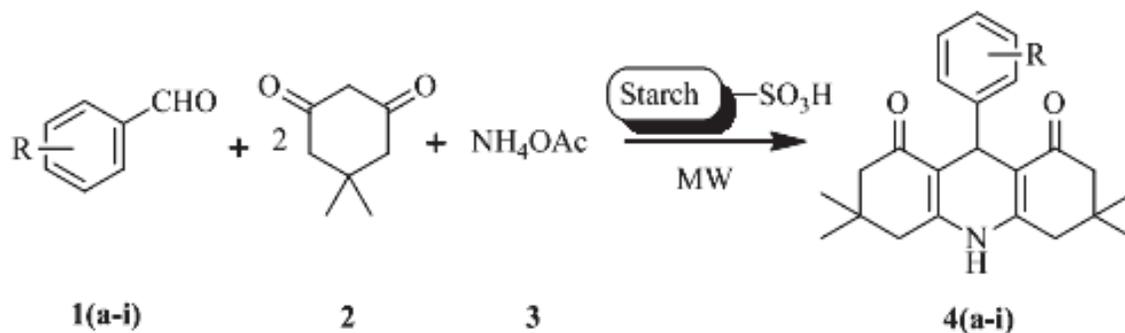
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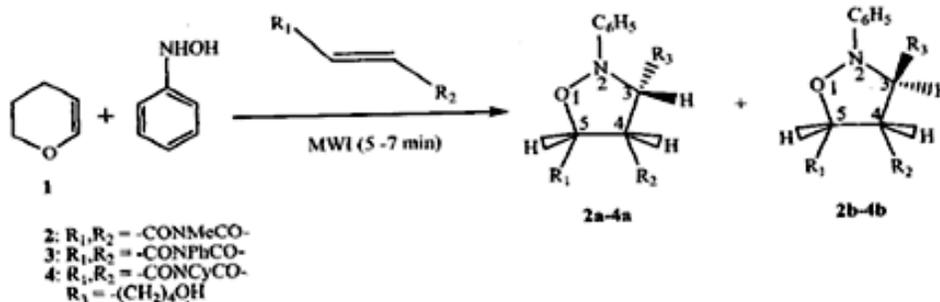
<sup>c</sup>S.R. College, Ghansangavi

**Keywords:** Acridinediones, Starch sulfuric acid, solvent free, microwave irradiation, reusability

A rapid, efficient and convenient protocol towards synthesis of acridinediones under solvent free condition. Synthesis of acridinediones were effectively carried out by one pot three component reaction of aldehyde, dimedone and ammonium acetate using starch sulfuric acid as reusable catalyst.



Scheme 1



## 85. Iron Mediated Reverse ATRP of *n*-Docosyl Acrylate

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**Keywords:** reverse atom transfer radical polymerization; *n*-docosyl acrylate; polymerization kinetics; polydispersity; comb-like polymers

Poly(*n*-docosyl acrylate) (PDA) with narrow molecular weight distribution have been synthesized by reverse atom transfer radical polymerization (ATRP) of *n*-docosyl acrylate (DA) using the FeCl<sub>3</sub>/2,22 -bipyridine initiation system in presence of 2,22 -azobisisobutyronitrile (AIBN) and benzoyl peroxide (BPO). The rate of polymerization ( $R_p$ ) for both the systems exhibit first-order kinetics, however peroxide initiated system shows slow  $R_p$  as compared to the azo-system. The reverse ATRP initiated by peroxides behaves differently than that of the azo initiators. In reverse ATRP with BPO, the  $R_p$  increased significantly with the increase of BPO resulting higher  $M_n$  and broader  $M_w/M_n$ . The reverse ATRP of DA did not exhibit living characteristics with BPO system.

## 86. Well-Defined Poly (Glycidyl Methacrylate) via Fe (III)-Mediated ARGET ATRP

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**Keywords:** Activators regenerated by electron transfer (ARGET); atom transfer radical polymerization (ATRP); glycidyl methacrylate; polymerization kinetics; polydispersity.

Activator regenerated by electron transfer (ARGET) in atom transfer radical polymerization (ATRP) is a new technique for synthesis of well defined polymers with predetermined architecture. In this work, ARGET ATRP of glycidyl methacrylate (GMA) was carried out in N,N-dimethylformamide (DMF) at 60 °C using ethyl 2-bromoisobutyrate (EBIB) as the initiator and ascorbic acid as reducing agent in presence of [Fe(DMSO)<sub>6</sub>](ClO<sub>4</sub>)<sub>3</sub>/1,1,4,7,7-pentamethyl-diethylenetriamine (PMDETA) catalyst system. The kinetic of the polymerization and the effect of different polymerization conditions are studied. The polymerization proceeded successfully while demonstrating characteristics of controlled/"living" radical polymerization.

**87. Sulfamic acid mediated convenient and efficient one-pot synthesis of novel 5-Substituted 1, 3, 4-thiadiazol-2-ylcarbamoyl) aliphatic amide acid derivatives**

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**Keywords:** 1, 3, 4-thiadiazols; sulfamic acid; one-pot synthesis, orthoesters, anhydrides, amide acid derivatives

Convenient and efficient one-pot synthesis of 5-substituted-1, 3, 4-thiadiazol-2-ylcarbamoyl) aliphatic amide acid derivatives were described and developed. Thiosemicarbazide and substituted triethylorthoester was efficiently condensed to furnish substituted ethyl acetate thiosemicarbazone intermediate. The latter gave clean sulfamic acid mediated cyclization and facile *insitu* condensation with variety of cyclic and acyclic anhydrides to afford 5-methyl-1, 3, 4-thiadiazol-2-ylcarbamoyl) aliphatic acid and acetamid derivatives in fair to good yields.

## 88. A Solvent-Free Green Synthesis and Biological Activities of Some New Heterocyclic Compounds

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**Keywords:** Solvent-free green synthesis, benzimidazole, antibacterial and antifungal activity.

Green synthesis of biologically active benzimidazole derivatives has been achieved under solvent-free green conditions, with incomparable atom economy. We have carried out the efficient solvent-free green synthesis of a series of benzimidazole derivatives in good yield. In this methodology, both reactants were thoroughly ground with a pestle in a mortar at room temperature in an open atmosphere until the mixture turned melt. For liquid starting materials, they were mixed thoroughly for a given period of time instead of grinding. The structures of the synthesized compounds were determined by the elemental and spectroscopic data. Finally the newly synthesized were screened for their antibacterial and antifungal activity. The solvent-free synthesis of benzimidazole derivatives provide a better results in term of yield, reaction time and atom economy as compared to conventional organic synthesis. The newly synthesized compounds were also found to be active against gram-positive bacteria (*S. aureus* and *S. mutans*), gram-negative bacteria (*P. aeruginosa*) bacteria and *Aspergillus Niger*. They showed less activity against gram-negative bacteria (*E. coli* and *S. typhi*) and *Candida albicans* in comparison to reference drug.

This synthesis offers very attractive features such as green synthesis, reduced reaction times and higher yields, all of which make it a useful and attractive strategy for the preparation of various benzimidazole derivatives. The simplicity of the procedure is also attractive, which offers wide scope in organic synthesis. These preparations have also proved to be effective against variety of bacterial and fungal strains.

**89. Theoretical calculations of infrared, NMR and electronic spectra of 2-nitroso-1, naphthol or 1-2 naphthoquinine-2 oxime and comparison with experimental data**

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**Keywords:** 2-nitroso-1-naphthol, 1-2 naphthoquinone-2-oxime, IR, NMR, Hartree Fock ,  
Electronic spectra

The geometry of the 2-nitroso-1,naphthol in solid state and 1-2 naphthoquinine-2, oxime in solution have studied by employing Hatree Fock ab initio calculations using 6-31 G\* level. IR wave number of 2-nitroso -1, naphthol is calculated and compared with experimental date. Further, 1-2, naphthaquinine-2, oxime in solution, NMR chemical shifts of 1H and 13C are calculated by HF method and 6.31 G\* level, experimental data was compared. Electronic spectra were also calculated and compared with experimental data. These results are discussed in detail in this work .

**90. A Physico-Chemical Approach and Solvent-Free Synthesis of Some New Benzimidazole Derivatives with Potent Biological Activities**

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**Keywords:** Green synthesis, benzimidazole, lipophilicity, molar refractivity antibacterial and antifungal activity.

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A Physico-Chemical approach towards solvent-free synthesis has gained a wide dimension in the last few decades in term of structure evaluation and biological activities of Benzimidazole derivatives. Green synthesis of pharmacologically active benzimidazole derivatives has been achieved under solvent-free green conditions, with incomparable atom economy. We have synthesized the efficient one-pot solvent-free green synthesis of a series of benzimidazole derivatives in good yield. The structures of the synthesized compounds were determined by the elemental and spectroscopic data. Finally the newly synthesized were screened for their antimicrobial activity. The solvent-free synthesis of benzimidazole derivatives provide a better results in term of yield, reaction time and atom economy in comparison to conventional organic synthesis. The newly synthesized compounds (*N*- [3-chloro -2-(substituted phenyl) -4- oxoazetidin-1-yl]-2-(2-methyl-1*H*- benzimidazol-1-yl) acetamide) were also found to be active against gram-positive, gram-negative bacteria and fungi. It was found that the tested compounds are more effective against the Gram positive bacteria and *Candida albicans*. The lipophilic character and molar refractivity of all synthesized compounds were also calculated and their structure activity relationship was studied. It may be concluded that lipophilic character of the molecules plays an essential role in producing antimicrobial effect. They showed less activity against *E. coli* and *Aspergillus flavus* in comparison to reference drug. This synthesis offers very attractive features such as green synthesis, reduced reaction times and higher yields, all of which make it a useful and attractive strategy for the preparation of various benzimidazole derivatives.

### 91. Synthesis of Novel Pyrazolo Dipyrimidines and Pyrazolo pyrimido pyridine

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**Keywords:** pyrazolo [1, 5-a] pyrimidines,

On the basis of the Zaleplon structure, novel pyrazolo [1, 5-a] pyrimidines were

designed and prepared. This paper reported the synthesis of new 5-methyl-7-substituted-pyrazolo [1, 5-a] pyrimidine-3-carbonitrile derivatives by using simple starting materials such as propane dinitrile and triethyl orthoformate. The Novel 5-amino Pyrazolo Pyrimidine in which amino functionality is utilized to construct further ring cyclization. The structures of the derived target compounds were confirmed by their IR and <sup>1</sup>H-NMR spectroscopic data. The preliminary pharmacological evaluations indicated that some compounds showed anticancer activity.

## **92. Silver Oxide Nanoparticles: Antibacterial Agent Synthesized by Electrochemical Reduction Method**

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**Keywords:** Electrochemical cell, Tetra butyl ammonium bromide, Silver oxide nanoparticles, Human pathogens, Antibacterial activity

Silver oxide nanoparticles were prepared by electrochemical reduction method which is environmental benign. The tetra butyl ammonium bromide (TBAB) used as stabilizing agent in an organic medium *viz.* tetra hydro furan (THF) and acetonitrile (ACN) in 4:1 ratio by optimizing current density. The parameters such as current density, solvent polarity, distance between electrodes, and concentration of stabilizers are used to control the size of nanoparticles. The synthesized silver oxide nanoparticles were characterized by using UV-Visible, FT-IR, XRD, SEM-EDS and TEM analysis techniques. The nanoparticles were tested for antibacterial activity against human pathogens like gram negative *Escherichia coli* (E.coli), *S. typhi* and gram positive *Staphylococcus aureus*, *B. subtilis* strains and which was proved to be excellent.

**93. Oxidative fragmentation of 1,5-cyclooctadiene derivative: A new entry into cembranoid group of diterpenoids.**

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**Keywords-** 1,5-cyclooctadiene, Oxidative fragmentation, diterpenoids, 14- membered macrocycle, domino intermolecular alkylation and cycloalkylation.

A number of diterpenoid natural products containing a 14-membered ring have been isolated from terrestrial and marine sources. Cembrane, the first naturally occurring 14-membered cyclic diterpene, is found in pine oleoresins and is an example of a simple hydrocarbon member.

The range of biological activity that has been recorded for 14-membered ring diterpenoids is remarkably wide: insect trail pheromones, termite allomones, neurotoxins, and cytotoxins, antiinflammatory and antimitotic agents.

14- membered cyclictetra ketone was synthesized from 1,5-cyclooctadiene derivative by Ruthenium oxide catalysed per iodate oxidation. The 1,5- cyclooctadiene derivative was synthesized by domino intermolecular alkylation and cycloalkylation of 2 (1-cyclopentenyl) ethanol, which was obtained from cyclopentanone by Reformatsky reaction followed by LAH reduction.

**94. Investigation of Proteins on Kabuli, Desi and Green Desi Chickpea.**

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**Key words:** Protein contents, Kabuli, Desi and Green seeded grams.

In the present communication nutritional quality and levels of protein in different varieties of gram has been evaluated. For this purpose protein content of grain and dhal samples of 14 desi, 20 kabuli and 11 green seeded gram varieties were examined. The mean values of three categories of gram revealed that relatively kabuli gram (mean 21.61 %) holds significantly superior position over desi gram (mean 19.78 %) followed by green seeded gram (mean 19.78 %). The varieties containing lower values of seed coat percentage showed higher values in grain protein contents. Statistical analysis of grain protein of the three categories of chickpea varieties indicated the variations recorded by kabuli, desi and green seeded gram were significant at 5 % level. The range and mean values of protein percent in dhal samples of the three categories showed that kabuli dhal samples contains highest protein content and lowest in green seeded gram varieties. It is interesting to note that the level of protein percent increased as the contents and intensity of colouration in seed coat is decreased.

**95. New Flavone Glycoside from Glossogyne Pinnatifida DC**

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Glossogyne pinnatifida DC<sup>1,4</sup> belongs to family Compositae. It is commonly known as 'Kamraj' in Hindi. It is found in Punjab, Kumaon, Chota Nagpur, W. Bengal. It is used both internally and externally in treatment of common troubles alone or in combination with other herbs. It is used as a sex tonic. The root is useless in the antidotal and symptomatic treatment of snake bite and scorpion sting.

Earlier workers<sup>5,6</sup> have reported various constituents from this plant. In the present paper, we report the isolation and structural elucidation of a new flavone glycoside 3, 5, 3', 4'-trihydroxy-7-methoxyflavone, 5-O- $\alpha$ -L-rhamnopyranosyl, (1'!3)O- $\beta$ -D-Xylopyranosyl, (1'!4)O- $\beta$ -D-glycopyranoside (A) from ethanolic extract of the stem.

**96. A Study on Altering Physico-Chemical Properties of Bengal Gram Starch by Estrification (Acetylation) for Various Food Applications**

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**Keywords:** Acetylation; Native Starch; Bengal gram; pasting properties; swelling; solubility  
Retrogradation; Gelatinization;

Bengal gram starch was isolated using wet milling *modus operandi* and the native starch was chemically modified to have a substituted acetylated starch. Both the moieties were characterized and the comparative study was done. Native and the acetylated starch

components were pure and composed of more than 98% carbohydrate fraction. Three levels of acetic anhydride *viz.* 6%, 8% and 10% were used for the reactive modification at 50°C keeping the reaction condition alkaline with 0.02M NaOH. The acetylated starch was found to have more amylose content to its native fraction. At 6%, 8% and 10% reactant level the percent acetyl content was 2.14%, 3.35%, 4.47% and DS 0.082, 0.130 and 0.176 respectively. Water absorption, oil absorption, solubility was higher but swelling power and percentage transmittance values on storage for the acetylated starch was lower than its native part. Pasting temperature ( $T_{0C}$ ) and pasting time ( $t_m$ ) was significantly lower for modified starch depicting that it requires lesser time and thermal energy for gelatinization hence while other preparative process as well. The stability of the formed gel was higher in terms of syneresis and the resulting starch gel confirmed lesser degree of retrogradation on DSC analysis. The FTIR spectra of the acetylated starch showed a specific peak at  $720.3\text{ cm}^{-1}$  depicting introduction of carbonyl stretch of acetyl group and this characteristic peak was absent in the native sample. Granule size and morphology of native and modified starch was similar with exceptional evidence of minute fissures.

**97. A Green Development for the Synthesis of Aryl/Alky1/Heteroaryl Bis (6-amino-1, 3-dimethyluracil-5-yl) methanes in Water**

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**Keywords:** Pyrimidine/green chemistry/heterocycle/uracil/water

Designing, choosing appropriate reaction path and reaction condition, to get outmost

and economical product; isolation keeping away purification and establish the structure of new compounds are great challenges for organic and biological scientists. Synthesis of aryl/alkyl/heteroaryl bis(6-amino-1,3-dimethyluracil-5-yl)methanes are carried out at room temperature with simple stirring in water without using any outdriving forces like heat, dehydrating agent, catalyst; coupled with easy work-up and excellent yield. No chromatography is required. If that strategy is used for the synthesis of bioactive molecules, like RNA-nucleobase uracil derivatives, then chemists feel the warmth and relax for not doing any harm to the environment while performing chemistry! The structures of the compounds were established using various spectroscopies and single crystal X-ray analysis.

## **98. SYNTHESIS AND BIO-ACTIVE STUDIES OF SOME SUBSTITUTED ARYL DIHYDRAZONES**

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**Keywords:** - Dithiodipropionic dihydrazide/Dithiodipropionic dihydrazone/ IR/NMR/Bio-active Studies)

Different dihydrazones viz. furfuryl-dithiodipropionic dihydrazone (FDTDPDHn), 2-a cetyl furan-dithiodipropionic dihydrazone (AFDTDPDHn) and 2-acef\tyl thiophene-dithiodipropionic dihydrazone (ATDTDPDHn) have been synthesized by the condensation of dithiodipropionic dihydrazide with different heterocyclic carbonyl compounds. All the synthesized compounds were characterized by their repeated M.P. determination, TLC for single spot elemental analysis, IR & NMR spectral data. On screening for their biological activities in vitro by Serial Dilution Method against two bacteria Staphylococcus aureus

and Escherichia coli and two fungi Aspergillus niger and Aspergillus flavus, all the compounds showed several folds increase in bio-activities as compare to their constituting fragments.

## **99. Synthesis and Antifungal Evaluation of Quinoxaline Derivatives**

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Kumar**

**and Mahesh Srivastava.**

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**Keywords:** - N-(aryl)-2-(3-oxo-1, 2, 3, 4 tetrahydroquinoxaline-2-yl) acetamide, o-phenylenediamine, maleic anhydride amines

A series of N-(aryl)-2-(3-oxo-1, 2, 3, 4 tetrahydroquinoxaline-2-yl) acetamide have been synthesized by condensation of substituted amines with maleic anhydride (MA) followed by cyclization with o-phenylenediamine. All the compounds have been screened for their antifungal activity against Candida albicans, aspergillus fumigatus, trichophyton rubrum,, and aspergillus flavus. In the primary screening, the compounds exhibited appreciable activity. The structures of the synthesized compounds 1b-5b have been established on the basis of elemental analysis and spectral data.

## **100. Syntheses and Antimicrobial Studies of 8-Substituted-2, 5-dihydro-2-(3-nitrophenyl)-1,5benzothiazepines**

**Seema Pant, Deepika Saxena and Raj Kumari Jadon**

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**Keywords:-** Chalcone, Staphylococcus aureus, Escherichia coli

Single step syntheses of 8-substituted-2,5-dihydro-2-(3-nitrophenyl)-4-phenyl-1,5-

benzothiazepines (3a-f) have been carried out by the reaction of six 5-substituted-2-aminobenzenethiols (1a-f), the substituent being fluoro, chloro, bromo, methyl, methoxyl and ethoxyl, with 3-(3-nitrophenyl)-1-phenyl-2-propenone (2) in dry ethanol saturated with dry HCl to obtain six new compounds. The structural assignments of the final products are based on the elemental analysis for C, H, N, and S and spectral analysis comprising IR, <sup>1</sup>H NMR and mass studies. The synthesized compounds have been screened for their antimicrobial activity against the gram-positive bacteria, *Staphylococcus aureus* and gram-negative bacteria, *Escherichia coli*, *Pseudomonas aeruginosa* and fungus, *Candida krusei* with a variety of reference compounds.

### **101. Syntheses and Antimicrobial activity of S-hepta-O-benzoyl lactosyl-1-aryl-5-phenyl-2,4-isodithiobiurets**

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**Keywords:** - Lactosyl arylisothiocarbamides, phenyl isothiocyanate

Per-O-acetyl and per-O-benzoyl derivatives of sugars are important intermediates in carbohydrate transformation and synthesis. In recent years the chemistry of dithiobiurets and related compounds show significant contribution to organic chemistry. Isodithiobiurets were reported for hypnotic and anticonvulsant properties. Condensation of S-hepta-O-benzoyl lactosyl-1-arylisothiocarbamides and phenyl Isothiocyanate resulted in the formation of S-hepta-O-benzoyl lactosyl-1-aryl-5-phenyl-2,4-isodithiobiurets. The required lactosyl arylisothiocarbamides were prepared by the interaction of S-hepta-O-benzoyl lactosyl bromide with aryl thiocarbamides. These newly synthesized compounds were characterized on the basis of chemical transformation, elemental analysis and IR, <sup>1</sup>H NMR and mass spectral studies. The polarimetric study of the titled compounds has been carried out. These compounds were screened for their antibacterial and antifungal activities against various pathogenic bacteria and fungi. The products showed good to moderate activity against above micro organisms.

**102. Thermodynamic, ultrasonic and refractive index studies of hydrazones in Dimethylformamide (DMF) at different temperatures**

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**Keywords:** Hydrazones; Speed of sound; salivation number; opartial molar volume; Molar refraction; Molecular interactions

Density ( $\rho$ ), speed of sound ( $u$ ), and refractive indices, ( $n_D$ ) of 2-hydroxy-5-chloroisonicotinoyl hydrazone and 2-hydroxy-5-methyl isonicotinoylhydrazone have been measured in N,N-dimethylformamide (DMF) at temperatures 298.15<sup>0</sup>K, 303.15<sup>0</sup>K, 308.15<sup>0</sup>K and 313.15<sup>0</sup>K. These measurements have been performed to evaluate some important thermodynamic and acoustic parameters. The apparent molar volume ( $V_{\hat{O}}$ ) and apparent molar Comopressibility ( $K_{\hat{O}}$ ), of hydrazones in DMF were also calculated. Partial molar volume, ( $V_{\hat{O}}^0$ ) and partial molar compressibility ( $K_{\hat{O}}^0$ ), were estimated bty using the values of ( $V_{\hat{O}}$ ), and ( $K_{\hat{O}}$ ), at infinite dilution. Refractive index data was used to calculate molar refractivity of solutions. The results have been discussed in the light of various types of interactions occurring in solution.

**103. SYNTHESIS OF N-3(4-CHLOROPHENYL THIAZOLE-2-Y1)-(2AMINO) METHYL)-QUINAOLINE-4(3H)-ONE AND THEIR DERIVATIVES FOR ANTITUBERCULAR ACTIVITY**

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**Keywords:** Mycobacterial activity, quinaolones, antitubercular, antitumour, antifungal, antithrombic, anticonvulsant.

A new series of N-[4-(4-chlorophenyl thiazole-2-yl)-2-amino methyl] quinaoline-4(3H)-one and their derivatives are synthesized. The structure of the title compounds are confirmed on the basis of IR and <sup>1</sup>H NMR. The compounds are screened for their antitubercular activity, using H<sub>37</sub>Rv strain on L J medium. All the compounds have showed moderate to promising antitubercular activity.

**104. Synthesis and antimicrobial activity of 4H,4-thio-2-hepta-O-benzoyl-â-D-lactosylimino-3-phenyl-2,3-dihydro-(1,3,5)-triazino-(2,1b)6,7 or 8-aryl benzothiozoles (hydrochlorides)**

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**Keywords:** Benzothiazoles, N-phenyl isocyanodichloride, 1,3,5 triazino compounds.

Carbohydrates play an important role in various molecular recognition events. They are found on the surface of cells, bacteria and viruses as glycoconjugates. Benzothiazole are bicyclic ring system with multiple applications. Benzothiazoles possess antitubercular,

anticancer, antitumor and antipyretic activity. N-lactosylated derivatives exhibit a wide range of medicinal activities, such as antiviral, antidibetic, analgesic and some other activities. The above applications of benzothiozoyl thiocarbamide as well as N-lactosylated derivatives and our interest in the carbohydrate chemistry prompt us to combine them s single entity. A series of novel 4H,4-thio-2-hepta-O-benolyl-â-D-lactosylimino-3-phenyl-2,3-dihydro-(1,3,5)-triaino-(2,1b)6,7 or 8 aryl benzoly-â-lactosyl-3-aryl benzothiozoyl-thiocarbamide with N-phenyl isocynodichloride. These compounds were screened for their antibacterial and antifungal activites against E. coli, P. vulgaris, S. aureus, S. Typhi, K. pneumonie, P. aeruginosa, A. niger and C. albicance. The newly synthesized compounds have been characterized by analytical and IR, <sup>1</sup>HNMR and Mass spectral studies.

**105. Green Chemistry Approach: Synthesis and spectral studies of hydrazones and their metal complexes**

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**Keywords:** Synthesis, microwave irradiation, spectral, IR, <sup>1</sup>HNMR, electronic spectra

Six new metal complexes of Co (II), Ni (II) and Cu (II) with bis-(furfuryl) adipic acid dihydrazone (FADH) and bis-(2-acetyl thiophene) adipic acid dihydrazone (2-ATADH) have been synthesized under microwave irradiation. The Microwave irradiation method was found remarkably successful and gave higher yield at less reaction time. All the synthesized compounds have been characterized by running their TLC for single spot, repeated melting point determination, elemental analyses, IR, <sup>1</sup>H-NMR and electronic spectral studies. The elemental analyses and spectral analysis results revealed their Metal : Ligand (1:1) stoichiometry. Electronic spectral studies suggested the octahedral geometry of the complexes.

**106. A NEW ANTHRAQUINONE GLUCOSIDE FROM THE STEM BARK OF CASSIA GRANDISLINN.**

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**Keywords:** Cassia grandis Linn, Stem bark, Aglycone, Anthraquinone, glucoside.

A new anthraquinone glucoside has been obtained from stem bark of C. Grandis. It has been extracted with ethyl acetate extract. The ethyl acetate extract after on concentration and cooling, subjected to column chromatography for purification. On concentration and leaving overnight it gave a light yellow coloured solid mp 190<sup>0</sup>C(d). as 1,3,5,8 tetra hydroxyl 6,7-dimethoxy-2-methyl anthraquinone and the glucoside was identified as 1,5,8 tri hydroxyl-6-7-dimethoxy-2-methyl anthraquinone-3-0-â-D(+) glycopyranoside.

**107. STUDIES ON COORDINATION COMPOUNDS SO SOME PYRAOLINE-5-ONE DERIVATIVE**

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**Keywords:** Pyrazoline, Isoniazid, Coordination compounds, hydrozone

Some tridentate ligands were synthesized by the reaction of ethyl 2-phenylhydrozoneo-3-oxobtyrate and its derivative with isoniazid by the method reported in literature.

The bivalent hexacoordinated complexes of Cu (II) and on the basis of their electronic, IR absorption properties and magnetic properties. The compositions of the

complexes were found as  $[ML_2]$ . The analysis shows that after deprotonation the ligand 1-isonicotinoyl-3-methyl-4-(phenylhydrazono)-2-pyrazoline-5-one (HL) behave as tridentate ligand (N, N, O donor).

The structural studies of metal complexes revealed that each metal ion is hexacoordinated. The electronic spectral band and IR spectral bands were interpreted.

### **108. Diastase immobilization by Gum Acacia-silica nanohybrids**

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**Keywords:** Amylase, immobilization, gum acacia-silica nano hybrid, enzyme kinetics

Gum acacia silica nanohybrids have been synthesized and extensively characterized by FTIR, XRD, SEM, TGA, PL and BET analyses. Experimental parameters such as precursor to H<sub>2</sub>O ratio, gum acacia concentration and thermal densification conditions dictate the final texture and properties of the synthesized nanohybrids. These hybrids are porous with high surface area and thermal stability. Structural characteristics of the materials indicate that the nanohybrids may be potentially exploited for enzyme immobilization, as catalysts, and in biomedical/optical applications. The material has been evaluated as immobilization support for diastase alpha amylase for the hydrolysis of soluble starch was monitored in comparison to free enzyme using 100 mg impregnation support at rpm 200, incubation time 10 minutes, pH 5, Temperature 313 K, where the enzyme the immobilized enzyme was found to have much higher activity as compared to free alpha diastase enzyme.

**109. Carboxymethyl tamarind gum-silica nanohybrids: Synthesis Characterization and Application**

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**Keywords:** Amylase, CMT-Si nanohybrids, immobilization/impregnation.

With an aim to synthesize efficient support for enzymatic reactions, carboxymethyl tamarind gum-silica nanohybrids have been synthesized by sol-gel polymerization of tetramethoxysilane. The optimization of the synthesis was carried out by focusing the enzyme activity immobilized on these supports taking alpha amylase as representative enzyme. The nanohybrids have been characterized by FTIR, XRD, SEM, TGA and BET analyses. The optimum nanohybrid sample © in terms of  $\alpha$  amylase immobilization was synthesized when water (H<sub>2</sub>O), tetramethoxysilane (TMOS) and methanol (MeOH) were used in 17:1:1 ratio at fixed template amount (0.5 g of carboxymethyl tamarind gum). Enzyme immobilization efficiency of this material was further enhanced upon calcinations (in nitrogen atmosphere), the optimum calcinations temperature being 400<sup>0</sup>C. Nanohybrid (C4) 49  $\mu$ g of  $\alpha$ -amylase was impregnated on the calcined hybrid and the immobilized enzyme was used for hydrolyzing soluble potato starch to glucose syrup taking hydrolysis by free enzyme as control.

**110. Synthesis of 2-(2-4, 5/5, 6/6, 7-Dichloro-1-(aminomethyl)-2-oxoindolin-3-ylidene) hydrazinyl -3-phenylquinazolin-4(3h)ones as Antifungal Agents**

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**Keywords:** Dichloroindolin-2, 3-dione, Schiff bases, Mannich bases, antifungal activity.

2-Mercapto-3-phenylquinazolin-4 (3H)-one 1 on hydrazinolysis with hydrazine hydrate gave 2-hydrazinyl-3-phenylquinazolin-4(3H)-one 2 which on condensation with 4,5/5, 6/6,7-dichloroindolin-2,3-diones gave 2-(2-(4,5/5,6/6,7-dichloro-2-oxoindolin-3-ylidene) hydrazinyl-3-phenylquinazolin-4(3H)-ones 3,5 (Schiff bases). Compounds 3-5 on being subjected to aminomethylation with different secondary amines in the presence of formaldehyde gave 2-(2-(4,5/5,6/6,7 dichloro-1-(aminomethyl)-2-oxoindolin-3-ylidene) hydrazinyl-3-phenylquinazolin-4 (3H)-ones 6-26 (mannich bases). The structures of the compounds have been established with the help of elemental analysis and spectral data. The compounds have been screened for their antifungal potential against human pathogenic fungi.

**111. A Simple and Efficient Synthesis of 3-Chloro-6,7-dimethoxy-9H-indeno[2,1-e]pyridine-4-carbonitrile and its ipso Substituted Derivatives**

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**Keywords:** Alkylidene malononitrile, Pinner reaction, 2-Chloronicotinonitrile, ipso substitution

#### *Section IV: Chemical Sciences*

The Knoevenagel condensation of 6, 7-dimethoxy indanone with malononitrile at ambient temperature afforded ylidinemalononitrile 2 which on further condensed with DMF-DMA furnished imine 3 with good yield. Dry HCl gas was purged in to the solution of imine 3 with IPA and/or methanol at room temperature produced chloronicotinonitrile 4 as major product and methoxynicotinonitrile 5a as minor product. Successful ipso substitution of various primary and/or secondary amines to chloronicotinonitrile 4 afforded new class of 2-substituted icotinonitrile derivatives with good yields.

### **112. Preparation and characterization of Jatropha Curcas oil based alkyd resin suitable for surface coating**

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**Keywords:** Jatropha curcas oil; Alkyd resin; Renewable resources; Surface coating

Jatropha Curcas oil was extracted from the seeds by solvent extraction method. Three different alkyd resins were prepared by varying the amount of phthalic and maleic anhydride based on Jatropha Curcas oil. The characterization of the resins for structure establishment is carried out using FTIR and <sup>1</sup>H NMR and the concomitant properties such as acid value, saponification value, viscosity etc. are also evaluated by standard methods. The prepared resins were cured by using MEKP (initiator) and Co-octoate (accelerator) at 120°C and the cured resins were characterized by chemical resistance, pencil hardness, adhesion, thermal stability and gloss. The resins may find potential applications in surface coating purposes.

**113. EFFECT OF DIHYDRIC ALCOHOL ON THE ALKALI CATALYSED SOLVOLYSIS OF PHTHALATE ESTER**

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**Keywords:** Dihydric alcohol, activation energy, entropy controlled, enthalpy dominating, salvation, transition state, entropy of activation, enthalpy of activation.

The solvent effect of dihydric alcohol (EG) on the alkali catalysed solvolysis of dimethyl phthalate was studied by carrying out the hydrolysis of the ester in water-EG media of varying composition consisting of 20 to 80% ethylene glycol (EG) (v/v) at different temperatures ranging from 20 to 40<sup>o</sup> C.

The specific rate constant values of the reaction were found to decrease with increasing concentration of ethylene glycol in the reaction media. The depletion observed in the values of iso-composition activation energy of the reaction shows that the transition is solvated and initial state is desolvated with addition of ethylene glycol in reaction media. From depletion in the values of “H\* and “S\* with simultaneous enhancement in “G\* values of the reaction, it has been concluded that the reaction is enthalpy dominating and antropy controlled and specific salvation is taking place in the water-EG media. From the values of iso-kinetic temperature, it may be concluded that water-EG reaction media obeys Barclay-Butler rule.

**114. Synthesis of hepta-*O*-benzoyl- $\alpha$ -D-lactosyl-3-(2)-substituted hydrazine-1,3-benzothiazolyl thiocarbamides**

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**Keywords:** Lactosyl isothiocyanate, hydrazino benzothiazoles, lactosyl hydrazine benzothiazolyl thiocarbamides

Benz-fused compound have been employed in the synthesis of various compounds which show very potential pharmacological activities. Carbohydrate is the key element in variety of biological phenomena and its *N*-linked sugar derivatives also exhibit wide range of medicinal activities. Keeping in this view, when one biological active molecule is linked to another, the resultant molecule generally has increased potency.

Hence for the first time, in present work, we have interacted two pharmacophores, hepta-*O*-benzoyl- $\alpha$ -D-lactosyl isothiocyanate and substituted 2-hydrazino-1,3-benzothiazoles in acetone medium to yield hepta-*O*-benzoyl- $\alpha$ -D-lactosyl-3-(2)-substituted hydrazine-1,3-benzothiazolyl thiocarbamides. The identities of these newly synthesized hepta-*O*-benzoyl- $\alpha$ -D-lactosyl-3-(2)-substituted hydrazine-1,3-benzothiazolyl thiocarbamides have been established on the basis of usual chemical transformations and IR,  $H^1$  NMR and Mass spectral studies.

**115. Studies on Synthesis, Characterisation and Electrochemical Behaviour of 2-(4-Hydroxyphenyl)-6[(E)-(4-methylphenyl) diazenyl]-4h-chromen-4-one**

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**Keywords:** Azo flavones, Voltammetry, Electrochemical Studies, Charge transfer coefficient, Forward rate constant.

The enormous growth in electrochemical studies in recent times was actually made possible by the development in electro analytical methods. Among the large number of analytical techniques available for the trace analysis, voltammetry has proven to be one of the most sensitive and reproducible techniques which is attributable to its features of being eco-friendly, in-expensive, facile and of course to its rapidity. In particular, organic electrochemistry has gained considerable interest and have become very powerful and versatile field of analysis for variety of organic compounds. It would be quite worthy of interest to perform comprehensive study on electrochemical behavior of synthesized azo compound bearing flavones nucleus at one of its ends. Therefore 2-(4-hydroxyphenyl)-6-[(E)-(4-methylphenyl) diazenyl]-4H-chromen-4one has been synthesized. The structure was established on the basis of IR, <sup>1</sup>H NMR, and elemental analysis data. Detailed evaluation of electroanalytical findings were targeted on 2-(4-hydroxyphenyl)-6-[(E)-(4-methylphenyl) diazenyl]-4H-chromen-4one. The mechanism of the electrode processes has also been deduced. The electro-reduction process is found to be two-electron, irreversible, and diffusion controlled. Various kinetic parameters such as charge transfer coefficient and forward rate constant have been calculated.

**116. Synthesis of New Class Of 3-Oxo-2-acetyl- $\beta$ -D-maltosyl-4-aryl-5-hepta-O-acetyl- $\beta$ -D-lactosylimino-1,2,4-thiadiazolidine (Hydrochlorides)**

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**Keywords:** Maltosyl aryl carbomides, N-hepta-O-acetyl- $\beta$ -D-lactosyl-S-chloro isothiocarbomoyl chloride, lactosyl-1, 2, 4-thiadiazolidine (hydrochlorides)

Heterocycles and medicines are both interrelated because human are totally dependent on the drugs derived from heterocyclic rings. Heterocycles and their derivatives have attracted the attention of chemists mainly because of broad spectrum biological and pharmacological activities associated with this class of the compounds specially having N, S or both heteroatoms which exhibited marked chemotherapeutic activities. A series of novel 3-oxo-2-hepta-O-acetyl- $\beta$ -D-maltosyl-4-aryl-5-hepta-O-acetyl- $\beta$ -D-lactosylimino-1,2,4-thiadiazolidine (hydrochlorides) were synthesized by the interaction of N-hepta-O-acetyl- $\beta$ -D-maltosyl-3-aryl carbomides. IR,  $^1\text{H}$  NMR, Mass spectral studies and elemental analysis characterized the newly formed products.

**117. Design, Synthesis and Antimicrobial Activities of Maltosyl-1, 2, 4-Dithiazolidines (Hydrochloride)**

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**Keywords:** Maltosyl thiocarbamides, N-phenyl-S-chloro isothiocarbomoyl chloride, N-hepta-O-benzoyl- $\beta$ -D-maltosyl-S-chloro isothiocarbomoyl chloride, 1-aryl-3-phenyl thiocarbamides, maltosyl-1, 2, 4-dithiazolidines (hydrochloride).

Development of glycobiology dealing with the role of carbohydrates in a plethora of biological processes has enforced the search for new and more practical methods for the synthesis of carbohydrate derivatives. The present study was related to synthesis and antimicrobial activity of novel maltosyl- 1, 2, 4-dithiazolidines (hydrochloride). A series of novel 3-hepta-*O*-benzoyl- $\alpha$ -D-maltosylimino-4-aryl-5-phenylimino-1,2,4-dithiazolidines (hydrochloride) were synthesized by the interaction of 1-hepta-*O*-benzoyl- $\alpha$ -D-maltosyl-3-aryl thiocarbamides with *N*-phenyl-*S*-chloroisoithiocarbamoyl chloride and 4-phenyl-5-hepta-*O*-benzoyl- $\alpha$ -D-maltosylimino-3-arylimino-1,2,4-dithiazolidines (hydrochloride) were prepared by the interaction of *N*-hepta-*O*-benzoyl- $\alpha$ -D-maltosyl-*S*-chloro isoithiocarbamoyl chloride with various 1-aryl-3-phenyl thiocarbamides. The newly synthesized compounds have been characterized by analytical and IR, <sup>1</sup>H NMR and Mass spectral studies. The compounds synthesized were investigated for their antimicrobial activities against *Proteus vulgaris*, *Escherichia coli*, *Salmonella typhimurium*, *Staphylococcus aureus*, *Pseudomonas aeruginosa* and *Aspergillus niger*. Some of these tested compounds exhibit moderate and strongest inhibitory against the tested strains of bacteria and fungus.

### **118. Intermolecular Inter-ligand Interaction in Mixed Ligand Complexes of Lanthanoids (III) Involving CDTA and Some O-N donor Amino Acids**

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**Keywords:-** Intermolecular, Inter-ligand, Interaction, Mixed ligand complexes, Lanthanoids, CDTA, Amino acids,  $\alpha$ -alanine, Valine, Leucine.

The formation constant studies on binary (logK) and mixed ligand complexes (logK) and stability quantifying parameters (“log k and —” log k) to examine the extra-stabilization

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due to inter-ligand interaction in Pr (III) and Nd (III) complexes involving cyclohexanediaminetetraacetic acid (CDTA) as primary ligand and  $\alpha$ -alanine ( $\alpha$ -ala), valine (val) or leucine (leu) as secondary ligands have been undertaken to evaluate the possible occurrence of intramolecular inter-ligand interaction. Stability quantifying parameters (“ $\log k$  and  $-\log k$ ”) indicate significant inter-ligand interaction.

**119. Roll of Stagnant Solution in Corrosion of Tin (Sn) Plates and Studies on Thin Canacious Plates**

**E.N. Nirapure, G. P. Sahu and S. C. Lavale\***

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Sahu et.al. reported the Metal Cancer “Corrosion brought anormous losses” excided Rs. 5000 Crore each year. This loss can be control with saving of nation’s productivity using researches on corrosion and taking preventive measurements. The tin (Sn) plates have been exercise in distinct salt solutions viz.  $\text{BaSO}_4$ ,  $\text{FeCl}_3$ ,  $\text{ZnCl}_2$ ,  $\text{FeSO}_4$ ,  $\text{NH}_4 \text{Cl}$  &  $\text{CuSO}_4$  in aqueous and non aqueous media could be successfully performed. The quick assessment of surface behaviour, potential pH diagraph, weight loss technique, linear polarization etc. reported. The thin films on the surface are responsible for passivation. The salt solution of  $0.01 \text{ mol dm}^{-3}$  to  $0.03 \text{ mol dm}^{-3}$  has been utilized. It is observed that decrease in pH at about 0.2 – 0.6 and weight loss is 32 – 120 mg. abnormal surface properties of the plates have been found. These depend on nature and concentration of ions used. The thin canacious films observed are photographed & investigation were made in detailed.

**120. Amberlyst® 15 DRY Resin: A Green and Recyclable Catalyst for Facile and Efficient One-pot synthesis of 3,4- Dihydropyrimidin-2 (IH)-Ones**

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**Keywords:-** Biginelli Reaction, 5-Unsubstituted 3,dihydropyrimidin-2 (IH)-ones, Amberlyst® 15 DRY, Heterogeneous Catalyst, Green Chemistry.

An environmentally benign green protocol for the synthesis of 5- Unsubstituted 3,4-dihydropyrimidin -2(IH)-Ones using Amberlyst® 15 DRY as a recyclable catalyst has been developed. The use of resinous, nontoxic, thermally stable and inexpensive Amberlyst® 15 DRY, as a recyclable heterogeneous catalyst, makes the process simple with negligible chemical waste. Among the various solid acid catalysts Amberlyst® 15 DRY was found to be the most efficient catalyst with regard to reaction time, yield and ease of work up procedure.

**121. Synthesis and Characterization of S-hepta-O-benzoyl maltosyl-1-arylthiocarbamides**

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**Keywords:-** Maltosyl bromide, aryl thocarbamides, arylisothiocarbamides.

S-Glycosides are those compounds in which Glycosyl group or its derivatives are

attached to the sulphur of sulphur containing compounds. Carbohydrate derivatives bearing N- and S-linked functionalities at anomeric position are known for their various biological activities and in medicinal chemistry. This class of compounds has several applications such as antifungal, antitumor, anticancer, antiviral and antimalarial activity. In view of applications in industry and also in medicinal chemistry it appeared interesting to carry out synthesis for some novel thiomaltosides.

Several S-hepta-O-benzoyl maltosyl-1-arylisothiocarbamides have been synthesized by the interaction of hepta-O-hepta-O-benzoyl maltosyl bromide and various aryl thiocarbamides. The identities of these newly synthesized compounds have been established on the basis of usual chemical transformation and IR, <sup>1</sup>H NMR and Mass spectral studies.

## **122. Exploration of antimicrobial and antioxidant potential of newly synthesized 2, 3-disubstituted quinazoline-4 (3H)-ones**

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A series of 2-(chloromethyl)—(4methyl-6-oxo-5-[(e)-phenyldiazenyl]-2-thioxo-5,6-dihydropyrimidine-1 (2H)-yl quinazoline-4(3H)-ones was synthesized by treating 2-(chloroethyl) amino benzoic acid with 3-amino-6-methyl-5-[(e)-phenyldiazenyl]-2-thioxo-5,6-dihydropyrimidine-4(3H)-one and was screened for in vitro antibacterial activities against a representative panel of Gram-positive and Gram-negative bacteria. The compounds were synthesized in excellent yields and all the synthesized compounds elicited the potent inhibitory action against all the tested bacterial strains. Furthermore, in order to explore the antioxidant potential of newly synthesized compounds, the free radical scavenging activity measurement were performed by the 1, 1-diphenyl-2-picryl-hydrazyl (DPPH) assay method. It is revealed from the antioxidant screening results that few compounds manifested profound antioxidant potential.

**123. Quercetin tetra-O-glycoside from the flowers of *Aconitum laeve* Linn**

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**Keywords:** - Quercetin-3-O- $\alpha$ -L-rhamnosyl, p-coumaroyl,  $\beta$ -galactopyranoside, antioxidant activity, *Aconitum laeve*.

*Aconitum laeve* Linn, an alpine herb of genus *Aconitum* (Family, Ranunculaceae) is native to alpine pastures of Central Himalayan's glaciers. Morphologically, the herb is characterized by the presence of pale-yellow flowers arranged in spike-like cluster, leaves with five to eight broad lobes and height is up to 1.5 meter. The genus *Aconitum* has been characterized by the presence of diterpenoid alkaloids, aconite and its derivatives. Aconite is life saving drug and has enormous biological activities. *Aconitum laeve* is a traditional medicinal plant and the extracts derived from its different parts have been used in curing number of diseases associated to inflammatory, cancers, heart ailments, neuro-degenerative and microbial, by some ethnic groups of tribal inhabitants of Central Himalayas. Alkaloid rich fractions derived from *Aconitum laeve* have been screened for various active alkaloid compounds. The cinnamyl flavonol glycosides from the genus *Aconitum* have been identified as potential antioxidative compounds.

Aqueous- methanolic extract from the flowers of botanically identified *Aconitum laeve* (Specimen N.48) was fractionated with benzene, diethyl ether and n-butanol and each partition was evaluated for antioxidant activity by DPPH-UV method. The n-BuOH fraction, a prominent antioxidative, was analysed for active principles. Antioxidant activity-guided fractionation of n-BuOH fraction led to isolation and characterization of active cinnamyl flavonol glycosides, quercetin-3-O- $\alpha$ -L-rhamnosyl (1'!2) -  $\alpha$ -L-rhamnosyl (1'!6)-3'-O-p-coumaroyl- $\beta$ -galactopyranoside. The structural elucidation was carried out by chromatographic, spectral (<sup>1</sup>HNMR, <sup>13</sup>CNMR, LC-MS) and hydrolytic (acid, enzyme, H<sub>2</sub>O<sub>2</sub>) studies.

**124. “CHEMICAL STUDIES FOR THE DISSOLUTION OF URINARY STONES”**

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**Keywords:** Amino Acids, Urinary stone, dissolution.

Human quest, over the yester decades, has led to spectacular advancement in medical science. Almost all specializations have witnessed remarkable achievements. Researches in areas like biogenetic engineering, genie therapy, cloning etc. have rather posed a challenge for the frontiers of human limitations. Biochemical studies have illuminated a number of disease mechanisms. Many molecntar diseases are curable now. However, despite all these progresses, some of the diseases of time immemorial, which are the functions of food, nutritional or metabolic disorders, have continued haunting the people. Urolithiasis i.e., formation of stones in the urinary tract is one such disease.

Keeping all these factors in mind, we have endeavored the possibilities of application of naturally occurring acids (amino acid) and their products in the dissolution of some samples of urinary stones, containing calcium phosphate, oxalate and carbonates. Different samples of stones were suspended in Glycine and  $\alpha$ -Alanine solutions. A substantial dissolution of stones was observed by loss in weight. Such studies would be helpful in designing drugs for dissolving, at least partially, the ‘Urinary Stones’.

**125. Tailoring wine yeast for the new millennium: Novel approaches to ancient art of winemaking**

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Gomtinagar, Lucknow*

Yeast are predominant in the ancient and complex process of wine making. *Saccharomyces cerevisiae* is known as wine yeast and is preferred for wine fermentations. Due to demining of modern wine making practices there is an ever growing yeast for wine yeast rains possessing a wide range of untapped indig-enous yeast with oenological potential, the complexity of wine yeast genetic features and genetic techniques often used in strain development.

**126. “Orgin and History of Chemia / Chemistry”**

**Dr. SUKHENDU KUMAR BAUR**

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The idea of Grostic philosophers to turn metal into gold, turned some inquisitive peoples into some experiments and researcher of metals, salts and other compounds which lead to preliminary state of chemistry i.e. chemia. English “chemistry” “Chimie” in French drived from the geek work chemia or xnuix. Emperor Dioclitan has ordered to perish all old manuscripts in which the word chemia was used at 296 A.D In ancient Chinese history, shih chi (historical memories), there is note of Chinese chemia by su-ma-Tan and his son su-ma-chun (145-87 BC). In the book chemia known Li-shao-chun, describad as having super natural powers said to emperor lute (156-87BC) – that he can turn cinnabar to gold. The tern Rasayan (chemistory) is derived from Atharva – Veda’s word Aayasyani – which denotes long life and methods to got good health. The paper deals with ancient chemia/ chemistry & use of chemistry in medicine in curlier eras.

**127. Mixed Ligand Complexes of Alkaline Earth Metal Salts of Some Organic Acids with Glycine**

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In the present study the mixed ligand complexes of alkaline earth metal salts of o-nitro phenol, Anthracitic acid, 8-hydroxy quinoline and 1-nitroso -2-naphthol with glycine have been discussed. Analytical data show that one molecule of Magnesium, Calcium and Strontium salts of organic acids combined with one molecule of Glycine, suggesting a coordination number six for the metal atoms, and general formula of the mixed ligand complexes have been established as  $ML_2 Gly$ . where  $M=Mg, Ca$  or or  $Sr$  and  $L=$  deprotonated o-nitro phenol, Anthracitic acid, 8-hydroxy quinoline and 1-nitroso -2-naphthol. The transition or decomposition temperatures of these complexes are higher than that of the ligand showing their greater stability. IR spectra of these complexes show a number of unexpected features. Firstly the O-H stretching frequency of the second ligand is either absent or shifted down by  $100-150\text{cm}^{-1}$  with reduced intensity. Secondly the  $-NH_2$  stretching region ( $3450-3200\text{cm}^{-1}$ ) show the very broad poorly resolved absorption typical of strongly hydrogen bonded  $-NH_2$  groups. In most of the cases this absorption is absent. Thirdly a new broad band of medium intensity with sub maxima between  $2710$  and  $2550\text{cm}^{-1}$  is seen in all the complexes. Which is absent in the metal salt or the second ligand.

**128. SYNTHESIS, CHARACTERIZATION OF NEW POTENTIAL INSECTICIDAL & ACARICIDAL AGENTS AND THE USE OF ITS IMPACT ON HUMAN HEALTH**

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Azamgarh (U.P.) India*

Ten 4-aryl-3-thio-semicarbazides & ten-5-aryl-amino-1, 2, 3, 4-thiazotriazoles<sup>1-3</sup> already reported in the literature, synthesized by the method Wahab & Rao, Characterized and tested for insecticidal & activities. 5-p-phenethylamino-1, 2, 3, 4-tetrazole has shown plants growth hormone, possess a serious environmental & public health problem due to exposure among farmers.

**129. Polymer-Support Lewis acid catalyst-III Reductive coupling of aromatic aldehydes and imines**

**Amajoyti Kalita<sup>a</sup>, Biju Basumatary<sup>b</sup> and Swapan K. Dolui<sup>\*</sup>**

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**Key words:** Polymer support; titanium tetrachloride; organic reaction.

Polymeric catalyst and polymer supported metal complex catalyst have been studied by many researchers, and this has been one of the important and rapidly developing fields of catalysis. As a part of our programme of investigating a polymer support, polypyrrole was combined with TiCl<sub>4</sub> in hexane to form a stable complex containing 2.1 wt% Ti as measured by colorimetric method. The resulting catalysts were characterised by FTIR, SEM-EDX, XRD and TGA. The complex showed good catalytic activity in organic reaction like synthesis of Di-ol and pyrrole. The catalyst showed good storability up to 90 days and can be reused six times without losing its activity.

**130. Preparation and physicochemical characterization of Ursodeoxycholic acid nanoparticles for colonic delivery**

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**Key words:** ursodeoxycholic acid, poorly soluble drug, eudragit RS100/RL 100, colon.

The objective of the present study was to formulate Ursodeoxycholic acid-eudragit® RS100 / RL100 nanoparticles and investigate the physicochemical characteristics of the prepared nanoparticles. The nanoparticles of Ursodeoxycholic acid with eudragit® RS100 / RL100 were formulated using solvent evaporation –nanoprecipitation technique.

The physicochemical characteristics of nanoparticles were studied applying particle size analysis, power X-ray crystallography, Fourier transform infrared spectroscopy and Atomic force microscopy. The release rate of Ursodeoxycholic acid from the nanoparticles prepared with various drug/polymer ratios was investigated. The drug/polymer ratio is found to affect the release of drug loaded nanoparticles. All the nanoparticles prepared using eudragit® RS100/ RL100 displayed lower crystallinity having relatively spherical and smooth morphology with particle size about 100nm and polydispersity index between 0.229 to 0.453. The drug loading was also recorded at a higher value of 76.53% to 94.97% and the in-vitro drug release in 48 hours study is 82.93% for formulation with drug polymer ratio 1:4. The intermolecular interaction between drug and the mixture of both polymers was detected in the FT-IR spectrum of the nanoparticles. According to these findings, formulation of the Ursodeoxycholic acid- eudragit® RS100/RL100 nanoparticles have been able to improve the physicochemical characteristics of the drug and hence is expected to successfully deliver the drug to colon.

**131. Dihydropyrano(c) chromenes and pyrano [2, 3-*d*] pyrimidines: DABCO catalyzed synthesis and their biological activity**

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**Key words:** - Multi-component, One-pot, DABCO, Dihydropyrano(c) chromenes, pyrano [2, 3-*d*] pyrimidines, Antibacterial activity.

A simple and efficient one pot synthesis of heteroaryl substituted dihydropyrano(c) chromenes and pyrano[2,3-*d*] pyrimidines has been developed via initial Knoevenagel, subsequent Micheal and final heterocyclization reactions of heteroaryl aldehyde, malononitrile and barbituric acid/ dimedone using 1,4-diazabicyclo [2.2.2] octane(DABCO) as catalyst. Short reaction time, environment friendly procedure and excellent yields are the main advantages of this procedure. All synthesized compounds have shown good antimicrobial activity against different microbial stains.

**132. Chemical Analysis of Betwa River Water : Special Reference to BOD & COD Surrounding Vidisha City (Mp) – India**

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**Keywords:** Betwa, BOD & COD, River pollution, Chemical analysis, Domestic nallah.

Chemical analysis is the most important fact to assess the quality of water of a river. For the same 12 sampling stations were formed on the river Betwa from the point where it enters the city to its final destination outside the city. Monthly sampling was

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conducted throughout the year at different stations on Bio-chemical Oxygen Demand (BOD) and Chemical Oxygen Demand (COD). For BOD method from workbook on Limnology and for COD potassium dichromate reflux ion method was adopted to reach to some conclusion. The Bio-Chemical Oxygen Demand (BOD) of river Betwa was found in between 1.1 to 14.2 mg/l throughout the year of the study period in different seasons of the year. Similarly COD was found in between 15.2 to 80.0 mg/l. Highest value was observed at station where the sewage nallah confluence with the river and lowest was near the water supply pump house. The entire study can be easily understood by observing the BOD and COD charts. The present study river Betwa shows that the main source of pollution which affects the chemical parameters of the system during most of the time is due to inflow of two domestic nallah from Vidisha city. The continuous threat of deterioration of water quality of this river in and around Vidisha city is only due to the inflow of domestic nallahs which may cause chronic diseases in man and animals. After the study it is important of mention that the pollution in te river on these parameters requires urgent attention for the well being of the environment and society.

### **133. Simple and efficient synthesis of imidazo [1, 2-a] pyridines using MgO in aqueous medium**

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**Keywords: imidazo [1, 2-a] pyridines, MgO, aqueous medium**

Various imidazo [1, 2-a] pyridines were synthesized from amino pyridines and aromatic phenacyl bromides by one step process in the presence of MgO in aqueous medium at room temperature. The salient feature of this method includes mild condition, short reaction time, high yield, easy purification and simple procedure.

**134. Biochemistry of Photosynthesis: A New Balanced Chemical Reaction.**

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**Key words:** Biochemistry, Photosynthesis, Enzyme, Light, Isotope, Photochemistry.

Photosynthesis is a biochemical process where green plants prepare their food from Carbondioxide from the atmosphere and water being absorbed from the soil in presence of sun light and Chlorophyll. From this definition it is clear that four reactants (Carbondioxide, Water, Light and Chlorophyll) are essential for the process to proceed and the product is a sugar or carbohydrate ultimately stored as starch. The entire process has Light Reaction (Photochemical) and “Dark Reaction” (Biochemical) Biochemical reactions are very much complicated being catalysed by various enzymes and the path of carbon is non as “Calvin Cycle” according to name of its discoverer. The overall reaction which is now universally accepted can be explained as follows. Six molecules of carbondioxide react with twelve molecules of water in presence of chlorophyll and sunlight to be only one molecule of sugar (Carbohydrate), six molecule of wear and six molecules of oxygen is being evolved in gaseous from this is the accepted equation and also chemiscally balanced. However while teaching the subject the author came across a new balanced equation. In the new balanced equation in place of twelve water molecules in the reactant side seven molecules can be expressed and accordingly in place of six molecules of water in the product side only one molecules of water is produced. As a Botanist teaching chemistry of Photosynthesis or more explicitly Photochemistry and Photophysics or biochemistry and biophysics in certainly beyond one’s grasp but question raised by students a undergraduate level is still more rewarding. If the newly devised chemistry well balanced equation is chemically accepted certainly it will be a nice interaction between Student and Professor in the class room for better academic and scientific excellence at tertiary level of higher education.

**135. Synthesis, Characterization and Application of some cold Brand Reactive Dyes on various fibres.**

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Various reactive dyes have been prepared by coupling diazotised 4, 41 – methylene-bis-o-brome aniline with cyanurated coupling components and their dyeing performance as reactive dyes has been assessed on silk, wool and cotton fibre. All the dyes gave yellow to maroon shades with good to very good light fastness on each fibre. The purity of dyes was checked by thin layer chromatography. The I.R. Spectra showed all characteristic bands and a representative dye's PMR spectra showed all the signals. The percentage dye-bath exhaustion on different fibres was reasonably good and acceptable. The dyed fibres showed moderate to very good fastness to light, washing and rubbing.

**136. SYNTHESIS AND ANTIMICROBIAL ACTIVITY OF 1-AMINOMETHYL-3-[4'-(4"-FLUROBOBENZYLOXY)-BENZO-HYDRAZONO]-ISATINS.**

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**Key words:** Isatin, Schiff bases, Mannich bases, Antimicrobial Activity.

A new series of 1-aminomethyl-3-[4'-(4"-fluorobenzyloxy)-benzohydrazono]-isatins (Mannich bases) have been synthesized and screened for their antimicrobial potential against human pathogenic bacteria and fungi. The structures of the compounds have been established by means of spectral data (IR, PMR and Mass spectrometry.).

**137. Design, synthesis and antimicrobial activity of some new derivatives of curcumin and sulphur drugs**

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New series of curcumin  $\alpha$ -enaminones of sulphur drugs is disclosed. The structures of the newly synthesized compounds have been confirmed on the basis of elemental analysis, melting points, optical rotations, UV visible, IR and mass spectral studies. All the newly synthesized derivatives of curcumin have been investigated for their in vitro anti-microbial activity using some bacteria viz. *Salmonella typhi*, *Escherichia coli* and *Staphylococcus aureus*, some fungi viz. *Aspergillus Niger* and *Aspergillus flavus*. Most of the sulphur drug derivatives showed excellent antimicrobial activity in comparison to parent sulphur drug and curcumin. Derivative of sulfamethoxy pyridazine showed good antifungal activity for the tested fungal species whereas derivatives of sulfaacetamide sodium, sulfamethoxazole and sulfapyridine showed better antibacterial activity.

**138. Synthesis and biological screening of some new types of azetidine derivatives**

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**Keywords:** Azetidinone, Antibacterial, Antifungal, Conventional and Microwave method and Indole.

A novel kind of azetidinone analogues containing indole moieties, were synthesized

and evaluated as antibacterial against a panel of Gram-positive and Gram-negative bacteria and antifungal against some selected fungi. The synthesis was carried out by conventional as well as microwave methods. The structure of all the synthesized compounds were confirmed by chemical and spectroscopic analyses such as IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and FAB-Mas

### **139. Estrogenic Pterocarponoids Extracted from Seeds of Plant *Crotalaria Mucronata***

**Dr. Swati Shrivastava**

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**Key words:** *Crotalaria Mucronata*, Pterocarponoids, Estrogenic Principles

*Crotalaria Mucronata*, commonly known as ‘san’, is a small sized plant belonging to family ‘Leguminosae’. Estrogenic properties of extracts isolated from seeds of plant *Crotalaria Mucronata* are being reported. The identification of the Estrogenic principles was carried out using color tests and separation techniques. The screening of various extracts prepared from seeds of the plant was carried out on female albino rats by uterine weight procedure. The substance was administered orally as well as intravaginally to the immature rats and the Estrogenic activity was evaluated on the basis of ‘uterine weight response’ and number of ‘vaginal openings’. It was found that out of various fractions attempted, Pterocarponoids present in ethyl acetate and acetone soluble fractions isolated from seeds of this plant showed adequate Estrogenic activity.

**140. Pyrazolines: A New Profile of Pharmacological Activities Review Article**

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**Keywords:** - Pyrazoline derivatives, Pharmacological activities.

Pyrazolines are prominent heterocyclic compounds and various procedures have been worked out for their synthesis. Pyrazoline compounds considered as a wonder nucleus which possess diverse biological activities and inspired chemists to utilize this skeleton in bioactive moieties to synthesize new compounds possessing pharmacological properties. This review article covers the latest information over active pyrazoline derivatives having different pharmacological action such as, antiinflammatory, analgesic, antimicrobial, antitubercular, anticonvulsant, insecticidal, antioxidant and anticancer activities.

**141. Polymer-Supported Lewis acid catalyst. III. Reductive coupling of aromatic aldehydes and imines**

**Amarjyoti Kalita<sup>a</sup>, Biju Basumatary<sup>b</sup> and Swapan K. Dolui\***

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Tezpur University*

**Keywords:** Polymer support; titanium tetrachloride; organic reaction

Polymeric catalyst and polymer supported metal complex catalyst have been studied by many researchers, and this has been one of the important and rapidly developing fields of catalysis. As a part of our programme of investigating a polymer support, polypyrrol was combined with TiCl<sub>4</sub> in hexane to form a stable complex containing 2.1 wt% Ti as measured by colorimetric method. The resulting catalysts were characterised by FTIR, SEM-EDX, XRD, and TGA. The complex showed good catalytic activity in organic reaction like

synthesis of Di-ol and pyrrole. The catalyst showed good storability up to 90 days and can be reused six times without losing its activity.

## **142. Facile Synthesis of Carbohydrate Based Potential Chemotherapeutic Agents Using Benzotriazole Methodolgy**

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The increasing demand for the significant amount of carbohydrate based molecules for their complete biological, medicinal, and pharmacological investigations have stimulated efforts to develop novel and facile procedures to achieve diverse glycoconjugates and related molecules.<sup>1</sup> The benzotriazole methodology has grown from an obscure level to the level of very high synthetic popularity, since it can easily be introduced into a variety of reactions, facilitates numerous transformations, recognized sufficiently stable during reaction and finally easily removed too at the end of the reaction sequence.<sup>2</sup> Recently, we have developed a facile protocol for N<sub>1</sub>-Aryl benzotrioles from diaomino arynes via CuI-mediated intramolecular N-arylation.<sup>3a</sup> Recently method has been modified for an easy access of N<sub>1</sub>-Alkyl benzotrioles.<sup>3b</sup>

## **143. SYNTHESIS OF SOME NITROGEN MUSTARDS (MANNICH BASES)**

**GIRISH KUMAR SINHA, R.K. MEHRA AND SHARAD KUMAR**

Post Graduate Centre of Chemistry (M.U.) College of Commerce,  
Patna-800020 (India)

**Keywords:** - Substituted phthalimides, ethanolamine, half nitrogen mustard, and mannich base.

Several Mannich base half nitrogen mustards have been synthesized by the condensation of 3-substituted phthalimides and 4-substituted phthalimides with (2-chloroethyl) amine in ethanolformalin.

**144. Studies on Biological activity of synthetic mannich base nitrogen mustard of 3-aminophthalimide-I**

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*Department of Botany & Biotechnology, College of Commerce, Patna 800 020*

**Key words:** - nitrogen mustard, 3-aminophthalimide, fungicidal effect, aspergillus sp.

Synthetically prepared N-bis (2-Chloroethyl) amino-methylene-3-aminophthalimide (m.p. 84<sup>0</sup>) showed definite fungicidal effect on Aspergillus species at 5% or higher concentration of the compound in ethyl alcohol. Lower doses did not show any degree of lethality when pure culture of Aspergillus flyus was treated by filter paper discs of the test solutions. The compounds may further be tested for its fungicidal property in which for its promotion as a possible antifungal drug and a compound active against aspergilluses.

**145. Synthesis of New Limonoids from Naturally Occurring Meliacins and Screening for Antifungal Activity**

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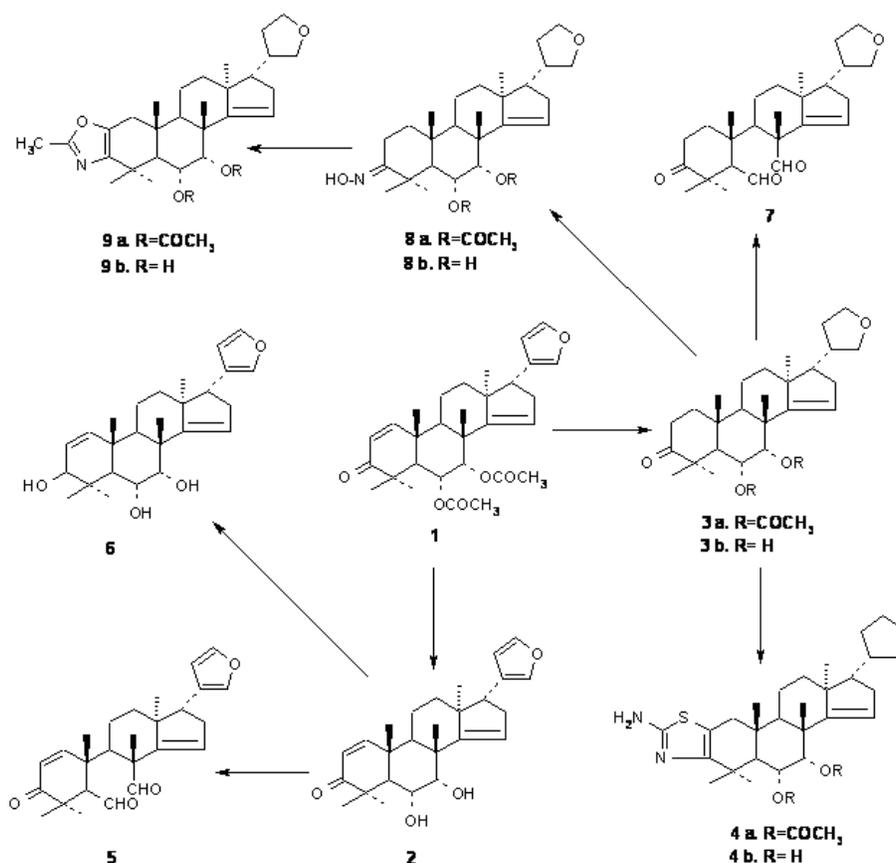
*E-mail: nkamalbhattacharya@yahoo.com*

**Key words:** Meliaceae, limonoids, paniculatin, heterocycles, antifungal activity

6-*acetoxyazadirone* (Paniculatin) (**1**) and dihydroxycompound of 6-*acetoxyazadirone*

Section IV: Chemical Sciences

acetoxyzadirone (Paniculatul) (**2**) are two naturally occurring meliacins have been isolated from the fruits and wood of *chisocheton paniculatus* Hiern. Chemical transformations of paniculatin and paniculatul gives 2-aminothiazolo [4,5-d] [1,2,20,21,22,23-hexahydro] paniculatin (**4a**), 2-aminothiazolo [4,5-d] [6á,7á -dihydroxy-1,2,20,21,22,23-hexahydro] paniculatul (**4b**), Dialdehyde (**5**), 3-hydroxy paniculatul (**6**), Dialdehyde (**7**), 2-methyloxazolo[4,5-d][1,2,20,21,22,23-hexahydro] paniculatin(**9a**), 2-methyloxazolo [4,5-d] [ 6á,7á –dihydroxy-1,2,20,21,22,23-hexahydro] paniculatin(**9b**). The structures of the new compounds have been elucidated on the basis of elemental analysis and spectral data. Antifungal activity and analysis of activity of the above compounds and their derivatives against two fungi *Rhizoctonia solani* and *Drechslera oryzae* are reported here.





# **99<sup>th</sup> Indian Science Congress**

3-7 January 2012, Bhubaneswar

**V**

## **ABSTRACTS OF ORAL/POSTER PRESENTATIONS**

### **II. INORGANIC CHEMISTRY**



**1. Synthesis, spectral and antimicrobial activity of Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> metal complexes of 1-(1-(furan-2-yl) ethylidene)-2-((3-methyl-2H-benzo[e][1,2,4]oxadiazin-2-yl)(phenyl)methylene) hydrazine**

**Devendra Kumar\* and Neelam**

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**Keywords:** Synthesis, spectral, IR, NMR, electronic spectral, TGA, hydrazone, antimicrobial activity.

Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> complexes of 1-(1-(furan-2-yl) ethylidene)-2-((3-methyl-2H-benzo[e][1,2,4]oxadiazin-2-yl)(phenyl) methylene) hydrazine have been synthesized and characterized by T.L.C, elemental analyses, IR, <sup>1</sup>H-NMR, magnetic moment values, electronic spectral and thermal studies. All the synthesized compounds, viz (3-methyl-2H-benzo[e][1,2,4]oxadiazin-2-yl)-phenyl-methanone (**2**), 3-phenyl-3-(3-methyl-2H-benzo[e][1,2,4] oxadiazin-2-yl) hydrazone (**3**), 1-(1-(furan-2-yl)ethylidene)-2-((3-methyl-2H-benzo[e][1,2,4]oxadiazin-2-yl)(phenyl) methylene) hydrazine (**4**) and their metal complexes (**5a-d**) were screened for antimicrobial activities *in vitro* against gram +ve bacteria (*Staphylococcus aureus*) and gram -ve bacteria (*Escherichia Coli*) and two fungi *Aspergillus niger* and *Aspergillus flavus*. Compound (**2**) exhibited significant antimicrobial activity which increased in its hydrazone (**3**). The activity further increased in the form of its derivative (**4**). However, metal complexes exhibited maximum activity against both bacteria and fungi.

**2. Synthesis, spectral and antimicrobial studies of macrocyclic complexes of transition metal ions of bioinorganic relevance**

**Devendra Kumar, Rubeena Akhtar, Neelam and Shivani Singh**

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**Key words:** Synthesis, spectral, antimicrobial, macrocyclic, transition metal

A novel series of macrocyclic complexes of the type  $[M(C_{32}H_{26}N_4O_4)X_2]$  and  $[M(C_{12}H_{18}N_4O_4S_2)]$  where  $M = Co(II), Ni(II)$  and  $Cu(II)$  and  $X = CH_3COO^-$ , were synthesized by template condensation reaction of diethylphthalate with 1,2-diaminobenzene and thiomalic acid with ethylenediamine respectively in presence of divalent metal salts in ethanolic solution. The complexes have been characterized with the help of various physico-chemical techniques, such as elemental analysis, IR and UV-Vis spectral studies. Spectral studies suggested an octahedral geometry for all the complexes. The biological activities of metal complexes and their fragments have been screened *in vitro* against two bacteria *Pseudomonas aeruginosa* and *Staphylococcus aureus* and two fungi *R.stolonifer* and *Pencellium notatum* to access their inhibiting potential. Metal complexes exhibited enhanced antimicrobial activity in comparison to their fragments.

**3. Synthesis and characterization of water soluble pentamethylcyclopentadienyl Rh(III) and Ir(III) complexes : Crystal structure of [Rh(h-C<sub>5</sub>Me<sub>5</sub>) (dpyam) Cl] PF<sub>6</sub> [dpyam = {(C<sub>5</sub>H<sub>4</sub>)C=NH(C<sub>5</sub>H<sub>4</sub>)}]**

**Keisham S. Singh<sup>a\*</sup>, Peng Wang<sup>b</sup> and Yuriy Mozharivskij<sup>b</sup>**

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**Key words:** Rhodium, amine, spectroscopy, crystal structure.

Water soluble complexes of general formula [(Cp\*) MCl (dpyam)] PF<sub>6</sub> were prepared by the reaction of [ $\{Cp^*MCl_2\}_2$ ] with two folds excess of dpNme ligand in methanol in the presence of NH<sub>4</sub>PF<sub>6</sub> [where; Cp\* = C<sub>5</sub>Me<sub>5</sub>, dpyam = {(C<sub>5</sub>H<sub>4</sub>)<sub>2</sub>C=NH}, dpNme = {(C<sub>5</sub>H<sub>4</sub>)<sub>2</sub>C=NMe}, M = Rh or Ir]. Complexes were isolated as their hexafluorophosphate in 67-80% yield. The complexes were characterized with the help of spectroscopic data and crystal structure of [Rh(Cp\*)(dpyam)Cl]PF<sub>6</sub> has been determined by X-ray diffraction study. The molecule crystallizes in orthorhombic crystal system in *pbcn* space group with a = 23.699, b = 13.951 and c = 14.783 Å;  $\alpha = \beta = \gamma = 90^\circ$ .

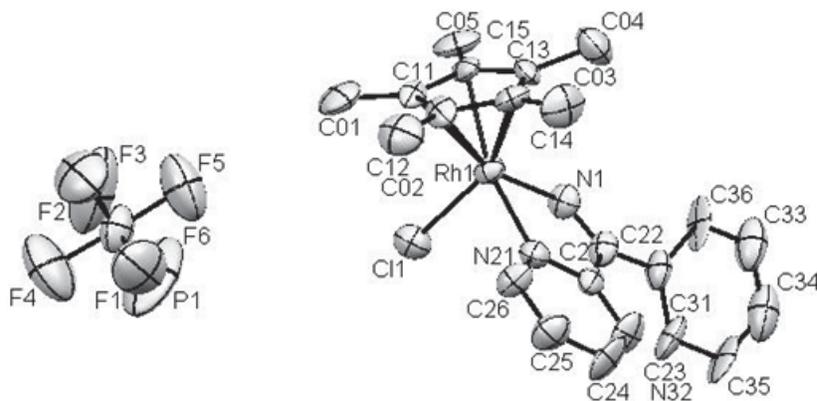


Figure: Crystal structure of [Rh(h-Cp\*)(dpyam)Cl]PF<sub>6</sub>. Hydrogen atoms have been omitted for clarity.

#### **4. Calculations of EPR Parameter Hyperfine Coupling Constants of Some Dipolar Metal Complexes Using Density Functional Methods**

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**Key words** – Density Functional Theory (DFT). Transition Metal Complexes, Hyperfine Coupling Constants.

Calculations of the EPR spectral parameter hyperfine coupling constants of Dipolar Metal Complexes  $[\text{Co}(\text{CO})_4]$ ,  $[\text{Mn}(\text{CN})_5\text{NO}]^{2-}$ ,  $[\text{Mn}(\text{CN})_4\text{N}]^-$ ,  $[\text{Ni}(\text{CO})_3\text{H}]$  have been carried out using density functional theory (DFT) with BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals and the results obtained have been compared with experimental values. The results obtained from the density functional methods have been found in close agreement with the result obtained from the experiments. The performances of the different functionals for different transition metal complexes have been found different. The performance of the functional BP86 have been found better for  $[\text{Ni}(\text{CO})_3\text{H}]$ ,  $[\text{Mn}(\text{CN})_5\text{NO}]^{2-}$ ; BHPW91 for  $[\text{Co}(\text{CO})_4]$  and B3LYP for  $[\text{Mn}(\text{CN})_4\text{N}]^-$  Dipolar Metal Complexes. We have not identified any such functional, the performance of which is excellent for calculation of EPR parameter hyperfine coupling constant for all transition metal complexes considered in this study.

**5. A comprehensive study on some Ln (III) – Ciprofloxacin complexes**

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**Keywords:** Ciprofloxacin, Gram (-) bacteria, Gram (+) bacteria, Antibacterial properties, FTIR

The complexes of trivalent lanthanides Pr(III) and Sm(III) with ciprofloxacin (1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinoline carboxylic acid) have been synthesized and these were characterized on the basis of their elemental analyses, molar conductivities, magnetic properties, IR-spectra, NMR-spectra and UV-spectral analyses. On the basis of these analyses it has been confirmed that the direct reaction of metal salts with ciprofloxacin leads to formation of complexes. The bidentate nature of ciprofloxacin and octahedral nature of the complexes has been established. The ligation centre in ciprofloxacin as carbonyl group at position-3 and oxo group at position-4 have also been confirmed other donor atoms do not participate in ligation because of chemical intuition. Solubility of the complexes has been determined by using different solvents. It has been found that complexes are insoluble in water but soluble in dimethyl sulfoxide, dichloromethane and ether. Melting point of the complexes was determined by the open capillary tube and hence is uncorrected. The complexes have been screened against gram negative and gram positive bacteria.

**6. Effect of Indoor Air Pollutants on Pulmonary System**

**Richa and Smriti**

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**Keywords:** - PEFR, PAH, POM N.Asth and Asth.

Indoor air pollution is associated with the contamination of urban air from automobile exhausts and industrial effluents. However, in developing countries, the problem of indoor air pollution far outweighs the ambient air pollution. There are four principal sources of pollutants of indoor air : (i) Incomplete combustion, (ii) building material, (iii) the ground under the building, and (iv) bio aerosols. In developed countries the most important indoor air pollutants are radon, asbestos, volatile organic compounds, pesticides, heavy metals, animal dander, mites, moulds and environmental tobacco smoke. However, in developing countries the most important indoor air pollutants are the combustion products of unprocessed solid biomass fuels used by the poor urban and rural folk for cooking and heating. The type of fuels used by a household is determined mainly by its economic status. In the energy ladder, biomass fuels namely animal dung, crop residues and wood, which are the dirtiest fuels, lie at the bottom and are used mostly by very poor people. Electricity, which is the most expensive, lies at the top of ladder and it is also the cleanest fuel. The study is conducted on the basis of candidate's exposure duration to indoor air pollutants with the help of peak flow gauge and its result shows that indoor air pollutants are responsible for breathing problem.

## **7. SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION AND PRELIMINARY ANTI- DIABETIC ACTIVITY OF OXOVANADIUM (IV) COMPLEXES WITH N<sub>2</sub>O<sub>2</sub> DONORS MACROCYCLES**

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**Key words:** Oxovanadium (IV), macrocyclic, triazoles, UV-Vis, Ir, EPR, insulin mimetic

A new series of diazadioxa oxovanadium(IV) macrocyclic complexes of type [VO(mac)] SO<sub>4</sub> have been synthesized via the condensation reactions of a 3-(phenyl/substituted phenyl)-4-amino-5-hydrazino-1,2,4-triazole (H<sub>2</sub>L) with salicylaldehyde / 2-

hydroxyacetophenone and 1,4-dibromobutane in the presence of oxovanadium (IV) sulphate in ethanol. All the newly synthesized compounds were characterized on the basis of elemental analyses, conductance measurements, magnetic properties, spectral (UV-Vis, IR, EPR) and XRD studies. All these macrocyclic complexes are conducting and monomeric in nature. The room temperature magnetic moments are normal for V (IV)  $d^1$  configuration. The ligands act as dibasic, tetradentate chelating agents with coordination sites at two azomethine nitrogens and two oxygen atoms ( $N_2O_2$  donors). All complexes are EPR active and at 77K, all complexes show axial anisotropy with two sets of eight line patterns. A square pyramidal geometry is proposed. The particle size of the complexes has been calculated from XRD spectra using Debye-Scherrer formula and these are found to be in nano range. The efficacy of two macrocyclic complexes was also studied in streptozotocin-induced diabetic rats over a period of 30 days. The administration of these complexes in diabetic rats reversed the diabetic effect due to their insulin-mimetic effects.

**8. Synthesis, Spectral and Antimicrobial Studies of Zinc (II) Complexes with Schiff Bases Derived from 2-Hydrazino-5- [Substituted Phenyl] -1, 3, 4-Thiadiazole**

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**Key words:-** Zinc(II), Schiff bases, Hydrazino thiadiazoles, IR, NMR, Antifungal and antibacterial

Zn (II) complexes have been synthesized by reacting zinc acetate with Schiff bases derived from 2-hydrazino-5[substituted phenyl]-1, 3, 4-thiadiazole and 2-hydroxyacetophenone/benzaldehyde/isatin. All these complexes are soluble in DMF and

DMSO; low molar conductance values indicate that they are non electrolytes. Elemental analyses suggests that the complexes have 1:2 metal to ligands stoichiometry of the type  $[ZnL_2(H_2O)_2]$  (LH=Schiff bases derived from 2-hydrazino-5-[substituted phenyl]-1,3,4-thiadiazole and 2-hydroxyacetophenone/isatin),  $[ZnL'_2(OOCCH_3)_2(H_2O)_2]$  (L'= Schiff bases derived from 2-hydrazino-5-[substituted phenyl]-1,3,4-thiadiazole and benzaldehyde) and they were characterized by IR,  $^1H$  NMR,  $^{13}C$  NMR and FAB mass. All these Schiff bases and their complexes have also been screened for their antibacterial (*Bacillus subtilis*, *Escherichia coli*) and antifungal activities (*Colletotrichum falcatum*, *Aspergillus Niger*, *Fusarium oxysporium* and *Curvularia pallescens*) by paper disc method.

**9. Synthesis, spectral characterization and in vitro antifungal and antibacterial studies of lanthanum (III) and praseodymium (III) complexes with Schiff bases derived from 5-substituted-4-amino-5-hydrazino-1,2,4-triazoles and isatin**

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The new lanthanum(III) and praseodymium(III) complexes of the general formula  $[LnCl(L)(H_2O)_2]$  (Ln= La(III) or Pr(III); LH<sub>2</sub>= Schiff bases derived from 3-substituted-4-amino-5-hydrazino-1,2,4-triazoles and isatin) have been prepared. The complexes have been characterized by elemental analyses, molecular weight by FAB-mass, thermogravimetry, electrical conductance, magnetic moment and spectral (electronic, infrared, far-infrared,  $^1H$  NMR and  $^{13}C$  NMR) data. The ligands and all prepared compounds were assayed for antibacterial (*Bacillus subtilis* and *Escherichia coli*) and antifungal (*Aspergillus niger*, *Aspergillus alternate* and *Helminthosporium oryzae*) activities. The activities have been correlated with the structures of the compounds.

**10. Synthesis and characterization of substituted amine complexes of Ni (II), Cu (II) and Zn (II) by using thiazolidinone alone or along with thiourea as a ligand**

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**Key words:** - Mixed ligand complexes, Mercaptyl thiazolidinone, Pyridine thiazolidinone, Thiourea, Ammine complexes

Mercaptyl thiazolidinone and Pyridine thiazolidinone were prepared to be used as ligands. Mixed ligand complexes of nickel(II), copper(II), and zinc(II) were prepared by involving either mercaptyl thiazolidinone (1) [2-(2-hydroxy benzoyl)-3-N-(2-mercaptyl)-1-Thiazolidin-4-one] or pyridine thiazolidinone (2) [2-(2-hydroxy benzoyl-3-N-(2-Pyridinyl)-1-Thiazolidin-4-one)] alone and along with thiourea. The products have been obtained by partial or complete replacement of the strongly coordinated ammonia of ammine complexes. The products were purified and separated by TLC and column chromatography. All the products have been characterized by elemental analysis, molar conductance, magnetic susceptibility and IR and electronic spectral measurements for their bonding and structures.

**11. Polarographic Determination and Antimicrobial activity of Cu (II) complex with 4-Chlorobenzylidene-4-aminoacetanilide**

**KRISHNA KUMAR RAJ AND RIYAZ AHMAD DAR**

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**Keywords:** 4-chlorobenzaldehyde; Polarography; Cu (II)-CAA complex, MIC

The electrochemical behaviour of the complex of Cu (II) with 4-Chlorobenzylidene-4-aminoacetanilide (CAA) was studied. It was observed that CAA forms 1:1 complex with Cu(II) in between pH 6.5 to 7.1. It was found that the reduction process of Cu (II)- CAA complex is two electron reversible reduction process at D.M.E. The logarithm value of stability constant of Cu (II)-4-Chlorobenzylidene-4-aminoacetanilide (CAA) complex has been found to be 4.85. The redox properties of the complex was extensively investigated by electrochemical method using cyclic voltammetry (CV). The Cu(II) complexes exhibited quasi-reversible single electron transfer process. The Schiff base and its complex has been screened for their *in-vitro* antibacterial (*Escherichiacoli*, *Staphylococcus aureus*, *Vibrio cholerae* and *Bacillus subtilis*) and antifungal (*Aspergillus Niger* and *Penicillium liliacinum*) activities by minimum inhibitory concentration (MIC) method.

## 12. Green Chemistry Approach: Synthesis and spectral studies of hydrazones and their metal complexes

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**Keywords:** Synthesis, microwave irradiation, spectral, IR, <sup>1</sup>HNMR, electronic spectra

Six new metal complexes of Co (II), Ni (II) and Cu (II) with bis-(furfuryl) adipic acid dihydrazone (FADH) and bis- (2-acetyl thiophene) adipic acid dihydrazone (2-ATADH) have been synthesized under microwave irradiation. The Microwave irradiation method was found remarkably successful and gave higher yield at less reaction time. All the synthesized compounds have been characterized by running their TLC for single spot, repeated melting point determination, elemental analyses, IR, <sup>1</sup>H-NMR and electronic spectral studies. The elemental analyses and spectral analysis results revealed their Metal:

Ligand (1:1) stoichiometry. Electronic spectral studies suggested the octahedral geometry of the complexes.

**13. Synthesis, spectral and antimicrobial activity of mixed ligand complexes of Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> with N, O and S donor ligands**

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**Keywords:** - Synthesis, spectral, antimicrobial, mixed ligand complexes.

Mixed ligand complexes of bivalent metal ions, viz: Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> of the composition (ML<sub>1</sub>L<sub>2</sub>) in 1:1:1 molar ratio, (where L<sub>1</sub>=diphenylamine-2-mercapto-2'-carboxylic acid (DPMC) and L<sub>2</sub>=2-furyl glyoxal-anthranilic acid (FGAA) have been synthesized and characterized by repeated melting point determination, elemental analyses, IR, <sup>1</sup>H-NMR, magnetic susceptibilities measurements and electronic spectral data. The synthesized ligands and their metal complexes were screened for their antimicrobial activity against two bacteria *Staphylococcus aureus* (gram +ve) and *Escherichia coli* (gram -ve) and two fungi *Apergillus niger* and *Apergillus flavus* by Serial Dilution Method. Metal complexes exhibited more activity than their ligands.

**14. Fabrication and Characterization of White Organic Light Emitting Device Using Blue and Orange Light Emitting Zinc Complexes**

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**Key words:** - WOLED, doped emissive layer, electroluminescence

Stable white electroluminescence (EL) was achieved from Organic LED in which bis (5,7-dimethyl-8-hydroxyquinolinato)zinc(II) [(Me<sub>2</sub>q)<sub>2</sub>Zn] was doped in bis {2-(2-hydroxyphenyl)benzoxazolato} zinc(II)[(HPB)<sub>2</sub>Zn]. The doped layer was used as emissive layer and the dopant concentration was optimized to achieve white light. Electroluminescence spectra, current-voltage-luminescence (I-V-L) characteristics of the device were studied by changing the dopant concentration in active layer. The best Commission International de L'Éclairage (CIE) coordinates i.e. (0.34, 0.38) were obtained with device structure ITO/áNPD (30nm)/30 % (Me<sub>2</sub>q)<sub>2</sub>Zn doped (HPB)<sub>2</sub>Zn/ BCP (6nm)/Alq<sub>3</sub> (28nm)/ Lif (1nm)/Al (100nm). The EL spectrum covers the whole visible spectra range from 400nm to 700nm. The color rendering index (CRI) for our best white light (device 4) was 47.4. The device showed very good color stability in terms of CIE coordinates with voltages. The maximum luminescence 1850 cd/m<sup>2</sup> was achieved at 23 V.

**15. Synthesis and optoelectronic properties of 5-ethyl-7-methyl-8-hydroxyquinolatoaluminium**

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**Keywords:**-OLED, 5-ethyl - 7 - methyl - 8 - hydroxyquinolatoaluminium ,  
electroluminescence.

5-ethyl-7-methyl-8-hydroxyquinolatoaluminium complex was synthesized and used as emitting material to produce orange light, the tetrahydrofuran (THF) solution of which fluoresced at 553 nm when excited by UV light at 258 nm and 337 nm. Electroluminescence (EL) spectra, current-voltage-luminescence (I-V-L) characteristics of the devices have been studied. The best results were obtained with the device structure ITO/TPD (30 nm)/Al (EtMeq)<sub>3</sub> (35 nm)/Alq<sub>3</sub> (25nm)/LiF (0.3nm)/Al (100nm). Maximum luminance of 969 Cd/m<sup>2</sup> was achieved when aluminium complex was used as emissive layer in the OLED at 14 V.

**16. Nanogram Determination of Mn (II) based on its catalytic effect on periodate oxidation of o-Anisidine**

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**Key words:** Nanogram Estimation of Mn (II), o-anisidine, periodate oxidation

The Mn (II) catalysed periodate oxidation of o-anisidine in acetone-water medium is first order with respect to catalyst, substrate and oxidant each. The progress of reaction was followed by monitoring the increase in the absorbance of reaction intermediate. The main reaction product characterized on the basis of melting point and spectroscopic studies, is methoxy-1,4-benzoquinone. The effect of pH, dielectric constant of medium, ionic strength and free radical scavengers was studied to develop the conditions for microgram determination of Mn(II) on the range 5.5-527.4 ng/ml. The characteristics of various calibration curves, Sendell's sensitivity, molar absorptivity, percentage recovery, effect of interferences and correlation coefficient have been evaluated. An attempt has been made for proposing a suitable mechanism for the reaction studied. Thermodynamic parameters are also reported.

**17. Microgram Determination of 2, 3-dimethylaniline based on its Manganese (II) catalyzed Oxidation by Periodate ion.**

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**Keywords:** - Microgram Estimation, 2, 3-dimethylaniline, Mn catalysed, periodat oxidation.

The Mn (II) catalysed periodate oxidation of 2,3-dimethylaniline in acetone-water medium is first order with respect to catalyst, substrate and oxidant each. The progress of reaction was followed by monitoring the increase in the absorbance of reaction intermediate. The main reaction product characterized on the basis of melting point and spectroscopic studies, is 2, 3-dimethyl -1, 4-benzoquinone. The effect of pH, dielectric constant of medium, ionic strength and free radical scavengers was studied to develop the conditions for microgram determination of 2,3-dimethylaniline in the range 1.2 – 19.4 µg/ml. The characteristics of various calibration curves, Sendell's sensitivity, molar absorptivity, percentage recovery, effect of interferrants and correlation coefficient have been evaluated. An attempt has been made for proposing a suitable mechanism for the reaction studied. Thermodynamic parameters are also reported.

**18. Development of cost effective process technology to produce biofuel**

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**Key words:** Biodiesel, Transesterification, syngas, biofuel, bioethanol

Development of process technology to produce biofuel such as biodiesel, biogas, bioethanol, etc from biomass has been taken up to replace fast depleting fossil fuel. Biodiesel from cheap oilseed of forest product for compression ignition (CI) engine at lower operating cost and the production of bioethanol from agricultural waste is the mode of research in the laboratory. The performance characteristics of CI engine using biodiesel brought novel explanation. Conversion of food waste materials of our vast canteen to methane rich biogas through anaerobic digestion is worked out but poor efficiency is noticed. Various drawbacks of producing biofuel attract to develop second generation technology using non-N<sub>2</sub> gasification agents producing high calorific gas such as CO and H<sub>2</sub> from biomass.

**19. EFFECT OF TEMPERATURE ON ABSORPTION OF CHLORINE AND BROMINE ON ABSORBENT CARBONS.**

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In the present research work, attention has been focused on the study of effect of temperature on adsorption of halogen gases by adsorbent carbons. Two samples of carbons of liquid bromine are adsorbed partially physically and partially chemically. It has also been observed that maximum percentage of chemisorbed gases occur at 120<sup>0</sup>C while the maximum uptake physical as well as chemical takes place at 30<sup>0</sup>C which was taken as lowest temperature studied. It was indicated that activated carbon, carbon blacks and charcoal differ markedly in their total chlorine uptake at 30<sup>0</sup>C.

The chemisorbed chlorine and bromine form stable complexes. The chemisorbed chlorine starts coming off on evacuation at increasing temperatures. On evacuating the treated samples at 100<sup>0</sup>C to constant weight a substantial amount of chlorine is retained particularly in the case of active carbons. The chemisorbed chlorine however, is expected

to be eliminated completely on evacuation at temperature around 150<sup>0</sup>C. The trends observed in case of bromine are similar.

**20. Polarographic study of In (III) & Tl (I) Complexes of N-Glycylglycine in Water & Aqueous Ethanol Media**

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**Keywords:-**Polarography, Indium, Thallium, N-Glycylglycine, complex, stability constants.

In (III) and Tl (I) form 1:3 complexes with N-Glycylglycine in aqueous & aqueous ethanol medium. The presence of ethanol in the medium considerably affects the nature and composition of the complex species. The natures of electrode processes were reversible and diffusion controlled. The successive formation of three complexes 1:1, 1:2, and 1:3 is established by Deford and Hume' method. The effect of change of temperature on the system has been investigated and the thermodynamic parameters  $DG^0$ ,  $DH^0$  and  $DS^0$  of the complexation reaction have also been determined. The formation of the metal complexes has been found to be spontaneous and exothermic in nature.

**21. Spectrophotometric determination of Hg(II) in water and soil samples using Schiff base.**

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**Key words: -** Schiff base, spectrophotometry, Mercury determination, soil and water.

An analytical application of bazo-thiophene 2-aldehyde and thio-semicarbazone (2-BTAT) is being reported for the first time. The reagent has been characterized using elemental analyses, IR, NMR and mass spectral data. This reagent has been used for the spectrophotometric determination of Hg (II). The reagent interacts with Hg(II) in pH range 7 ~ 8 . Brown colored complex with 1:2 (M: L) ratio is obtained. The colour is stabilized for 8-10 hrs. The molar absorptivity and sandell's sensitivity of (2-BTAT) were observed as expected. This method has been applied to potable, polluted water and soil sample containing Hg (II).

## **22. Synthesis, Characterization of Cu-TiO<sub>2</sub> Nanocomposites and Their Application in Photodegradation of Eriochrome Black-T**

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**Keyword:** - Photocatalyst, Nanocomposites, Eriochrome Black-T, Photodegradation.

Photocatalysis deals with reactions which are initiated by electronically excited molecules generated by absorption of suitable radiation in the visible or near ultraviolet region. Photocatalytic reactions occurring in the presence of semiconductor and light. Researchers are using photocatalysts for oxidative degradation of various non-biodegradable wastes.

Titanium dioxide (TiO<sub>2</sub>), commonly known as Titania, is one of the most commonly used photocatalysts. Because of its high oxidative power, stability, and non-toxicity, it promises a broad range of uses as a photocatalysts. Advantage of using TiO<sub>2</sub> as photocatalyst are: (a) using TiO<sub>2</sub>, the process occurs under ambient conditions. (b) using TiO<sub>2</sub>, the oxidation of the substrate to CO<sub>2</sub> is complete in most cases and (c) it is comparatively inexpensive and remains quite stable in contact with different substrate.

In the present study, to prepare the nanocomposites of Titania by solution impregnation method. The prepared sample of Titania and copper Titania were subjected

to photocatalytic degradation of Eriochrome Black T was done.

The degradation of Eriochrome Black T was more prominent in case of 2 hour study, in the presence of Cu-TiO<sub>2</sub> than the commercially obtained TiO<sub>2</sub>. The degradation of Eriochrome Black T is 40 % - 50 % observed in case of 2 hour study.

### 23. Syntheses, spectral and biological studies of new imines derived from 5-Bromothiophene-2-carboxaldehyde & their Si(IV), Sn(IV) complexes

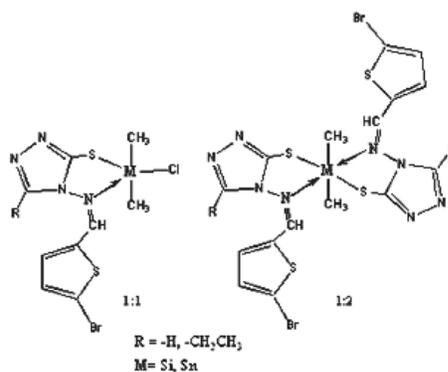
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**Keywords:** 4-Amino-5-mercapto-s-triazole, Schiff-bases, silicon-complexes, tin-complexes, Antimicrobial activity.

The imines HL<sup>1-2</sup> have been synthesized by the reaction of 5-Bromothiophene-2-carboxaldehyde with 4-Amino-5-mercapto-3-substituted-s-triazole. Organosilicon (IV) and organotin (IV) complexes having general formulae R<sub>2</sub>MCl (L<sup>1/2</sup>), and R<sub>2</sub>M (L<sup>1/2</sup>)<sub>2</sub> were synthesized from the reaction R<sub>2</sub>MCl<sub>2</sub> with these Schiff bases in 1:1 and 1:2 molar ratio, where M= Si/Sn, R= CH<sub>3</sub>. The synthesized compounds have been characterized with the aid of elemental analyses, molar conductance and spectroscopic studies including UV, IR, <sup>1</sup>H, <sup>13</sup>C, <sup>29</sup>Si and <sup>119</sup>Sn NMR spectroscopy. On the bases of these studies, the resulting complexes have been proposed to have trigonal bipyramidal and octahedral geometries. *In vitro* activities of compounds against some bacteria and fungi have been carried out.



**24. Growth and thermal stability of Ta<sub>2</sub>O<sub>5</sub> on Si (100) surface**

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Tantalum pentoxide (Ta<sub>2</sub>O<sub>5</sub>) is one of the most promising stable high dielectric oxide which can be used in miniaturization of electronic memory devices. The dielectric constant of pur Ta<sub>2</sub>O<sub>5</sub> is about 25 and it can be increased to 100 by introduction of nitrogen into Ta<sub>2</sub>O<sub>5</sub>. We have prepared thin layers of about 1nm Ta<sub>2</sub>O<sub>5</sub> by e-beam deposition of Ta onto clean p-type Si(100) surface under oxygen pressure in-situ in the preparation chamber of hard X-ray photoelectron spectrometer on BW2 beamline, DORIS III, DESY, Hamburg, Germany. Ta 4f and O 1s core levels have been investigated using hard X-ray photoemission with a photon energy of 3 keV with in-situ annealing in oxygen pressure. Our results indicate that the as deposited Ta<sub>2</sub>O<sub>5</sub> on Si is in amorphous phase and it transforms to crystalline Ta<sub>2</sub>O<sub>5</sub> on annealing in oxygen pressure of 1.5x10<sup>-4</sup> mbar at 650°C. O 1s peak intensity increases by a factor of two after annealing and O 1s exhibits unusually large chemical shift of about 1 eV. The amorphous phase of Ta<sub>2</sub>O<sub>5</sub> contains lot of oxygen defects and is capable of consuming oxygen upon phase transformation to crystalline phase.

25. **Mixed – ligand complexes of  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Zn}^{2+}$  with 2, 2' Bipyridine as a primary ligand and L-2-amino-3-imidazolyl propionic acid as secondary ligand.**

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Jaipur 302017(INDIA),*

**Keywords:** - formation constants, mixed ligand, L-Histidine, 2,2' Bipyridine

Modified form of Irving Rossotti titration technique has been applied to study the formation constants of mixed ligand complexes of the type MAL where  $M = \text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Zn}^{2+}$ ;  $A = \text{Bipyridyl}$  and  $L = \text{L-2-amino-3-imidazolyl propionic acid(L-Histidine)}$  at  $30^\circ\text{C}$  ( $\mu=0.1\text{M}$ ). The values of the formation constants obtained in the mixed ligand system are little less than first formation constant of M-L simple systems.

26. **A Mild and Efficient Method for Synthesis of Benzils from Benzoin with Different Metal Salts supported over Silica**

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**Key words:** Benzoin, Benzils, oxidation, metal salts, silica.

In order to develop a cost-effective and green procedure for the oxidation of benzoin

to benzils, the use of different metal salts supported over silica for the oxidation of benzoin to benzils is described.

**27. Adsorption of Pb (II) from aqueous solution by hybrid precursor from rice husk**

**Awanish Patel<sup>1</sup>, M. K. Bhatnagar<sup>\*</sup>, Ashok Tripathi<sup>2</sup>, Mukesh Singh<sup>3</sup>**

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**Key words:** -Rice husk hybrid precursor (RHHP), Pb (II), Sorption, Metal ion.

A carbon adsorbent derived from rice husk by nitric acid treatment was used for the removal of Pb (II) from aqueous solution. Sorption of metal ion has been studied as a function of contact time, temperature, pH of the solution and metal ion concentration. These factors have remarkable positive effect on sorption process. The adsorption data of RHHP at different initial concentration was fitted to Freundlich & Langumir adsorption isotherms and monolayer sorption capacity determined was 72.04 (pH 6.0 and temperature 20<sup>o</sup>c). Thermodynamic parameter indicated that the sorption is exothermic, spontaneous with a greater affinity of metal species for the adsorbent.

**28. “Metal Complex Formation and Anticancer activity of Complex Drug Zinc II- Dacarbazine”**

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**Keywords:** - Dacarbazine, Raper’s Method, Polarographic Study, Amperometric- titrations, and Invitro and Invivo study.

Dacarbazine is an antineoplastic chemotherapeutic drug also known as Imidazole Carboxamide impede the formation of new tissues by interfering with cell growth .The complexation properties of dacarbazine (dac),with metal being a compound of interest for anticancer research. The physiochemical, microbial and pharmacological studies of Zn-II Dacarbazine complex have been done in solid & aqueous phase. According to their polarographic studies,elemental analysis, IR spectral study, the formula of complex has been formed 1:1 Zn(II) Dacarbazine by using polarographic method at 251<sup>0</sup>C and ionic strength of the metal ligand interaction of complex has been found.

The amperometric titration & polarographic studies shows that there is a (1:1) (M:L) metal ligand interaction . On the basis of obtained data the microbial and pharmacological studies of metal drug complex revealed that anticancer activity of Zn (II) Dacarbazine as compared to synthetic drug.

**29. SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL STUDIES OF SOME THIOCYANATO BRIDGED DIMETALLIC COMPLEXES CONTAINING Co(II), Cd(II), Hg(II) and N, N', -BIS (BENZYLIDENE)-1,2 -PHENYLENEDIAMINE SCHIFF BASE.**

**N. Upadhyay,<sup>1</sup> Aradhana Mishra<sup>2</sup> & K. Kumar<sup>3</sup>**

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*3 : Dept of zoology, Pt. SNS Govt. PG College Shahdol (MP)*

**Key words:** - bimetallic, thiocyanato, Schiff base.

The coordination chemistry of Transition metal complexes has been progressing at a tremendous pace. These complexes were finding use in the field of homogeneous catalysis, analytical chemistry and biological system. The presence of thiocyanato group in mixed ligand coordinated complexes of transition metal was reported to have an ability to influence the biochemical behaviour of the complexes. Complexes of  $MM^*(SCN)_4$  ( $M = Co^{2+}$ ;  $M^* = Cd^{2+}$ ,  $Hg^{2+}$ ) with N, N\* -Bis (benzylidene) – 1,2, phenylenediamine Schiff base of molecular formula  $[MM^*(SCN)_4 (BENDAMB)(1,2)]$  have been synthesized and characterized by elemental analyses, molar conductance magnetic moment, IR, electronic,  $^1H$  NMR spectral studies. The softness parameter  $TEn^{\#}$  of complexes have also been calculated to derive the binding site of the thocyanate ligand. The insecticidal activity against Red cotton bug (*Dysdercus koenigii*) of complexes also been investigated and was compared with solvent and Schiff base.

**30. Synthesis and Spectral Studies of isomeric Copper (II) Complex Salts With Phenylbiguanide [PhBigH<sup>+</sup>/C<sub>8</sub>H<sub>11</sub>N<sub>5</sub>]**

**R.K.Prasad<sup>a\*</sup>, (Mrs) Bina Rani<sup>b</sup>, and Dhananjai Singh<sup>b</sup>**

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**Keyword:** Phenylbiguanide, Magnetic susceptibilities and Absorption spectra

Isomeric cis trans bis(phenylbiguanidinium)copper(II) salts of composition [Cu(PhBigH<sup>+</sup>)<sub>2</sub>]X<sub>2</sub>.nH<sub>2</sub>O where PhBigH<sup>+</sup> = C<sub>8</sub>H<sub>12</sub>N<sub>5</sub>, X<sup>-</sup> = OH<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup> or I<sup>-</sup> and n = 1,2 or 6 have been isolated and characterized from the studies of their colour, magnetic susceptibilities, infrared vibrations and electronic absorption spectra. The cis variety is isolated at lower temperature and in moderately alkaline medium (pH ~ 10 -12) which is transformed to stable trans form by boiling in neutral aqueous medium.

**31. NEW ORGANOTITANIUM (IV) COMPOUNDS WITH FERROCENYLMORPHOLINE-N-THIOHYDRAZONES**

**Kartik Kumar Nandi\***

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**Keywords:-** Organotitanium, Ferrocene, Thiohydrazone, etc.

In continuation of our works on studies on biologically significant organometallic

ligands containing ferrocenyl moiety, this paper is based on isolation of two new organotitanium (IV) compounds of organometallic ligands containing ferrocenyl moiety. Reactions of two organometallic ligands, 1-formyl-ferrocenemorpholine-N-thiohydrazone [HFfmth] & 1-acetyl-ferrocenemorpholine-N-thiohydrazone [HAFmth], with  $\text{Cp}_2\text{TiCl}_2$  have studied. Two new organotitanium (IV) compounds,  $\text{Cp}_2\text{Ti}(\text{Ffmth})_2$  &  $\text{Cp}_2\text{Ti}(\text{AFmth})_2$  are isolated from the *in situ* reaction mixture of corresponding ligands with more than 75% yield. Both the ligands are found to function in a monobasic & bi-dentate fashion. Isolated complexes are found soluble in DMSO, DMF & chloroform. The characterization of the new compounds are attempted with elemental and spectroscopic [UV-VIS, IR and  $^1\text{H-NMR}$ ] data analysis.

**32. SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL STUDIES OF SOME THIOCYANATO BRIDGED BIMETALLIC COMPLEXES CONTAINING Co(II), Cd(II), Hg(II) & N, N', - BIS (BENZYLIDENE)-1, 2 -PHENYLENEDIAMINE SCHIFF BASE.**

**N. Upadhyay,<sup>1</sup> Aradhana Mishra<sup>2</sup> & K.Kumar<sup>3</sup>**

*1: Dept of Chemistry, Pt. SNS Govt. PG College Shahdol (M P)*

*2: Dept of Chemistry, Govt. PG College Maihar (MP)*

*3: Dept of Zoology, Pt. SNS Govt. PG College Shahdol (MP)*

**Key words:** - bimetallic, thiocyanato, Schiff base.

The coordination chemistry of Transition metal complexes has been progressing at a tremendous pace. These complexes were finding use in the field of Homogeneous catalysis, Analytical chemistry and Biological system.

The presence of thiocyanato group in mixed ligand coordinated complexes of transition metal was reported to have an ability to influence the biochemical behaviour of the complexes.

Complexes of  $\text{MM}'(\text{SCN})_4$  ( $\text{M} = \text{Co}^{2+}$ ;  $\text{M}' = \text{Cd}^{2+}, \text{Hg}^{2+}$ ) with N, N'-Bis

(benzylidene) - 1, 2, phenylenediamine Schiff base of molecular formula  $[MM'(SCN)_4(BENDAMB)(1, 2)]$  have been synthesized and characterized by elemental analyses, molar conductance magnetic moment IR, Electronic,  $^1H$  NMR spectral studies.

The softness parameters  $TEN?$  of complexes have also been calculated to derive the binding side of the thiocyanate ligand. The insecticidal activity against Red cotton bug (*Dysdercus koenigii*) of complexes also been investigated and was compared with solvent and Schiff base.

### **33. Synthesis structural characterization and biological screening of oxovanadium (IV) complexes derived from Schiff base ligand containing thiosemicarbazone.**

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The synthesis and characterization of the complexes of oxovanadium (IV) is reported here-in of  $[VO L_1 (H_2O)_2] SO_4$  ( $L_1$  = Schiff bases ligands containing thiosemicarbazone moiety). Complexes of oxovanadium (IV) with bis (p-methoxybenzaldehyde) thiosemicarbazone (MBATSCZ), bis (N, N' di-methyl-4-aminocinnamaldehyde) thiosemicarbazone (DMABATSCZ), bis (pyridine-2-aldehyde) thiosemicarbazone (PATSCZ), bis (p-chlorobenzaldehyde) thiosemicarbazone (CBATSCZ) bis (indole-3aldehyde) thiosemicarbazone (IATSCZ), bis(3-methylsalicylaldehyde) thiosemicarbazone (MSATSCZ), bis(5-methylsalicylaldehyde) thiosemicarbazone (M'SATSCZ), bis(furfuryl-2-aldehyde) thiosemicarbazone (FATSCZ) and bis (5-bromosalicylaldehyde) thiosemicarbazone (BSATSCZ) have been synthesized and characterized by elemental analyses, molar conductivity, magnetic moments, thermal studies, EPR, IR and electronic spectra. These studies show octahedral geometry around the metal ion. These complexes were also screened for their anti-bacterial and anti-fungal activities.

**34. Cobalt, Nickel, Copper and Zinc complexes with 1, 3-diphenyl-1H-pyrazole-4-carboxaldehyde Schiff bases: Antimicrobial, spectroscopic, thermal and fluorescence studies.**

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**Keywords:** - 1, 3-diphenyl-1H-pyrazole-4-carboxaldehyde, Antimicrobial activity, Thermal studies, 1, 2, 4-triazole, fluorescence.

Two new Schiff bases of 1,3-diphenyl-1H-pyrazole-4-carboxaldehyde and 4-amino-5-mercapto-3-methyl.H-[1,2,4]triazole [HL1-2] and their cobalt, Nickel, Copper and Zinc complexes have been synthesized and characterized by elemental analyses, spectral (UV-Vis, IR, <sup>1</sup>HNMR, Fluorescence) studies, thermal techniques, magnetic and conductance measurements. IR results demonstrate the bidentate binding of the Schiff bases through azomethine nitrogen and thiol group. A square planar geometry for Cu(II) and octahedral geometry for Co(II), Ni(II) and Zn(II) complexes have been proposed. The pyrazole Schiff bases and their metal complexes have been studied in vitro antibacterial against *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli* and *Pseudomonas aeruginosa* and in vitro antifungal against *Aspergillus Niger* and *A. flavus*.

**35. NIOBATES FOR ADVANCED TRANSDUCER APPLICATIONS**

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Lead Barium Niobates has morphotropic phase boundary (MPB).when barium is

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partially substituted in place of lead. The maximum concentration that can be introduced is 0.4 in MPB system. The lead niobates belong to tungsten bronze structures and this type of ferroelectric materials are found to be technologically important for device applications due to their superior properties. The search for these properties in this family has stimulated much interest in a number of potential MPB system. This phase boundary occurs generally at nearby constant composition over a wide temperature range. Francombe had mentioned that a mixed phase of tetragonal and orthorhombic structures occurs at barium concentration of 0.375-0.475 it's a fact that the materials near MPB are more suitable towards piezoelectric application. The solid solutions of lead barium niobates are the most studied and developed morphotropic in Tungsten Bronze family. Rare earth doped lead barium niobates were synthesized by another technique hot pressing by Nagata. A rare earth modification leads to higher values of certain piezoelectric coefficients. The following rare earth doped lead barium niobate ceramics were prepared by conventional ceramic techniques, characterized by XRD and SEM. Material processing and characterization by XRD, SEM and measurements: The rare earth doped lead barium niobates were synthesized by using high pure oxides, through ceramic technique. The calcination temperature is fixed at 850 °C for 3 hours and sintering temperature is fixed at 1280 °C for 1 hour. A little care has been taken to avoid lead losses during sintering at high temperatures.

### **36. Template synthesis, spectral studies and antibacterial studies of tetraaza macrocyclic complexes of trivalent metal ions**

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**Keywords:** macrocyclic complexes, trivalent metal salts, template synthesis, magnetic measurements, infrared, electronic spectra

A new series of the complexes has been prepared by template condensation of dimedone and carbohydrazide in the methanolic medium forming the complexes of the type  $[M(TML)X]X_2$ ; where TML is a tetradentate macrocyclic ligand;  $M=Cr(III), Fe(III)$ ;  $X=Cl^-, NO_3^-, CH_3COO^-$ . The complexes have been characterized with the help of elemental analyses, conductance measurements, molecular weight determination, magnetic measurements, electronic, infrared and far infrared spectral studies. Molar conductance values indicate them to be 1:2 electrolytes. Electronic spectra along with magnetic moments suggest the five coordinate square pyramidal geometry for these complexes. The complexes were also tested for their *in vitro* antibacterial activity. Some of the complexes showed satisfactory antibacterial activity.

### **37. SYNTHESIS OF POLY (ACRYLATE-ACRYLIC ACID-CO-MALEIC ACID) HYDROGEL FOR REMOVAL OF HEAVY METAL IONS OF EFFLUENT WATER**

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**Key words: Hydrogels, acrylic acid, swelling, maleic acid, networks**

New methods are being developed to correct the imbalances of water system caused by effluents as removal of metal ions from sewage and industrial waste is posing a big problem. Super absorbing hydrogel i.e., cross linked hydrophilic polymer of three dimensional network having porous structure, were reported to be an effective material for the safe and convenient treatment of industrial effluents. The comparatively moderate cost and the ease of preparation make the hydrogels a promising candidature for the said application. Here we report a new hydrogel for removal of heavy metals. It is observed that the swelling ratio vary markedly with the amount of cross linker added. Swelling kinetics

in distilled water is shown to be non-Fickian. Heavy metals such as Zinc, Nickel, Lead and cadmium effectively removed by the hydrogel. Desorption of loaded hydrogel and its reuse also possible.

### 38. Microwave assisted synthesis, characterization and biological activities of metal complexes with tridentate Schiff bases

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**Key words:** Microwave, biological, tridentate, Schiff bases

A new series of cadmium complexes with general formula  $M(L)_2X_2$  L= (Z)-1-(1-benzyl-2,3-dihydro-8-methyl-1H-pyrido [3,2-b]indol-4(5H)-ylidene) semicarbazone and (Z)-1-(1-benzyl-2,3-dihydro-8-methyl-1H-pyrido[3,2-b]indol-4(5H)-ylidene)thiosemicarbazone have been prepared. These are characterized by elemental analysis, molar conductance measurement and molecular weight determinations. A spectral study (IR, <sup>1</sup>HNMR, UV-Vis and XRD) indicates coordination of azomethine nitrogen, and oxygen/ sulphur atoms with metal center. Bio-efficacy of the ligands and their complexes has been examined against the growth of bacteria *in vitro* to evaluate their antimicrobial potential.

### 39. DFT and QSAR Studies of Artemisinins: an *In Silico* approach for better antimalarial

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**Key words:** Antimalarial drug, artemisinin, DFT, reactivity parameters, QSAR

A comparative study on the structure and chemical reactivity of antimalarial drug, artemisinin and some of its selected derivatives were performed using density functional theory (DFT). DFT based global reactivity descriptors such as global softness and global electrophilicity calculated at the optimized geometries are used to investigate the usefulness of these descriptors for understanding the reactive nature of the molecules. Local descriptors, Fukui function and philicity values successfully describe the reactive sites of the molecules. Antimalarial activities of artemisinin derivatives were investigated by quantitative structure-activity relationship (QSAR) analysis using DFT based descriptors as well as some molecular mechanics (MM) parameters.

#### 40. Simple and efficient synthesis of imidazo [1, 2-a] pyridines using MgO in aqueous medium

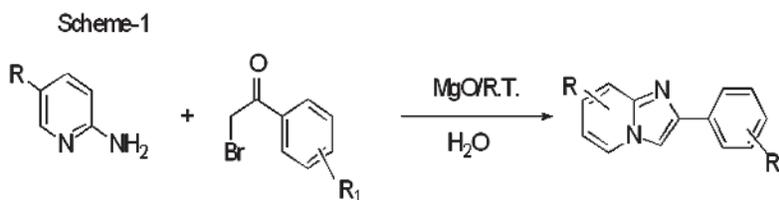
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**Keywords:** imidazo [1, 2-a] pyridines, MgO, aqueous medium

Various imidazo [1, 2-a] pyridines were synthesized from amino pyridines and aromatic phenacyl bromides by one step process in the presence of MgO in aqueous medium at room temperature. The salient feature of this method includes mild condition, short reaction time, high yield, easy purification and simple procedure.



R=H, Cl. R<sub>1</sub>=4-Cl, 4-Br, 4-NO<sub>2</sub>, 3-NO<sub>2</sub>, 4-OMe.

**41. Structural studies of complexes of 2- Mercaptobenzothiazole and 2-benzothiozoyl acetic acid with Palladium (II) and Platinum (II)**

**Rajnish Kumar Singh<sup>a</sup>, Krishna Mohan Singh<sup>b</sup>, Ashwani Kumar Singh<sup>c</sup>, Arun Kumar Yadav<sup>d</sup>, Ravindra Singh<sup>e</sup>, Shamshad Ahmad<sup>f</sup>, Naushad Alam<sup>g</sup>, Krishna Kumar Tinku<sup>h</sup>, Sanjay Kumar<sup>i</sup>, Irshad Ali<sup>j</sup>.**

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**Keywords:** - 2- Mercaptobenzothiazole, 2-benzothiozoyl acetic acid, Palladium (II), Platinum (II)

The complexes of Thiozole and benzothiozole derivatives are of immense interest due to their antibacterial, antifungal, herbicidal, pesticidal, antiviral, sedative, antihistaminic and anti-inflammatory properties. In the present communication the complexes of Pd(II) and Pt(II) with 2- mercaptobenzothiozole (MBtzH) and 2-mercapto benzothiozoyl acetic acid (BtaH) of composition  $[M(MBtzH)_2X_2]$  and  $[M(Bta)_2]$  (M= Pt(II) and Pd(II), X= Cl, Br, I) have been prepared and characterized by elemental analysis, molar conductance, magnetic susceptibility, infrared and electronic spectral studies. The electrical conductance values of complexes in dimethylformamide indicated nonionic character of almost all complexes of Pd(II) and Pt(II). The complexes were found to be diamagnetic suggesting their square planar geometry. The IR spectra of complexes indicated deprotonation of carboxyl acid group (COOH). The IR spectra of 2-mercaptobenzothiozole complexes  $[M(MBtz)_2]$  (M= Pd<sup>2+</sup> or Pt<sup>2+</sup>) indicated deprotonation of thiol SH and bonding through deprotonation of thiol 'SH' and benzothiozole ring nitrogen as well. In case of bis ligated dihalo complexes  $[M(MBtzH)_2X_2]$ , the ligand appears to be bonded through thione sulphur atom of 2-mercaptobenzothiozole as indicated by lowering of  $\nu(C=S)$  of ligand around 960-980 cm<sup>-1</sup> in infrared spectra.

**42. Stabilization of acrylamide based bicontinuous high internal phase emulsions and their polymerization for highly porous materials synthesis**

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**Keywords:** HIPEs, Hydrophilic polyHIPEs, morphology, highly porous mate

High internal phase emulsions (HIPEs) are concentrated emulsions which are used to template highly porous polymer materials synthesis. This work describes the synthesis of novel acrylamide (AAM) based polyHIPEs cross-linked with ethyleneglycol dimethacrylate (EGDMA). In the case of bicontinuous o/w HIPEs, the structural aspects of surfactant are important rather than their HLB value. Dielectric constant and Hildebrand solubility parameter have found to influence the HIPE stability rather than the dipole moment. The kinetically stable o/w HIPEs obtained in this work were polymerized by free radical thermal polymerization which yielded highly porous poly(AAM-co-EGDMA) polyHIPEs. The porous and physical characteristics of these polyHIPEs were conducted.

**43. Synthesis and characterization of Tamarind seed kernel polysaccharide-silica hybrids for sorption applications**

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**Keywords:** TKP, TEOS, Sol-gel, Silica, nano bio-composite, adsorption.

Tamarind (*Tamarindus indica L*) seed kernel polysaccharide (TKP) was reinforced by silica to produce its monolithic nanohybrids in a sol-gel reaction. Tetraethylorthosilicate (TEOS) was used as silica precursor and TKP served as template and porogen for the ensuing silica matrix. The nanohybrids were found photoluminescent and efficient in Hg(II) removal from solution. The ratio of various reactants (Polysaccharide: TEOS: H<sub>2</sub>O: EtOH) and reaction conditions were optimized to tailor the Hg(II) sorption by the material. The optimum sample was sintered to further enhance its properties. The nanohybrids have been characterized using Fourier Transform Infra-red spectroscopy (FTIR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Thermogravimetric Analysis (TGA), Differential Thermal Analysis (DTA) and Photoluminescence analysis (PL) and a mechanism for the sorption has been proposed.

#### **44. Fabrication of a novel CdS-pillared Zirconium-Titanium Phosphate (ZTP) for photodegradation of organic pollutants under solar light**

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**Keywords:** CdS-pillared zirconium-titanium phosphate; Methylene blue; Band gap energy; Leuco-methylene blue

With an attempt to extend the light absorption towards visible range and inhibit the rapid recombination of excited electrons and holes during photoreaction, new type of photocatalysts, cadmium sulfide pillared zirconium-titanium phosphate (CdS-ZTP) were synthesised by two step sulfurisation route. The photocatalysts were characterized by SAXS, DRUV-vis, PL, etc.. CdS pillaring has increased the photocatalytic efficiency of ZTP by three folds by increasing surface area, visible light sensitivity and decreasing band gap energy to 2.81 eV. 15CdS-ZTP showed the best photoactivity in the range of 70-94% and 64% towards the degradation of dyes and phenol in 180 min under solar light.

**45. Synthesis, Structural characterization and Solid-state Reaction kinetics of Co(II) and Cu(II)- Schiff base complexes**

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**Keywords:** Spectral, TGA, Co (II), Cu (II), Schiff-base 4-aminoacetophenon, 1-acetonaphthone and 2-imino-4-thiobiuret.

The coordination complexes of Co (II) and Cu (II) with the Schiff base derived from 4-aminoacetophenone and 1-acetonaphthone with 2-imino, 4-thiobiuret have been synthesized and characterized by micro analytical data, UV-vis, FT-ir and FAB mass spectral studies. FAB mass and thermal data show degradation of complexes. Synthesized complexes have been tested for the reactivity and substitution behavior. The thermal behavior of metal complexes shows that the hydrated complexes lose molecules of hydration first; followed by decomposition of ligand molecules in the subsequent steps. The activation thermodynamic parameters, such as activation energy ( $E^*$ ), pre-exponential factor ( $Z$ ), entropy of activation ( $DS^*$ ), enthalpy of activation ( $DH^*$ ) and Gibbs free energy ( $DG^*$ ) are calculated with the help of TG, DTA and DTG curves using Coats–Redfern (C-R) method.

**46. Design and Development of Vanadium Phosphate Materials towards Liquid Phase Reactions**

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**Key words:** Esterification; Vanadium phosphate; Acetic acid; n-butyl acetate

Novel aluminium promoted vanadium phosphate (Al-VPO) catalyst has been synthesized. The catalysts were unambiguously characterized by N<sub>2</sub> adsorption-desorption, XRD, FT-IR techniques, UV-vis DRS and the total amount of the acidity of the catalysts was estimated by NH<sub>3</sub>-TPD. The catalytic activities were checked in the heterogeneous catalytic esterification of acetic acid with n-Butanol in a solvent free medium. The optimization of reaction was carried out by varying temperature from 75°C-150°C, molar ratio (butanol: acetic acid) from 1:1-1:4. Under optimum conditions, the catalytic esterification runs revealed a significant effect of the vanadium phosphate giving 62% conversion with 100% selectivity to butyl acetate.

#### **47. VISIBLE-LIGHT DRIVEN Gd<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>/GdCrO<sub>3</sub> COMPOSITE FOR HYDROGEN EVOLUTION**

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**Key words:** Photocatalyst, water splitting, composites, photocurrent measurements

A series of Gd<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>/GdCrO<sub>3</sub> composites are prepared by solid state combustion method using Gd (NO<sub>3</sub>)<sub>3</sub>, TiO<sub>2</sub>, Cr<sub>2</sub>O<sub>3</sub> as metal source and urea as a fuel. The composites are characterized by X-ray diffraction, UV–Visible diffuse reflectance spectra, Brunauer-Emmett-Teller (BET) surface area measurement, photoluminescence spectra, X-ray photoelectron spectroscopic studies, photocurrent measurement etc. The photocatalytic activity of the composites is examined towards hydrogen production without using any co-catalyst under visible light illumination. The rate of formation of hydrogen is measured by the photocatalytic activity measurement device and gas chromatography. The highest efficiency is observed over the composite GTC (Cr:Gd:Ti=1:1:1). On the basis of photocurrent measurement and PL, the mechanism of enhanced photocatalytic activity has been discussed.

- 48. Mixed – ligand complexes of Cu<sup>2+</sup>, Ni<sup>2+</sup>, Co<sup>2+</sup>, Zn<sup>2+</sup> with 2,2' Bipyridine as a primary ligand and L-2-amino-3-imidazolyl propionic acid as secondary ligand.**

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**Keywords:** - formation constants, mixed ligand, L-Histidine, 2,2' Bipyridine

Modified form of Irving Rossotti titration technique has been applied to study the formation constants of mixed ligand complexes of the type MAL where M = Cu<sup>2+</sup>, Ni<sup>2+</sup>, Co<sup>2+</sup>, Zn<sup>2+</sup>; A = Bipyridyl and L = L-2-amino-3-imidazolyl propionic acid(L-Histidine) at 30°C (μ=0.1M). The values of the formation constants obtained in the mixed ligand system are little less than first formation constant of M-L simple systems.

- 49. Cationic cobaltamines as anion receptors: synthesis, spectroscopic characterization and crystal structure of cis-diazidobis (ethylenediamine) cobalt (III) C<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>5</sub>-**

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**Keywords:** Cobalt (III), second sphere coordination, supramolecular chemistry, spectroscopy, hydrogen bonding, anion receptor.

Crystals of [*cis*-Co(en)<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>](C<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>5</sub>) have been obtained by slowly mixing

the separately dissolved *cis*-diazidobis(ethylenediamine)cobalt(III) nitrate and 2,4-dinitrophenolate, in aqueous medium in 1:3 molar ratios. Elemental analysis and spectroscopic techniques (IR, UV/vis,  $^1\text{H}$  and  $^{13}\text{C}$  NMR) were employed for the characterization of the complex salts. Single crystal X-ray structure determinations showed that the new complex salt crystallizes in the orthorhombic space group *Pbca* with  $a = 8.8263(6)$   $b = 12.0292(7)$   $c = 33.339(2)$  Å,  $V = 3539.7(4)$  Å<sup>3</sup>,  $Z = 8$ ,  $R = 0.0447$ . Supramolecular assemblies *via* hydrogen bonding network between the anionic groups and the  $\text{NH}_2$  groups of the coordinated ethylenediamine molecules, involving second-sphere coordination have been observed.

#### 50. **Destruction of Resinous compounds by use of Natural Enzymes from waste paper**

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*Scientist and Research Analyst*

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**Keywords:** Resinous compound, Ginger, Onion, Garlic, Waste paper, pH, Temperature

Resinous compound like urea formaldehyde resins, melamine formaldehyde resins, starch, coated resins are present in waste papers. It is very difficult to remove these resins from waste papers. In these experiment natural enzymes of Ginger, Onion & Garlic have been used to destroy resins.

Waste paper containing high resinous compounds has been treated with the different combination of ginger, garlic & onion extract ratios, by maintaining pH & temperature of reactions. As resins generally dissolved in highly polar solvent so energy increases due to increase in their ionization power, hence they are able to break bonds the strong bonding between resin and paper.

**51. EXPERIMENTAL INVESTIGATION OF CONTROL OF NO<sub>x</sub> EMISSIONS IN DIESEL-FUELED COMPRESSION IGNITION ENGINE**

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Diesel fueled engines produce less carbon monoxide (CO), unburned hydrocarbon (HC), and particulate emissions but with higher NO<sub>x</sub> emissions. Exhaust Gas recirculation (EGR) is effective to reduce NO<sub>x</sub> from diesel engines because it lowers the flame temperature and the oxygen concentration in the combustion chamber. However, EGR results in higher particulate matter (PM) emissions. Thus the drawback of higher NO<sub>x</sub> emissions while using diesel may be overcome by employing EGR.

The objective of this project work is to investigate the usage of diesel and EGR Simultaneously in order to reduce the emissions of all regulated pollutants from diesel engines. A single cylinder, water cooled, high speed direct injection diesel engine was used for experiments. HCs, NO<sub>x</sub>, CO and smoke opacity of exhaust gas were measured to estimate the emissions.

Various engine performance parameters such as brake thermal efficiency, brake specific fuel consumptions (BSFC), and brake specific energy consumptions (BSEC), etc were calculated from the acquired data.

The experimental results show that EGR with diesel resulted in reductions in NO<sub>x</sub> emissions without affecting any performance and slightly increased in smoke opacity. 15% of EGR gives better performance in terms of NO<sub>x</sub> and smoke compared to 11%, 23% and 30% of EGR.

**52. “THE STUDY OF Pb & Cd CONTAMINATION IN SOIL OF WATER BODIES AROUND BALCO CITY, DISTRICT – KORBA (C.G.)”**

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The sediment of water bodies in around the Balco city contain toxic element Pb & Cd. Belgiri Nallah and Dengur Nallah both are important water body system of Balco city of Korba District. Belgiri Nallah passes through Village - Belakshar, Neharu Nagar, Parsabhatha, Belgiri Basti, Rumgara and Dengur Nallah passes - Bhadrpara, Lalghat & Kohdiya. Both are spread about 10-12 Km distance in around the Balco city and ultimately joined with Hasdeo River. Hasdeo River is the main water body system of Korba – District. Various industries situated near at Belgiri Nallah & Dhengur Nallah. Plant effluents discharge in these water body system, many compounds settle in surface of soil of water bodies.

In the present paper deals with the contamination of  $Pb^{2+}$  &  $Cd^{2+}$  ions in the sediment of water body system. These are important toxic ions. Normal erythrocytes have defense system against the oxidative stress in the cell. The most important of them is the hexose monophosphate shunt Glucose 6-phosphate dehydrogenase is first enzyme of this metabolic path-way. This enzyme has multiple sulphhydryl groups. These toxic elements form mercaptides with sulphhydryl groups. Resulting in the loss of enzymatic activity. Excessive daily dose of  $Pb^{2+}$  &  $Cd^{2+}$  ion in the body, exchanges with  $Zn^{2+}$  ion in the enzymatic system. Resultant loss of enzymatic activity. The study was carried out during May 2009 to April 2010. In present investigation is to assess whether  $Pb^{2+}$  and  $Cd^{2+}$  ion contamination in soil of water body increases or not and compare to WHO limits.

**53. THERMODYNAMICS OF BINARY ALLOYS OF  
PHARMACEUTICAL ACTIVE IMIDAZOLE WITH o -  
PHENYLENEDIAMINE**

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**Keywords:** Phase diagram, Partial and integral thermodynamic functions, activity, and activity co-efficient.

The present study describes the investigation of entectic and non-eutectic alloys of imidazole (IM) with o - Phenylenediamine (OPD). the solid-liquid equilibrium (SLE) data determined by the melt method in the form of melting temperature with their corresponding composition construct the solid-liquid equilibrium phase diagram which suggest simple eutectic behaviour is followed by the binary system. The activity co-efficient model based on enthalpy of fusion was employed to calculate the partial and integral thermodynamic functions such as  $g^E$ ,  $h^E$  and  $s^E$ . These values help to predict the nature of molecular interaction, ordering and stability between the components. The spontaneity of mixing of eutectic and non eutectic alloys was discussed by the partial and integral mixing quantities  $DG^M$ ,  $DS^M$  &  $DH^M$ . Using Gibbs-Duhem equation the solution of partial molar heat of mixing, activity and activity co-efficient of the component in the binary mix have been resolved.

**54. SPECTROPHOTOMETRIC MICRODETERMINATION OF DYSPROSIUM (III) AND HOLMIUM (III) WITH CHROME AZUROL-S IN PRESENCE OF CETYLPYRIDINIUM BROMIDE**

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**Keywords:** Spectrophotometric, chrome azurol-S (CAS), Cetylpyridinium bromide (CPB), Dysprosium (Dy), Holmium (Ho).

With the growing applications of lanthanoids in science and technology, the study of coordination compounds of these elements has received great attention. A large number of chromogenic reagents form soluble colored complexes with rare earths. Chrome azurol-S has been reported to form green colored complexes with rare earths and has been used for microdetermination of these metal ions. The addition of cationic surfactant, cetylpyridinium bromide (CPB), sensitizes the color reactions of Dy(III) and Ho(III) with chrome azurol-S. The formation of a water soluble ternary complex of stoichiometric ratio 2:1:2 (e.g. Dy(III) - R - CPB) is responsible for the observed enhancement in molar absorptivity at shifted wavelength, when a surfactant is present. The ternary complexes exhibit absorption maxima at 632nm with a bathochromic shift of about 88nm. Beer's Law obeyed between 0.2 to 6.40ppm. Effective photometric range and molar absorptivity of these ternary complexes have been calculated. The optimum reaction conditions and other analytical parameters were evaluated. The effects of interfering ions on determination of both the metal ions were studied. A simple, rapid and highly sensitive method for the determination of Dy (III) and Ho (III) with chrome azurol-S is proposed

**55. “REFRACTOMETRIC INVESTIGATIONS OF SYMETRICAL TRIZINO THIOCARBAMIDES IN AQUOUS DIOXANE”**

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**Keywords :-** 1-(4-Hydroxy-6-methyl)-s-triazino-3-phenylthiocarbamides (L<sub>1</sub>), 1-(4-Hydroxy-6-methyl)-s-triazino-3-ethylthiocarbamide (L<sub>2</sub>), 1-(4-Hydroxy-6-methyl)-s-triazino-3-methylthiocarbamide (L<sub>3</sub>), Dioxane-Water percentage composition, Refractrometry study.

Refractrometric measurements of recently synthesized drugs viz. 1-(4-Hydroxy-6-methyl)-s-triazino-3-phenylthiocarbamide (L<sub>1</sub>), 1-(4-Hydroxy-6-methyl)-s-triazino-3-ethylthiocarbamide (L<sub>2</sub>), 1-(4-Hydroxy-6-methyl)-s-triazino-3-methylthiocarbamide (L<sub>3</sub>) were carried out at different percentage composition of solvent to investigate effects of structure, groups on s-triazino thiocarbamides. The data and the results obtained during these investigations gave detail information regarding drug absorption, transmissions activity and effect of these drugs. Taking all these things in to consideration this research work was carried out

**56. Studies on some novel hetero binuclear Schiff base complexes of Cu<sup>II</sup> and Ni<sup>II</sup> with organic chelates of Ag<sup>I</sup>**

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**Key words:** Schiff base, heterobinuclear complexes, IR spectra, UV-Vis spectra.

#### *Section IV: Chemical Sciences*

A series of novel hetero binuclear complexes of Cu<sup>II</sup> and Ni<sup>II</sup> with Schiff base derived from condensation of salicylaldehyde and ethylenediamine have been synthesized. These complexes have been characterized by elemental analysis, electronic and IR spectral analysis and molar conductance measurements. The IR spectra suggest that the bonding between Cu<sup>II</sup> or Ni<sup>II</sup> metal chelate and silver metal to be dative in nature which bonds via phenolic C–O bond. Low value of molar conductance suggest for their non-electrolytic nature.

### **57. Simple and Rapid Spectrophotometric Determination of Metal Ions**

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**Key words:** - Simple, Hydroxamic acid and Rapid

Simple spectrophotometric methods have been developed for the determination of trace amounts of metals (Fe, Mn and Cr) by using N-substituted Hydroxamic acid. The metal ions give colored complexes with Hydroxamic acid. The complexes show maximum absorption in the visible range. Beer's law is also obeyed and major cations and anions do not interfere. The developed method has been successfully applied for analysis of metals in water samples of selected areas of Bhopal city.

Rapidity of color development with hydroxamic acid is an advantage in analyzing various water samples. Use of cost effective chemicals is an added advantage to the proposed method.

**58. Microgram Determination of o-Anisidine Based on its Manganese (II) Catalyzed Oxidation by Periodate ion.**

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**Key words:** - Microgram Estimation, o-anisidine, Mn catalysed, periodate oxidation.

The Mn (II) catalysed periodate oxidation of o-anisidine in acetone-water medium is first order with respect to catalyst, substrate and oxidant each. The progress of reaction was followed by monitoring the increase in the absorbance of reaction intermediate. The main reaction product characterized on the basis of melting point and spectroscopic studies, is methoxy-1, 4=benzoquinone. The effect of pH, dielectric constant of medium, ionic strength and free radical scavengers was studied to develop the conditions for microgram determination of o-anisidine in the range 2.463-924.8565 µg/ml. The characteristics of various calibration curves, percentage recovery, effect of interferences and correlation coefficient have been evaluated. An attempt has been made for proposing a suitable mechanism for the reaction studied. Thermodynamic parameters are also reported.

**59. Structural aspects of Complexes of Isatin morpholin-N-thihydrazone with Pd (II) and Pt (II)**

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**Key words:-** Isatin morpholin-N-thihydrazone, Pd(II) Pt(II)

The complexes of Isatin and its derivatives are of immense interest due to their potential application in analytical, medicinal and pharmaceutical fields. It is established that some Isatin derivatives show anti-HIV activity. In view of above a multidentate Schiff base has been synthesized and its complexes are reported in present communication. The Schiff base has been derived by condensation of Isatin and morpholin-N-thiohydrazone ( $C_{13}H_{14}N_4O_2S = HIstmth$ ). The complexes of Schiff base with Pd (II) and Pt (II), having composition  $[M (HIstmth) Cl_2]$  and  $[M (HIstmth)_2]$  have been prepared and characterized. The dichloro complexes  $[Pd (HIstmth) Cl_2]$  and  $[Pt (HIstmth) Cl_2]$  were obtained in acidic medium where ligand coordinates as neutral bidentate chelating molecule. The ligand gets deprotonated in neutral or basic medium and formed bis chelated inner complexes  $[M (Istmth)_2]$  ( $M = Pd^{II} \& Pt^{II}$ ). The complexes are all diamagnetic and qualitatively have been found to be non conducting in DMF. The UV spectra of complexes showed very strong absorption below 430nm. The diamagnetism and ligand to metal ratio indicated four coordinated planar structure to the both Pd (II) & Pt(II) complexes. The IR spectra of ligand and complexes showed uncoordinated nature of isatin carbonyl group. ( $\delta_{CO} - 1680 - 1690 \text{ cm}^{-1}$ ). The IR spectral study indicated bidentate coordination of ligand as neutral molecule in  $[M (HIstmth) Cl_2]$  and as anionic deprotonated chelating molecule in  $[M (HIstmth)_2]$ .

**60. Studies on dinuclear Complexes of Ni<sup>II</sup> and Cu<sup>II</sup> metal ions with some N, N, N, O donor ligands**

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**Key words:** -2-aminobenzothiazole/2-carboxybenzothiazole/IR/UV/ Magnetic moment

Some tetradentate ligands HL were synthesized by the condensation of 2-aminobenzothiazole derivative with 2-carboxy benzothiazole by the methods reported in literature. The dimeric complexes of Ni (II) and Cu (II) with these ligands were synthesized, structurally characterized on the basis of electronic and IR absorption properties and magnetic properties. The composition of metal complexes were found as  $[M_2L(CH_3COO)_2Cl(H_2O)_3]$ . Analysis shows that after deprotonation HL behaves as tetradentate ligand by N,N-coordination with one metal ion and N,O coordination with another metal ion. The structural studies of complexes revealed that each metal ion is hexacoordinated. While the coordination position of one metal ion is satisfied by N,N atoms of ligand and two acetate ions, the coordination position of another metal ion is satisfied by N,O atoms of ligand, three water molecules and one Cl ion. The electronic absorption bands, IR-bands and magnetic moment data were interpreted.

**61. Synthesis, spectral and antimicrobial activity of mixed ligand complexes of Co<sup>II</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup> with N, O and S donor ligands**

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**Keywords:** -Synthesis, spectral, antimicrobial, mixed ligand complexes.

#### Section IV: Chemical Sciences

Mixed ligand complexes of bivalent metal ions, viz:  $\text{Co}^{\text{II}}$ ,  $\text{Ni}^{\text{II}}$ ,  $\text{Cu}^{\text{II}}$  and  $\text{Zn}^{\text{II}}$  of the composition  $(\text{ML}_1\text{L}_2)$  in 1:1:1 molar ratio, (where  $\text{L}_1$ =diphenylamine-2-mercapto-2'-carboxylic acid (DPMC) and  $\text{L}_2$ =2-furyl glyoxal-anthranilic acid (FGAA) have been synthesized and characterized by repeated melting point determination, elemental analyses, IR,  $^1\text{H-NMR}$ , magnetic susceptibilities measurements and electronic spectral data. The synthesized ligands and their metal complexes were screened for their antimicrobial activity against two bacteria *Staphylococcus aureus* (gram +ve) and *Escherichia coli* (gram -ve) and two fungi *Apergillus Niger* and *Apergillus flavus* by Serial Dilution Method. Metal complexes exhibited more activity than their ligands.

### **62. PH Metric Study of Complexes of Copbalt (II), Copper (II), Aluminum (III) and Iron (III) with 2- Hydroxy – 5- Chloro Phenyl Chalcone in 70% DME – Water**

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**Key words:** -Metal Complexes, Chalcone, Stability Constants

The pH Metric technique has been for determination of stability constants of complexes of Cobalt (II) Copper (II), Aluminum (III) With 2-Hydroxy – 5- chloro phenyl chalcone in 70% DME – Water at constant ionic strength (0.1M) and constant temperature  $30 \pm 0.1^\circ \text{C}$  The PH metric data obtained have used to determine the values of proton-ligand and metal – ligans stability constants using Lrving-Rossotti's expression.

**63. STUDY OF BAND STRUCTURE OF ENERGY OF LIQUID ALKALIMETALS (Li, Na, K, Rb, &Cs)**

**Amar Nath Choushary**

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**Key words:** Band Structures, Ionic Co-ordinate, Fermi surface

Band structure of energy of liquid alkali metals has been presented. In the structure of the theory the important in gradients are the form factors and the structure factors, As the approach rests heavily on the assumption that the potential is considerable weak. The alkali metals have been favourite of theoretical account of their simple free surface measurements. The discrepancy in the computed results can also be attributed to the neglect of various harmonic effects such as multiphonon processes and partially due to magnitude of form factors and energy wave number characteristics. The various properties can be evaluated from total energy depending on ionic co-ordinate.

**64. Synthesis and Characterization of Diaminoalkyl Polysiloxane Nano Emulsion for Water Repellent Finishing of Cotton Fabric**

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**Keywords:** -Synthesis, diaminoalkyl polysiloxane, cotton fabric, water repellent

Diaminoalkyl polysiloxane (DAAPS) has been synthesized using ring opening polymerization and characterized by analyzing FTIR and <sup>1</sup>H NMR spectra. The nano emulsion of DAAPS has been applied on to cotton fabric by a pad-dry-cure technique at different concentrations (5-25gpl) with 70% expression at padding. The results showed that the treatments of nano emulsion of DAAPS not only improved the water repellency but also influenced the tensile strength of the fabric sample positively without hampering the comfort properties with respect to air permeability and bending length. No significant change in water repellency was observed even after continuous rubbing with skin simulating friction partner under significant load. The treatment was found to enhance the colour depth and fastness properties of cotton samples dyed with direct dye.

**65. MANGANESE (II) CATALYZED PERIODATE OXIDATION OF 2, 3-DIMETHYLANILINE IN ACETONE-WATER MEDIUM—A KINETIC AND MECHANISTIC STUDY**

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**Key words:** Periodate oxidation, 2, 3-dimethylaniline, Kinetics and mechanism

The Mn (II) catalysed reaction between 2, 3-dimethylaniline (AMX) and periodate ion in acetone-water medium Rate of reaction decreases on increasing the ionic strength and decreasing the dielectric constant of the medium. Free radical scavengers do not affect the reaction rate. One mol of AMX reacts with two moles of periodate during the initial part of reaction. Results of kinetic studies under pseudo first order conditions,  $[\text{IO}_4^-] \gg [\text{AMX}]$ , are in agreement with the rate law:  $d[\text{C}]/dt = kK_3K_4K_w[\text{Mn}^{\text{II}}] [\text{S}] [\text{IO}_4^-]_0 [\text{H}^+] / \{K_2 K_w + (K_w + K_b K_2)[\text{H}^+] + K_b [\text{H}^+]^2\}$  where  $kK_3K_4$  is the empirical composite rate constant,  $K_w$  is ionic product of water,  $K_2$  is acid dissociation constant of  $\text{H}_4\text{IO}_6^-$  and  $K_b$  is base dissociation constant of TOL.  $[\text{S}]$  is the concentration of AMX and  $[\text{IO}_4^-]_0$  represents the concentration of periodate which has been taken in excess. The  $1/k_{\text{obs}}$  versus  $[\text{H}^+]$  profile passes through the minimum. The reaction products were subjected to solvent extraction, TLC, melting point, and spectroscopic studies and characterized as 2,3-dimethyl-*p*-benzoquinone. The values of thermodynamic parameters are:  $E_a = 5.16 \text{ kcal mol}^{-1}$ ,  $A = 4.19 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ;  $S^\ddagger = -37.44 \text{ cal mol}^{-1} \text{ K}^{-1}$ ,  $G^\ddagger = 16.17 \text{ kcal mol}^{-1}$  and  $H^\ddagger = 4.54 \text{ kcal mol}^{-1}$ . Suitable mechanism has been proposed.

**66. Synthesis, characterization antimicrobial activity studies of some transition metal complexes derived from 5-chloro-N<sup>1</sup>- ((2-mercaptoquinolione-3yl) methylene) -3-phenyl -1H- indole – 2 earbohydrazide**

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**Key words:** Schiff base, Metal complexes and antimicrobial activity

A series of new coordination complexes of Fe (III), Co (II), Zn (II) and Cd (II), with Schiff base 5-chloro N<sup>1</sup>-((2-mercaptoquinolione-3yl) methylene) -3-phenyl -1H- indole – 2 earbohydrazide have been synthesized and characterized by elemental analysis, IR spectra, NMR spectra, mass spectra, TGA and powder X- ray diffraction data. The Schiff base behaves as tridentate ONS – donor ligand and forms the complexes of the type ML<sub>2</sub> – stoichiometry in case of Fe(III) Co,(II), Ni(II), Nz(II), Cd(II). All the complexes exhibited octahedral geometry. The ligand and its complexes have been screened for their antibacterial and antifungal activity against S. aureus, P. aureus and A. Niger and A. flavus, respectively.

**67. Estimation of Glucose from Blood/Serum Sample**

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**Key words :-** Estimation, blood, serum, diabetic patient

Many excellent methods are available for the estimation of glucose in blood/blood serum. To carry out this program of estimating glucose in diabetic patient the new method is described here. The chemical method by using o-toluidine which is based upon the spectrophotometric analysis which gives the quantitative determination of glucose from blood/blood serum.

## **68. Synthesis and Characterization of Layered Double Hydroxides**

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**Key words:** -Mg (II) Al-NO<sub>3</sub>-, Zn (II) Al-NO<sub>3</sub>, XRD, SEM, TG, analysis

Layered Double Hydroxides (LDH) of various elements like Mg (II) Al-NO<sub>3</sub> and Zn(II) Al-NO<sub>3</sub> have been prepared by co-precipitation method. They have been characterized by elemental analysis, power X-ray diffraction. FTIR spectroscopy, TG-DTG and scanning electron microscopy. The X-ray analysis showed that both the cations (M<sup>2+</sup> and M<sup>3+</sup>) were located in same layer and only carbonates and water are present in interlayer. H-NMR studies revealed that water and carbonates are perpendicular to the layer. TGA analysis indicated formation of stable Mg-Al and Zn-Al metal oxides at 750<sup>0</sup>C. Various stoichiometric conditions have also been used for the synthesis of compounds.

## 69. MAGNETIC NAD SPECTROSCOPIC CHARACTERIZATION OF SOME COPPER (II) COMPLEXES

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**Key words:** - Square pyramidal, tetragonally distorted octahedral

1- (Phenylazo)-2 naphthol (PANH) has three potential donor sites and thus it acts as a very good chelating agent. This ligand has been used for complexation with Cu(II) ions to synthesize the complexes of general formula  $[Cu(PAN)_2L]$  where L = secondary ligands like pyridine, picoline,  $H_2O$  and  $n=O$ , a and 2. These complexes have been characterized by their elemental analysis, conductivity measurement & magnetic moment & at room temperature, infrared and electronic spectra. The ligand PANH is found to be co-ordinated through deprotonated phenolic oxygen and azonitrogen forming a six membered chelate with two conjugate  $\pi$ -bonds in chelate ring. The magnetic moment values reveal the mononuclear nature of the complexes while their electronic spectra reveal the square planar geometry of the complexes  $Cu(PAN)_2$  while  $[Cu(PAN)_2L]$  and  $[Cu(PAN)_2L_2]$  are found to be square pyramidal and tetragonally distorted octahedral, respectively

## 70. Spectroscopical and biochemical aspects of complexes of Co (III) with mixed ligands biguanide $C_2H_7N_5$ and pyridine $C_5H_7N$

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Complexes of transition metal cobalt with oxidation state III with mixed ligands

biguanide and pyridine had been prepared so far and its elemental studies were studied. In this research paper, an effort is made in order to characterize their spectroscopic characters and unravels the hidden truth behind its biochemical properties. The blue prints of the structure of the coordination complexes which were prepared are illustrated with the help of UV & IR spectroscopical data. The antifungal properties of the complexes have been studied in PDA and SDA medium against two fungus *Aspergillus niger* & *Aspergillus versicolor* which has showed a good response.

**71. “SYNTHESIS AND CHARACTERISATION OF SOME VO (IV) COMPLEXES WITH BIOLOGICALLY ACTIVE LIGANDS”**

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**Key words:** Carbazone Complexes: IR and e.s.r spectra

Carbazones and hydrazones are known to be biologically active compound. The structural aspects of transition metal complexes of carbazones and hydrazones are correlated to their biological activities. In the present paper we report the structural aspects of complexes of VO(IV) with 2-formylpyridine semicarbazone (FPS), 2-acetylpyridine semicarbazone (APS), 2-formylpyridine thiosemicarbazone (FPTS) and 2-acetylpyridine thiosemicarbazone (APTS) on the basis of their IR, electronic and e.s.r spectra.

**72. Binuclear complexes of Cu (II) and Ni (II) Schiff base of Salicylaldehyde and 1, 2- propylenediamine with alkaline Earth metal salts of some organic acids**

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**Keywords:** Binuclear complexes, Schiff base, Salicylaldehyde, 1, 2- Propylenediamine, Infrared spectra

A number of stable binuclear complexes of Cu(II) or Ni(II) Schiff base of salicylaldehyde and 1,2- propylenediamine with alkaline earth metal salts of some organic acids of general formula  $[MaPS.MbL_2]$  Where  $Ma = Cu (II) \text{ or } Ni(II)$ ,  $Ps = n,n'-1,2$  propylene-bis (Salicylaldimine),  $Mb = Mg, Ca, Sr \text{ or } Ba$ ,  $L =$  deprotonated o-nitrophenol (ONO), (2,4-dinitrophenol (DNP), 2,4,6-trinitrophenol (INP) or 1-nitroso-2-naphthol (1N2N) have been synthesized and characterized by elemental analyses infrared, electronic absorption spectral data, conductivity and magnetic moment measurements IR spectral data confirm the coordination of oxygen atom of phenolic group and nitrogen atom of –NO, –NO<sub>2</sub>, etc. to alkaline earth metals values suggest the square planar structure of Ni<sup>2+</sup> for metal chelates as well as binuclear complexes. The compounds are tested against one Gram +ve bacteria (S. aureus) Gram- ve bacteria (E.coli) and fungi (C.albicans).

**73. EFFECT OF VARIATION ON AXIAL LIGANDS ON DISTORTION FROM OCTAHEDRAL SYMMETRY**

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**Keywords:** - Anisotropic g values, Polycrystalline ESR spectra

In this work we present the investigation of the influence of the variation of axial legends on the distortion of distortion of symmetry from octahedron. Complexes of general formula  $ML_2X_2$  (where L= Vanillin semicarbazone (VSCH) and X =Cl CH<sub>3</sub> COO and NO<sub>3</sub> and M = V(II), Mn(II) and Cu(II) have been prepared and they have been characterized by their elemental analyses, conductivity, i.r. Spectra magnetic moment electronic neutral bidentate one, co-ordinationg through N and Oxygen atoms forming five memebred chelate ring All the complexes are found to be tetragon ally distorted Dq. (ax) forV(II) complexes are 819.76-833 cm<sup>-1</sup> minimum for Cl. and maximum for NO-3 ligands along z-axis Dt values are for Cl- complex indicating grater distortion when Cl. occupations. The values of Racah Parameters B and C for Mn(II) complexes are 753-764cm<sup>-1</sup> and 3075-3312 cm<sup>1</sup> respectively Cu.(II) complexes show strong tetragonal distortion with Dt Values 546 to 594 cm<sup>-1</sup> due to strong Jahn –Teller effect in d<sup>9</sup> system The g<sup>II</sup> & g<sup>I</sup> values of V(II) complexes are 2.0018-2.0021and 2.0004-2.0007 respectively with G>4. for Mu (II) complexes g<sup>I</sup> & g<sup>II</sup> values are 2.0556-2.0681 and 2.2624-2.2754 respectively. For Cu(II) complexes g<sup>I</sup> & g<sup>II</sup> values are 1.972-1.980 and 1.969-1.978. The greater values of G than 4 in all the complexes are indicative of negligible or no exchange interaction among the parameters and esr tensors favour tetragonal distortion in all the complexes.

**74. Synthesis Structural Elucidation and Antimicrobial Studies of Chromium (III) and Ruthenium (III) Complexes with Schiff Bases Derived From Isatin and Various Sulpha Drugs**

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**Key words:** Metal Chelates Schiff bases, spectroscopic studies biological activity

The syntheses and spectral characterization of the chromium (III) and ruthenium(III) complexes of the formula  $[M(L)_2(H_2O)_2] Cl$  where  $M=Cr(III)$  and  $Ru(III)$   $LH =$  Schiff bases derived from isatin and series of various sulpha drugs [viz. sulphanilamide (ISHAH), sulphamerazine, (ISHMH), Sulphaguanidine (ISHGH), sulphadiazine [ISHAH] sulphacetamide (ISHACH) and sulphapyridine (ISHPH) on the basis of elemental analyses, molar conductance, magnetic susceptibility, electronic and infrared studies it can be concluded that the LH act as a monomeric bidentate O,N donor towards the studied metal ions. The complexes are monomeric and their geometry is octahedral. The ligands and their metal complexes have been screened in vitro for antibacterial (*Bacillus subtilis* and *Escherichia coli*) and antifungal (*Aspergillus Niger*, *Aspergillus alternate* and *Helminthosporium oryzae*) activities. The activities. have been correlated with the structures of the compounds.

**75. STUDIES ON SCHIFF BASE COMPLEXES OF SN (II) AS ANTIMICROBIAL AGENTS**

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*Institute of Basic Science & khandari Agra*

**Key words:** Schiff – bases, I.R. spectral biocidal studies

Metal chelates of hydroxy benzalidine anhrtranillic acid and 2- hydroxy benzalidine – o – aminothiophenol and 2 – hydroxy benzalidine – o- aminophenol and with Tin (II) have been prepared and characterized by their elemental analyses T.L.C. and I.R. spectral studies All the synthesized ligands and their metal chelates were screened for their anti-bacterial properties against the bacteria Staphylococcus aureus (gram+ve) and E. Coli (gram-ve) bacteria and two common fungi (Aspergillus niger and Candida albicans) A comparative study of biocidal activities of metal complexes and ligands indicate an enhanced activity of the ligand in the form of their metal complex.

**76. ANALYSIS OF VARIOUS GROUND WATER QUALITY PARAMETERS OF MALPURA TEHSIL OF TONK DISTRICT. RAJASTHAN, INDIA**

**Girja Shanker Tailor and C.P. Singh chandel**

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**Key words:-** USSL diagram, Piper trilinear diagram, Ground water Chemical indices, Hydro Chemical facies

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To evaluate the major suitability of water for drinking irrigation and domestic use, the chemical characteristics of groundwater in Malpura Tehsil (Tonk district, Rajasthan) have been investigated and evaluated. Water samples from hand pumps, open wells and bore wells were collected during monsoon season 2010 and analyzed for major cations ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ) and major anions ( $\text{Cl}^-$ ,  $\text{F}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ). To understand the water quality and utilitarian aspects of ground water, chemical indices like %Na, RSC, SAR, piper trilinear diagram and USSI diagram were calculated based on the analytical results. According to EC and SAR calculation the dominant classes C2S1, C3S1, C3S2, C3S3, C4S3, and C4S3 were found. On the basis of hydro chemical facies the water in the study area is  $\text{Na}^+$ ,  $\text{K}^+$ -Cl –  $\text{SO}_4^{2-}$  typed.

#### **77. Micro determination of furosemide pure & some of its pharmaceutical Preparations with CE (IV) reagent.**

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**Key words:** Determination, furosemide, CE (IV) Micro methods

A new method has been developed for the micro determination of furosemide pure and some of its pharmaceutical preparations by using Ce(IV) reagent as oxidant. The method is simple accurate, sensitive and gives reproducible results within  $\pm 1\%$  error. Effects of different variables have been studied and SD & CV calculated. Recovery experiment is carried out by standard drug addition method. A probable reaction mechanism has also been suggested. Interference of various ions had been studied.

**78. XAFS Investigations of same binuclear copper (II) Schiff base complexes**

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**Key words:** Cu (II) complexes. Salen; salophen; Cu K-EXANES; XANES; theoretical model

X-ray absorption fine structure (XAFS) have been investigated at the K<sub>edge</sub> of copper in some binuclear copper(II) salen/salophen complexes: [Cu(salen)]<sub>2</sub> (1), [Cu(salen)CuCl<sub>1</sub>]H<sub>2</sub>O (2) [Cu(salophen)]<sub>2</sub> [Cu(salophen)]<sub>2</sub> (3) and pCu(salophen)CuCl<sub>2</sub>] (4) (where salen = N,N = ethylenebis(salicylideneiminato) dianion and salophen = N,N'-o- phenylenediaminebis (salicylideneiminato) dianion and salophen – N,N'-o- phenylenediaminebis(salicylideneiminato) dianion) Crystallographic data is available for 1 and it has been used to generate the theoretical model, which has been fitted to the experimental extended X-ray absorption fine structure (EXAFS) data of 1 to obtain the structural parameters, which include bond-lengths, coordination numbers and thermal disorders. The results obtained have been found to be comparable with the crystallographic results. The same theoretical model which was generated for 1 has been used as standard to fit the experimental EXAFS data of 3, to investigate the coordination geometry around Cu1 center in 3 Binuclear complexes 2 and 4 have two copper centers, (Cu1) and (Cu2), having different coordination geometry. The theoretical model of 1 has been used as standard to fit the EXAFS data of 2 and 4 to investigate the geometry around Cu2 center in these 2 and 4 by generating theoretical model from the crystal structure of another copper (II) complex of a structural parameters of 2, 3 and 4 so determined have been reported. From EXAFS analysis it has been found that (Cu1) centers have square pyramidal geometry in all the four complexes and (Cu2) centers gave distorted tetrahedral geometry in all four complexes and (Cu2) centers have distorted tetrahedral geometry in complexes 2 and 4. The different X<sub>ray</sub> absorption near edge structure (XANES) features for the four complexes have been identified and discussed. The values of the chemical shifts and presence of typical Cu(II) XANES features suggest that copper is in +2 oxidation state in these complexes. The XANES features also support the assignment of five-coordinated square-pyramidal geometry around Cu1 center in the four complexes. The intensity of 1s – 3d pre-edge feature has been used to investigate the geometry and binuclear nature of the complexes.





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**V**

**ABSTRACTS OF**  
**ORAL/POSTER**  
**PRESENTATIONS**

**III. PHYSICAL CHEMISTRY**



**1. Surface and physicochemical Properties of Gemini of Gemini Surfactants and their role in kinetics**

**Deepti Tikariha, Namrata Singh, Birendra Kumar, Kallol K.Ghosh\***

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**Keywords:** CMC, Gemini Surfactants, Micellar Catalysis, Ethylene Glycol, Surface Tension Nucleophiles

The interfacial and physicochemical properties of some cationic Gemini surfactants viz. alkanediyl-a, w-bis (hydroxyethylmethylhexadecylammonium bromide) have been investigated in aqueous and ethylene glycol by conductivity and tensiometric methods. The critical micelle concentration (cmc), surface excess concentrations, minimum area per molecule at the air-water interface and the surface pressure at the cmc has been determined. The thermodynamics of micellization of gemini surfactants have also been evaluated. In order to see the micellar kinetic effects the hydrolysis of p-nitrophenyldiphenyl phosphate (PNPDPP) using some oximate and hydroxamate nucleophiles have been studied in gemini surfactants. Kinetic constants were observed to be dependent on spacer chain length of gemini surfactants and on the nature of nucleophiles used.

**2. Effect of Added Alcohols on Micellar Properties of Cationic Monomeric and Gemini Surfactants in Non-aqueous Solutions**

**Birendra Kumar, Deepti Tikariha, Kallol k.Ghosh\***

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**Keywords:** Surfactant, critical micelle concentration, micelles, gemini surfactant, monomeric surfactant

Effect of added alcohols (methanol, ethanol and propanol) on Micellar properties of cationic monomeric surfactants viz. cetyltriphenylphosphonium bromide (CTPB), tetradecyltriphenylphosphonium bromide (TTPB), cetylpyridinium bromide (CPB) and gemini surfactant, decanediy-1,10-bis (dimethylhexadecylammonium bromide) abbreviated as C<sub>16</sub>-10-C<sub>16</sub>,2Br) have been investigated at 300 K. The effects of alcohols (methanol, ethanol and propanol) on critical micelle concentration (cmc), degree of micellar ionization ( $\alpha$ ) and on the polarity of the micellar interfacial region were investigated by using conductivity measurements. The cmc values of cationic surfactants increase with addition of methanol to ethanol but in case of n-propanol cmc values are decreasing. The Gibbs energy change, standard enthalpy and standard entropy of micellizations are also evaluated. The dependence of these thermodynamic parameters on the concentration of alcohols are determined in terms of the effect on micellization of CPB.

### **3. Recent Trends in Kinetics in Analytical Chemistry: Monitoring of Environmental Pollutants Using Kinetic Methods**

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Environment*

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Recent years have seen an upsurge in the use of kinetics in analytical chemistry. “Kinetic Method of Analysis” is a newly growing field in the area of analytical and environmental chemistry. During the past decade considerable efforts have been directed towards developing increasingly sensitive kinetic methods for the determination of trace environmental pollutants. This is a rate-based technique rather than equilibrium based one. The ‘Kinetic Catalytic Methods (KCM)’ continues to be the most popular method in the literature of Kinetic Methods of Analysis. Because of their high sensitivity, Kinetic Catalytic Methods have been recognized as offering a valuable approach to trace analysis of environmental pollutants. The growing popularity and gradual acceptance of KCM is due to high specificity, sensitivity and precision combined with simple photometric procedure and economy

compared to the other methods of comparable analytical merits used for pollution control.

Several reactions such as redox reactions, ligand substitution reactions and metalloporphyrin formation have been utilised as indicator reactions for the development of kinetic catalytic methods of trace analysis of environmental pollutants. Many methods have been reported for kinetic determination of inorganic species like mercury, copper, ruthenium, nitrate, nitrite while few for organic species, based on their catalytic/inhibitory effect on ligand substitution or oxidation reactions.

While the principles have general validity, the discussion will be mainly centered around the recent work done using catalysed ligand substitution or oxidation reactions on hexacyanoferrate(II) or hexacyanoferrate(II) complexes. In this presentation, an attempt will be made to highlight brief principles and procedures for trace determination of environmental pollutants based on their catalytic effect on selected indicator reactions.

#### **4. Anodic Stripping Voltammetry to Identify Phases of Electrodeposites**

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*CSIR Emeritus scientist, Alagappa University, Karaikudi-3*

**Keywords:** Anodic stripping voltammetry, Pulse plating, Zinc nickel alloy, Phases

Anodic stripping voltammetry is used as an insitu tool to identify the phases formed during electro deposition. DC plated and pulse plated Zinc nickel alloy electro deposits were analyzed. Anodic voltammograms revealed two dissolution peaks in sodium sulphate containing EDTA. The first peak corresponds to d- Ni<sub>3</sub>Zn<sub>22</sub> and the second phase g- Ni<sub>5</sub>Zn<sub>21</sub>.

## **5. The study of B-Z oscillatory reactions: Bromate-Gallic acid System**

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**Keywords:** Oscillatory reaction, Gallic acid, B-Z reaction, Oscillation, excitability,

An Oscillating reaction system, far from equilibrium, has most interesting property called excitability. The behavior of Belousov-Zhabotinsky reaction the bromate/gallic acid/ $H_2SO_4$  system, in presence of electrolytes and nonionic surfactants; with and without ferroin indicator: Studied by potentiometric method has been reported. The solvents 1, 4-dioxan, acetonitrile, dimethylformamide and tetrahydrofuran have retarded the oscillatory reaction. The salts have also exhibited inhibitory effect in the system. The n lowering effect of ferroin at higher concentration may be due to complex formation of ferroin. The n has been found to decrease with the increase in concentration of the electrolyte up to a certain threshold value. Above which there was no oscillation.

## **6. NSAID POISONING IN MEDICO LEGAL CASES**

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**Keywords:** Forensic management, Toxicology, Forensic Medicine, toxicity, free radical

The non-steroidal anti-inflammatory drugs are among the most commonly prescribed drugs

due to their high efficacy in the treatment of pain. Fever and inflammation, but having estimated gastrointestinal tract bleeding/perforation (UGIB) risk. And in the post mortem examination reports the gastric mucosal and sub mucosal hemorrhages and bleeding episodes in unnatural death cases are frequently observed. Thus it is essential to find out the cause of stomach bleeding and lesions to rule out the possibilities of any foul play. However, a plausible mechanism and/or any strategic overview in autopsy are yet to be studied in detail. The objective of this communication was to evaluate the chemical events underlying the hemorrhages/bleeding to gastric toxicity with or without poisoning and in relation to its impacts on the examination of FM&T. The experimental observations reveal the possible mechanisms of gastric lesion formation, and involvement of an oxidative pathway through the free radical toxicity. It also points out that zinc status of an individual may reflect as a marker of gastric lesions. Recording of true medical status of the deceased is very much essential for detecting the cause of unnatural death. This preliminary investigation provides a baseline of strategic forensic evidence management and evaluation of prosecution witness status of a medico legal case profile.

**7. The effect of sodium dodecyl sulphate micelles on the kinetics of oxidation of L-cysteine by iron(iii)-1,10-phenanthroline complex**

**N.Annapurna<sup>1</sup> A.Kalyan Kumar<sup>2</sup> and P,Vani<sup>3</sup>**

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*2 & 3. Department of Inorganic and Analytical Chemistry,  
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**Keywords:** Kinetics and mechanism, L-cysteine, iron (iii)-1, 10-phenanthroline and sodium sodium dodecyl sulphate

The effect of sodium dodecyl sulphate micelles on the kinetics of oxidation of L-cysteine by iron(iii)-1-10-phenanthroline complex in perchloric acid medium was studied at 30<sup>0</sup>C. The progress of the reaction is followed by measuring the absorbance of tris-

phenanthroline iron(II) formed at 510 nm. The reaction showed first order dependence with respect to iron(III). The rate of the reaction increases with increase in phenanthroline concentration and [cysteine] as well and the order with respect to cysteine was found to be two. The rate of the reaction decreases with increase in [SDS] and [H<sup>+</sup>]. Stochiometric study and product analysis confirmed that the product of oxidation of cysteine to be cystine. A suitable mechanism has been proposed to explain the observed kinetics involving the reaction between [Fe(phen)<sub>2</sub>RSH]<sup>3+</sup> and zwitterionic form of cysteine in rate-determining step. The activation parameters of the reaction were computed using linear least squares method and the values of E<sub>a</sub> and "S<sup>#</sup> were found to be 64.8±1.1 kJ mol<sup>-1</sup> and -50.5±3.5 J k<sup>-1</sup> mol<sup>-1</sup> respectively.

## **8. MANGANESE (II) CATALYZED PERIODATE OXIDATION OF 2,3-DIMETHYLANILINE IN ACETONE-WATER MEDIUM-A KINETIC AND MECHANISTIC STUDY**

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Haridwar-249404(U.K.), India*

**Key words:** periodate oxidation, 2, 3-dimethylaniline, Kinetics and mechanism.

The Mn (II) catalysed reaction between 2, 3-dimethylaniline (AMX) and periodate ion in acetone-water medium rate of reaction decreases on increasing the ionic strength and decreasing the dielectric constant of the medium. Free radical Scavengers do not affect the reaction rate. One mol of AMX reacts with two moles of periodate during the initial part of reaction. Results of kinetic studies under pseudo first order conditions, [IO<sub>4</sub>]<sup>-</sup> >> [AMX], are in agreement with the rate law:

$$D[C]/dt = k k_3 k_4 k_w [Mn^{II}][S][IO_4]_0 [H^+] / \{K_2 K_w + (K_w K_b k_2)[H^+] + K_b [H^+]^2\}$$

Where  $k k_3 k_4$  is the empirical composite rate constant,  $k_w$  is ionic product of water,  $k_2$  is acid dissociation constant of H<sub>4</sub>IO<sub>6</sub> and  $K_b$  is base dissociation constant of TOL. [S]

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is the concentration of AMX and  $IO_4^-$  represents the concentration of periodate which has been taken in excess. The  $1/b_{obs}$  versus  $[H^+]$  profile passes through the minimum. The reaction products were subjected to solvent extraction, TLC, melting point, and spectroscopic studies and characterized as 2,3-dimethyl-p-benzoquinone. The values of thermodynamic parameters are  $E_a=5.16 \text{ kcal mol}^{-1}$ ,  $A=4.19 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ;  $\Delta S^\ddagger = -37.44 \text{ cal mol}^{-1} \text{ K}^{-1}$ ,  $\Delta G^\ddagger = 16.17 \text{ kcal mol}^{-1}$  and  $\Delta H^\ddagger = 4.54 \text{ kcal mol}^{-1}$ . Suitable mechanism has been proposed.

### **9. Effects of Electrode geometry on contact Glow Discharge Electrolysis**

**Dr Rajeshwar Singh**

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Contact glow discharge electrolysis is a novel electrolysis in which plasma is sustained by dc glow discharges between an electrode and the electrolyte surrounding it. It develops spontaneously during normal electrolysis at sufficiently high voltages and is characterized by a stable gaseous sheathing around the anode or the cathode across which glow discharges occur. The Chemical results of CGDE are remarkable: the products are novel for ordinary electrolysis and their yields exceed greatly the Faraday law value. The location, however, changes to the cathode whenever the relative anode-to-cathode dimension (diameter, length, or surface area) is sufficiently large. Usually the smaller electrode (rather sufficiently smaller electrode) is the location of the breakdown of normal electrolysis. The influence of relative anode-to-cathode length is significantly stronger than that of the relative diameter in determining the location of the CGDE

**10. Synthesis and Characterization of a new organic nonlinear optical crystal: 4- methoxy benzoin**

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**Keywords:** Synthesis, Characterisation, Intermolecular hydrogen bonding, NLO application

4- Methoxy benzoin (MB4), a new organic nonlinear optical crystal was grown by slow evaporation technique. Single crystals of MB4 have been subjected to X-ray diffraction analysis to estimate the lattice parameters and the space group. The molecular structure was confirmed using FTIR and NMR spectral analyses. Optical behavior and the thermal stability of the crystal were determined by using UV-Vis spectroscopy and TG-DTA curves. The nonlinear optical property of the crystal was tested by Nd: YAG laser source. SHG efficiency of 4MB is found to be 4 times that of potassium dihydrogen phosphate.

**11. Use of concept Maps in Teaching Electro Chemistry**

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**Keywords:** - Chemical, Biochemical, In-vitro biological dosimeters, detection of low doses, characteristics and applications of these dosimeters

Physical chemistry courses particularly topics like electrochemistry are often considered as difficult and not so interesting by most of the under graduate students because of their limited familiarity with the underlined abstract concepts of basic principle of electricity and the lengthy derivations and tedious numerical along with very preliminary types of laboratory exercises. The difficulties experienced by the students are further enhanced mainly due to surface understanding concepts of other related topics like thermodynamics, chemical equilibrium and other topics of the physical chemistry course

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without appreciating their interrelating links with the concepts of electrochemistry. Concept mapping technique which is a knowledge graph with network of interrelated concepts connected to the main central theme has been found more effective teaching strategy for the present course of electrochemistry in limited available time for classroom teaching. These have been used in the different stages of classroom teaching which include

- Introduction and interrelation between of concepts of electrochemistry.
- Identification of individual and general difficulties/problems in problem solving sessions based on linkages.
- Minimize repetition and duplication due to overlapping of concepts of curriculum.
- Conduction of mini tests to get feedbacks from the students.
- Coverage of maximum contents of the curriculum in limited available time for classroom teaching.

An attempt has been also made to develop correlation between experimental observations made during laboratory course work with the concept maps discussed in the classroom sessions in the form of VEE and fishbone diagrams.

## **12. Some Radiation Dosimeters and Their Use**

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UV radiation as well as ionizing radiations (e.g. X-ray, gamma rays and neutrons) are used for therapeutic and radio-protective purposes mostly in the low doses of radiation (maximum dose up to 100 Gy). For that purpose it is necessary to develop suitable chemical, biochemical and in-vitro biological tissue-equivalent dosimeters which should respond proportionately with increasing doses of radiation.

The recent paper elucidates the dosimeter aspects of a few such dosimeters. UV lamps are used for phototherapy. Radio-nuclides and radiopharmaceuticals are used for both therapeutic and diagnostic purposes. During their use for patients the amount of internal dose delivered by these compounds are passable to be measured by suitable dosimeters. Even during radiotherapy, brachy-therapy and photodynamic therapy absorbed dose

measurement is a fundamental necessity, Radiation-induced changes in biological systems, if known thoroughly, can produce suitable biological dosimeters that are of immense utility in research institutions.

Hospitals, nuclear installations etc. throughout the work. The principles and applications of dosimeters described here are:-

- (i) Potassium Ferri-oxalate actinometer for UV radiation.
- (ii) FBX system for gamma and X-rays.
- (iii) Modified FBX system for gamma rays and thermal neutrons.
- (iv) 5-Hydroxy-L-tryptophan and 5-Hydroxytryptamine and Diltiazem as biochemical dosimeters for radiation induced neuro-degeneration and cardiovascular systems.
- (v) DNA, Nucleohistone, H1-DNA and H4-DNA complexes as in vitro death and nucleosomal aberration.

### **13. Interfacial and Physicochemical Studies of Gemini Surfactants and the Micellar Kinetic Effects**

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**Keywords:** - CMC, Gemini surfactants, Micellar Catalysis, Ethylene Glycol, Surface Tension, Nucleophiles

The Interfacial and Physicochemical properties of some cationic Gemini surfactants viz. alkanediyl-1-a, w-bis (hydroxyethylmethylhexadecylammonium bromide) have been investigated in aqueous and ethylene glycol by conductivity and tensiometric methods. The critical micelle concentration (cmc), surface excess concentrations, minimum area per molecule at the air-water interface and the surface pressure at the cmc have been determined. The thermodynamics of micellization of Gemini surfactants have also been evaluated. In order to see the micellar kinetic effects the hydrolysis of p-nitrophenyldiphenyl

phosphate (PNPDPP) using some oximate and hydroxamate nucleophiles have been studied in Gemini surfactants. Kinetic constants were observed to be dependent on spacer chain length of Gemini surfactants and on the nature of nucleophiles used.

#### **14. Studies on the Solvent effect on the Solvent-Solute Interaction and The Mechanism of the Solvolysis Reaction**

**Rashmi Sinha<sup>1</sup> and R T Singh<sup>2</sup>**

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**Keywords:** - Iso-Kinetic temperature, Intraction, Uni and Bimolecular, Mechanistic path, Specific Solvation, Aquo Aprotic.

The iso-kinetic temperature value of the reaction has been found to be nearly 300 which clealy indicates that there is an ppreciable interaction between solvent and solute present in the reaction. The number of water molecules associated with the transition state has been found to be decreasing with rise of temperature which indicates that with gradual addition of the organic co-solvent (Dioxan) in the reaction media and with rise of temperature the mechanistic path of the reaction is changed from unimolecular to bimolecular.

#### **15. STUDIES OF EFFECT OF NON-AQUEOUS SOLVENT ON THE ACTIVATION THERMODYNAMIC PARAMETERS AND MECHANISM OF ALKALINE SOLVOLYSIS OF CAPRYLATE ESTER**

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**Key Words:** Thermodynamic Parameters, Activation, Solvolysis, Dense and bulky, Enthalpy dominating, Entropy controlled, Polarisation energy.

The solvent effect on the activation thermodynamic parameters and mechanism of alkali catalysed hydrolysis of methyl caprylate ester was studied in Water-Propan-2ol media having varying concentration of Propan-2-ol from 30 to 80% (v/v) at different temperatures ranging from 20 to 40°C. The rate of reaction was found to decrease with increasing proportion of the organic cosolvent in the reaction media. The numbers of water molecules associated with the activated complex were found decreasing from 1.696 to 0.763 with increasing temperature and from this was inferred that in water- Propan-2ol media, structure of water is being changed from its bulky form to its dense form. Out of the three thermodynamic activation parameters  $\Delta H^*$ ,  $\Delta S^*$  and  $\Delta G^*$ , all are found to increase simultaneously. Hence, it is concluded that in this reaction, increase in enthalpy dominates over enhancement in entropy and the reaction is enthalpy dominating reaction.

## **16. Kinetics and Isotherm Analysis of Pb(II) Adsorption onto Lemon grass**

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**Keywords:** Adsorption; Lead ions; Lemon grass; Batch studies; Kinetics Isotherms

A new adsorbent for removing lead ions from aqueous solutions in a batch mode system using Lemon grass (L-G). A comparison of the kinetic models on the overall adsorption rate showed that the adsorption system was best described by the pseudo second-order kinetics. The adsorption isotherm fitted by Langmuir's model showed maximum adsorption capacity (108.2 mg/g). Factors influencing lead adsorption such as initial Pb(II) concentration (12.5-100mg/L), pH (1-6), contact time (5-120 min) and adsorbent dosage (0.1-1.0 g) were investigated. The adsorption process was relatively fast and equilibrium was established within 120 min. maximum adsorption of Pb(II) occurred at pH~5. The experimental results demonstrated that complexation is one of the major adsorption mechanisms for binding Pb(II) ions to sorbents.

**17. A Density functional Study of CO Adsorption on gas phase and NaY zeolite supported gold monomers**

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**Keywords:** Gold nanoparticles, Zeolite support, Co oxidation, Density Functional Theory

The interaction of carbon monoxide with the gold monomer in two oxidation states 0 and +1 both in the gas phase and on a NaY zeolite support is studied using density functional theory (DFT). Three structures of the zeolite having different Na ion content are considered. CO vibrational frequency shows a blue shift on going from the oxidation state 0 to +1. For our T9 zeolite cluster containing three aluminum atoms, CO binding energy values of 1.21 and 1.16 eV, for the oxidation states 0 and +1 respectively, have been found for the cluster containing two Na ions.

**18. Performance of DFT for the Calculation of Hyperfine Coupling Constants of Some Isotropic Metal Complexes**

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**Keywords:** Density Functional Theory (DFT). Isotropic Metal Complexes, Hyperfine coupling Constant.

The performance of DFT methodology to predict with accuracy the hyperfine coupling constants (hfccs) of isotropic metal complex  $[\text{Mn}(\text{CN})_4]^{2-}$ ,  $[\text{Cr}(\text{CO})_4]^+$  and  $[\text{Co}(\text{CO})_4]$  have been investigated. For this investigation, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals have been used. The hyperfine coupling constants values obtained from different density functionals have been found in the order of BLYP > BP86 > BPW91 > B3LYP > B3PW91 > BHPW91 > EXP for  $[\text{Mn}(\text{CN})_4]^{2-}$ , BLYP > BP86 > BPW91 > B3LYP > B3PW91 > BHPW91 > EXP. For  $[\text{Cr}(\text{CO})_4]^+$  and BHPW91 > BHP86 > BHPW91 > EXP. For  $[\text{Co}(\text{CO})_4]$  > B3LYP > EXP. The performance of the functional BHPW91 has been found better for  $[\text{Mn}(\text{CN})_4]^{2-}$  and  $[\text{Cr}(\text{CO})_4]$  and B3LYP for  $[\text{Co}(\text{CO})_4]$ . We have inferred that DFT functional BHPW91 is best functional for the estimation of hyperfine coupling constant of isotropic metal complex  $[\text{Mn}(\text{CN})_4]^{2-}$  and  $[\text{Cr}(\text{CO})_4]$  and B3LYP for isotropic metal complex  $[\text{Co}(\text{CO})_4]$ .

## 19. Density Functional Theory and Chemical Concepts

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**Keywords** : Density functional (DF), Local Density approximation (LDA), Local spin density approximation (LSDA).

Quantum mechanics and theoretical chemistry has contributed significantly to our understanding of nature of chemical bonding, interaction between electrons and atomic nuclei in a molecule and chemical properties. The Nobel Prize in chemistry was given jointly to Walter Kohn and John Anthony Pople for their revolutionary contribution in the field of quantum chemistry in 1998. The properties that can be most commonly estimated using DF method are molecular geometry in ground and excited states, charge and spin

density distribution, potential energy surfaces (PES), spectroscopic properties, thermodynamic properties etc. The Hohenberg-Kohn theorem, Hohn Sham method and use of gradient corrected and hybrid functionals are useful to calculate the energy, geometry and molecular properties of the complex chemical systems.

**20. Ab initio studies on the Monoadducts and Biadducts of Mitomycin C analogues with DNA**

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**Keywords :** Mitomycin C, monoadduct, biadduct

Alkylation mechanisms of mitomycins to form monoadduct and biadducts formation are relevant to drug toxicity. Both the mechanisms have been studied for few selective mitomycins with quantum mechanical methods. The cationic behavior of C1 and C10 are not similar for these MCs, which may be related to the monoalkylation or bialkylation mechanisms of these drugs. The bialkylation mechanisms are expected for MC2 and MC3, whereas the other MCs may be sufficiently stabilized through monoalkylation, and bialkylation may be secondary reactions. The effects of substituents to the monoadduct and biadducts formations are found significant.

**21. Molar Conductance of Thiamine Hydrochloride in Water at 310.15 K**

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**Keywords:** electrolytic conductance, molar conductance, limiting molar conductance, Debye-Huckel-Onsagar equation, Walden constant.

Drug thiamine hydrochloride is a potent drug commonly known as vitamin B<sub>1</sub>. Electrolytic conductance of thiamine hydrochloride (IUPAC Name: thiazolium3- [(4-amino-2-methyl-5-pyrimidinyl) methyl]-5- (2-hydroxyethyl) -4-methyl-, chloride, monohydrochloride) have been measured in water at normal human body temperature 310.15 K and atmospheric pressure. Experimental data have been used for calculating specific conductance, molar conductance limiting molar conductance and Walden constant. Experimental results have been explained on the basis of Debye Huckel Onsagar equation.

## **22. Polarographic study of in (III) & TI (I) Complexes of N-Glycylglycine. In Water & Aqueous Ethanol Media**

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**Keywords:-** Polarography, Indium, thallium, N-Glycylglycine, complex, stability constants.

In (III) and TI (I) form 1:3 complexes with N-Glycylglycine in aqueous & aqueous ethanol medium. The presence of ethanol in the medium considerably affects the nature and composition of the complex species. The successive formation of three complexes 1:1, 1.2, and 1:3 is established by Deford and Hume method. The effect of change of temperature on the system has been investigated and the thermodynamic parameters “G°”, “H°” and “S°” of the complexation reaction have also been determined. The formation of the metal complexes has been found to be spontaneous and exothermic in nature.

**23. Densities and viscosity measurement of  $K_3[Cr(C_2O_4)_3].3H_2O$  in water, methanol- water, Isopropanol- water and DMSO-water at 303.15kK.**

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**Keywords:** - density, viscosity, solute-solute interaction, solute-solvent interaction

Densities and viscosity of  $K_3[Cr(C_2O_4)_3].3H_2O$  in water, methanol-water, isopropanol- water and DMSO- water have been measured at 303.15 k. from the density data, the values of apparent molar volume and limiting molar volume have been determined. The result of viscosity data have been fitted to Jones-Dole equation to get the Falkenhagen coefficient and Jones-Dole coefficient. The main thrust of the study is to correlate such physicochemical properties and relevant interaction parameters with the nature of molecular interactions.

**24. Comparative Study of the Kinetics of Alkali Catalysed Hydrolysis of Ethyl-Iso-Valerate in Aquo-Acetone and Aquo-Propan-2-ol.**

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**Keywords** – Hydrolysis, Ethyl-Iso-Valerate, Acetone, Propan-2-ol.

Kinetic studies of alkali catalysed hydrolysis of Ethyl-Iso-Valerate in Aquo-acetone and Aquo-propan-2-ol solvent system at various compositions 20% to 60% (V/V) of Acetone

and propan-2-ol have been reported. The specific rate constant have been found to increase with rise in temperature in both solvents. In aquo-actone medium the rate constant value has been found to increase with increasing proportion of acetone but in aquo propan-2-ol medium to decrease with increasing proportion of propan-2-ol at all temperatures, Iso - composition activation energy ( $E_c$ ) increases in acetone while decreases in propan-2-ol on increasing proportion of organic co-solvent. Iso- dielectric activation energy( $E_D$ ) Decreases in acetone while increases in propan-2-ol on increasing proportion of the solvent. The rate variations and other thermodynamic parameters have been explained on the basis of specific solvation phenomenon of solvent.

## **25. AB-INITIO STUDIES OF PYRIDINE-2-CARBALDEHYDE THIOSEMICARBAZONE: A BIOLOGICAL ACTIVE NOVEL COMPOUND**

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**Keywords:** Pyridine-2-carbaldehyde thiosemicarbazone, HF/STO-3G, HF/3-21G & HF/6-31G ab-initio methods, Correlation Coefficient (CC) HOMO-LUMO energy, Net atomic charge, Electron density and Thermodynamic parameters.

The molecular geometry, net atomic charge and atom electron densities, HOMO-LUMO energy, Hardness- Softness and thermodynamic parameters of the pyridine-2-carbaldehyde thiosemicarbazone a novel biological active compound, are examined theoretically at the ab-initio HF/STO-3G, HF/3-21G & HF/6-31G levels. The correlation coefficients are reported for bond lengths and bond angles at different levels of calculations. Net atomic charge and atom electron density data reveal the coordination sites in Pyridine-2-carbaldehyde thiosemicarbazone when it undergoes complexation with transition metal ions. Consequently, performance of ab-initio method at different levels of calculations has

been tested to find the best auxiliary tool for the designing of a novel material

**26. Synthesis of graphene filled polypyrrole nanocomposites by interfacial polymerization: their optical, electrical and electrochemical behavior**

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**Keywords:** Polypyrrole, graphene oxide, interfacial polymerization, nanocomposite

Polypyrrole (PPy)/graphene oxide (GO) nanocomposites were successfully prepared via liquid/ liquid interfacial polymerization where GO and initiator was dispersed in the aqueous phase and the monomer was dissolved in the oil phase. The synthesized samples were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), ultraviolet-visible absorption (UV-vis), X-ray diffraction (XRD), electrochemical and electrical conductivity measurements. Good dispersion of the GO sheets within the PPy matrix was observed from the morphological analysis. A noticeable improvement in thermal stability and electrical conductivity of the composites were observed. The composites showed excellent electrochemical reversibility at the scan rate of 0.1 Vs<sup>-1</sup> and good cyclic stability even up to 100<sup>th</sup> cycle. Newly developed graphene oxide based polypyrrole composite could be applied in electrochemical energy storage device.

**27. STUDIES ON THE CHANGES OBSERVED IN MECHANISM AND SOLVENT-SOLUTE INTERACTION DUE TO SOLVATION**

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**Keywords:** Solvation changes, Iso-dielectric, Solvoysis, Solvent-solute Interaction, Specific Solvation, Entropy, Mechanistic Pathways, Inhibitor

In order to highlight the salvation changes, the kinetics of acid catalysed hydrolysis of amyl methamoate in water t-butanol media having different concentrations, 30 to 80% (V/V) of the organic component at different temperatures ranging from 20°C to 40°C.

From the number of molecules associated with the activated complex which increases from 0.267 to 1.368 with increase in temperature, it is inferred that bimolecular mechanistic path of the reaction is changed to unimolecular.

Depletion observed in both the values of “H\* and “S\* with simultaneous enhancement in “G\* values of the reaction with increasing concentration (mole %) of the organic content of the reaction media reveals that the reaction is entropy controlled.

From the evaluated values of iso-kinetic temperature which is 324, it is concluded on the basis of the guidelines of leffler that there is stronger solvent-solute interaction in water-t-butanol media.

After studying the effect of increasing ionic strength and hydrogen ion concentration of the media, it is inferred that the reaction is ion-dipolar one and it follows AAC 2 mechanism.

## **28. MODIFICATION OF NATURAL POLYMER AND TO STUDY THE SOME PROPERTIES**

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**Keywords:** - Graft copolymer/ Acrylamido-2-methyl-I-propane sulphonic acid (AMPS) mandelic acid Potassium Bromate/ Guargum

Guar gum has been modified by grafting 2-acrylamido-2-methyl-I-propane sulphonic acid (AMPS) onto guar gum in aqueous medium. The graft copolymerization reaction was studied under different experimental conditions such as monomer concentration, redox pair concentration, backbone concentration, hydrogen ion concentration, time of reaction

and temperature. It has been observed that grafting ratio, add on and conversion decrease on increasing the bromate ion concentration. A similar trend has been observed with hydrogen ion concentration. The grafting ratio, add on and conversion have been found to increase with mandelic acid concentration. On increasing the AMPS concentration in the concentration range  $2.0 \times 10^{-2}$  to  $8.0 \times 10^{-2}$  mol dm<sup>-3</sup>, the grafting parameters show increasing trend. However, the grafting ratio and add on decrease while conversion increases with increase in guar gum concentration. All the grafting parameters show increasing trend with time and the optimum temperature has been observed as 35 °c the graft copolymer has been sent for characteriziton by infrared spectroscopy and thermogravimetric analysis.

**29. Synthesis and Antibacterial activity of 6-(5<sup>D</sup> – substituted-2-2benzofury)-4-aryl-4H-2-thiopyrimidines.**

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**Keywords:** á, â.-Unsaturated ketones, benzofuran, thiopyrimidines.

Various 2- thiopyrimidines can be usually synthesized starting from ethyl acetoacetate, ethyl malonate, ethyl cyanoacetate, acetyl acetone Or á, â unsaturated ketones by cyclocondensation with thiourea . In the present work The target thiopyrimidine have been synthesized starting from á, â unsaturated ketones and thiourea in presence of alcoholic potash. This synthetic method is simple, yields are good and the products obtained are unambiguous

These 2- thiopyrimidines can be synthesized by the Condensation of different 1-(5<sup>D</sup> – substituted-2<sup>D</sup> -benzofury)-3- (4-substituted aryl)-2-propene-1-ones with thiourea in presence of alcoholic potassium hydroxide. This cyclocondensation route was select because of readily availability of the required á, â unsaturated ketones and unambiguous product formation with good yield. Screenings of antibacterial activity of synthesized 2-

thiopyrimidine were also carried out by qualitative methods.

**30. Kinetics and Mechanism of Oxidative Decarboxylation of Amino acid with Bi (V) as Oxidant in HClO<sub>4</sub> - HF Mixture**

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**Keywords:** Kinetics, Mechanism, Oxidation, Amino acids, Bi (V), Pseudo first order, Aldehyde, Energy of activation, Electron transfer, Bridged outer sphere mechanism.

Kinetics and mechanism of oxidation of Histidine with Bi(V) has been studied in HClO<sub>4</sub> - HF Mixture. Pseudo first order rate constant ( $k^D$ ) was calculated from  $\log [Bi(V)]$  vs time. The initial rates were calculated by plane mirror method. The plots of initial rates vs  $[Bi(V)]$  is linear passing through the origin showing first order in Bi (V). The values of second order rate constant ( $k$ ) were calculated.

The rate of reaction was found to be independent of hydrogen ion concentration,  $[NaF]$  and  $[Bi(III)]$ . The reaction rate decrease with increasing ionic strength. Rate of reaction was studied at three different temperatures viz 298 K, 303 K and 308 K. The values of thermodynamic parameters  $E_a$ ,  $\Delta G^*$ ,  $\Delta H^*$ ,  $\Delta S^*$  of oxidation reaction was calculated.

**31. Surface Tension and Refractive Indices of Diacetone Alcohol + Benzene at Different Temperatures**

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**Key words:** Diacetone alcohol; refractive indices; surface tension

The studies of refractive indices and surface tension are being increasingly used as tool for investigation of the properties of pure components and the nature of intermolecular interactions between the liquid mixture constituents. Refractive indices ( $n_D$ ), and surface tension ( $\sigma$ ) have been measured for the binary liquid mixture of diacetone alcohol+ Benzene over the entire composition range at 303.15 K, 313.15 K and 323.15 K. The Redlich-Kister model was used to correlate the measured properties. It was found that in all cases, the experimental data obtained fitted with the values correlated by the corresponding models very well. The molecular interactions existing between the components were also discussed.

**32. Title: Preparation of conductive hydrogel based on poly (acrylamide-co-acrylic acid) and polyaniline and their actuation behavior.**

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**Key words:** Hydrogels, conducting polymers, electroactive behavior, crosslinker.

Electrically conducting composite hydrogels of poly (acrylamide-co-acrylic acid)

and polyaniline were prepared by two- step synthesis process. The hydrogels were prepared by aqueous polymerization technique at room temperature by varying the amount of crosslinker. Then hydrogel film was immersed in oxidative media and subsequently in aniline solution. Aniline was absorbed on the surface of the film and polymerized. The structural confirmations were by FTIR, UV-visible analysis, XRD and SEM. The electrical conductivities were evaluated by Four-probe method. The electroactive behaviour of composite hydrogels was investigated by measuring effective bend angles at different applied voltages.

### **33. Kinetics of Hydrolysis of Di-4-Methyl-2-Nitro Aniline phosphate in Buffer Medium**

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**Key words:** Hydrolysis, Di-4-methyl-2-nitroanilin phosphate.

Kinetic study of hydrolysis of Di-4-Methyl-2-nitroaniline phosphate has been investigated in the pH range 0.00 to 7.46 in 30% dioxane- water (v/v) medium at 60°C. The pH log rate profile has a rate maximum at pH 4.17. Hydrolysis of diester carried out in buffer shows that neutral and mononegative species are reactive at pH 0.00 to 2.00 and pH 2.00 to 7.46 respectively. The theoretical rate determined from specific rates and fraction of the neutral and mononegative species agrees closely with the experimental rates. Bimolecular nature of hydrolytic reaction has been decided on the basis of temperature and solvent effect study. Di-4-methyl-2-nitroaniline phosphate involves P-N bond fission, which is strengthened by isokinetic relationship. Probable mechanism has been proposed for the hydrolysis of diester via its neutral and mononegative species.

**34. APPARENT MOLAR VOLUMES AND TRANSPORT BEHAVIOUR OF GLYCINE AND L-VALINE IN AQUEOUS SOLUTIONS OF TRIPOTASSIUM CITRATE AT T= (308.15 AND 318.15) K**

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**Key words:** Apparently molar volume; Tripotassium Citrate; Amino acids; Viscosity.

Densities and viscosities of glycine and L-valine have been measured at 308.15 and 318.15 K in aqueous tripotassium citrate solutions ranging from 0.2 to 0.8 mol kg<sup>-1</sup> of tripotassium citrate. The values of apparent molar volume, partial molar volume at infinite dilution and relative viscosities of each amino acid in various aqueous tripotassium citrate solutions have been evaluated from the density and viscosity data. Transfer volume data have been used to calculate the pair and triplet interactions. The results have been discussed in terms of solute-solute and solute-solvent interactions and the structural changes of the solutes in solutions.

**35. VISCOMETRIC STUDIES OF BINARY LIQUID MIXTURES OF CYCLOPENTANE (1) + 2-PROPANOL (2), + 1-BUTANOL (2), AND + 2-BUTANOL (2) AT T = (298.15 AND 308.15) K**

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**Keywords:-** Viscosities; Deviations in viscosity; Bloomfield and Dewan Model; Correlating equations

Viscosities at  $T = (298.15 \text{ and } 308.15) \text{ K}$  and atmospheric pressure for binary liquid mixtures of cyclopentane with 2-propanol, 1-butanol, and 2-butanol over the whole composition range have been measured as a function of composition using an Ubbelohde viscometer. The deviations in viscosity and excess free energy of activation for viscous flow have been calculated from experimental data. Different correlations were used to correlate the viscosity data. The Bloomfield and Dewan model has been used to calculate viscosity coefficients which are compared with experimental data of the mixtures.

### 36. Thermodynamics of molecular interactions in ternary mixtures: Excess molar enthalpies

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**Keywords:** Connectivity parameter of third degree of a molecule, Excess molar enthalpies,  $H^E_{ijk}$ ; Interaction energy parameter, X; characteristic volume,  $V^*$ ; characteristic temperature,  $T^*$ .

Excess molar enthalpies,  $H^E_{ijk}$  of o-toluidine (i) + tetrahydropyran (i) + Picoline or (k) ternary mixtures have been measured over entire mole fraction at 308.15K using 2-drop calorimeter. The experimental data have been fitted to Redlich-Kister equation to evaluate ternary parameters along with their standard deviations. The topology of the constituents of the mixtures has been utilized to (Graph theory) predict  $H^E_{ijk}$  values of the investigated mixtures. The observed data have also been analyzed in terms of Prigogine-Flory-Patterson theory, it has been observed that  $H^E_{ijk}$  values predicted by Graph theory compare well with their corresponding experimental values.

**37. Excess molar volumes and excess isentropic compressibilities of ternary mixtures at 298.15K**

**Neeti<sup>a</sup>, S.K. Jangra<sup>a</sup> and V.K. Sharma<sup>a\*</sup>**

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**Keywords:** Excess molar volumes  $V_{123}^E$ ; Excess isentropic compressibilities,  $(k_{123}^E)_s$ ; Connectivity parameter of third degree of a molecule, Interaction parameter,  $x$ .

The densities,  $\rho_{123}$  and speeds of sound  $u_{123}$ , data of ternary OT(1) + THP (2) + Py or benzene or toluene (3) mixtures have been measured as a function of composition at 298.15K. The excess molar volumes,  $V_{123}^E$  and excess isentropic compressibilities,  $(k_{123}^E)_s$  values of the studied mixtures have been determined by employing measured experimental data. The observed thermodynamic properties have been fitted to Redlich-Kister equation to predict ternary adjustable parameters and standard deviations. The  $V_{123}^E$  and  $(k_{123}^E)_s$  values have been analyzed in terms of Graph theory. It has been observed that  $V_{123}^E$  and  $(k_{123}^E)_s$  data determined by Graph theory compare well with experimental values.

**38. Densities and Refractive Indices of Tetrahydrothiophene-1, 1-dioxide-Alcohol Liquid Mixtures at 303.15-318.15K**

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**Keywords:** Density, refractive index, excess refractive indices, Redlich-Kister polynomial equation

Densities and refractive indices of binary solutions of tetrahydrothiophene-1,1-dioxide with 2-propanol and 2-methyl-1-propanol, have been measured as a function of composition at 303.15-318.15K and atmospheric pressure. Experimental values have been used for calculating excess densities, excess refractive indices, Excess parameters have been fitted to redlich-Kister polynomial equation using least squares method.

### **39. QUANTUM CHEMICAL STUDIES ON MOLECULAR STRUCTURES OF COPPER-BIPYRIDENE COMPLEXES**

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**Keywords:** Copper, bipyridines, quantum chemical calculations, metal-ligand bonding

The Cu-bipyridene complexes were studied by quantum chemical calculations by B3P86 and MP2 methods using 6311+G(d,p) or larger basis sets with the GAUSSIAN 2003 program package. The monodentate structures of neutral and ionic Cu-(4,4'-bipyridine) have  $C_2$  symmetry with about  $40^\circ$  rotation angles between the two pyridine rings, while the neutral and ionic Cu-2,2'-bipyridine complexes have planar conformations in  $C_{2v}$  symmetry.

### **40. Study of Acoustic properties of 2-hydroxy-5-methyl acetophenone in DMF at different temperatures**

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**Keywords:** 2-hydroxy-5-methyl acetophenone; Speed of sound; solvation number; partial molar volume; Molecular interactions

Density ( $\rho$ ), speed of sound ( $u$ ), and refractive indices, ( $n_D$ ) of 2-hydroxy-5methyl acetophenone have been measured in N,N- dimethylformamide (DMF) at temperatures 298.15<sup>0</sup>K, 303.15<sup>0</sup>K, 318.15<sup>0</sup>K and 313.15<sup>0</sup>K. These measurements have been performed to evaluate some important thermodynamic and acoustic parameters. The apparent molar volume ( $V_\phi^0$ ), and apparent molar Compressibility ( $K_\phi$ ), of hydrazones in DMF were also calculated. Partial molar volume, ( $V_\phi^0$ ) and partial molar compressibility ( $K_\phi^0$ ), were estimated by using the values of ( $V_\phi$ ), and ( $K_\phi$ ), at infinite dilution. Refractive index data was used to calculate molar refractivity of solutions. The results have been discussed in the light of various types of interactions occurring in solution.

#### **41. Designing of novel copolymers using an artificial intelligence method: some exciting results**

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**Keywords:** Artificial intelligence, Genetic algorithm, electrically conducting polymers, Electronic structure, Copolymers, Donor-acceptor polymers, Band gap

Designing of organic conjugated polymers with desired conduction properties continues to remain a challenge. For successful molecular designing of such polymers, one needs to have a complete understanding of the structure-property relationship in these polymers. A successful and exciting route in this direction is provided by donor-acceptor polymers. Using an efficient designing route of genetic algorithm, we present some new and exciting results for copolymers of donor-acceptor polymers. Our results are important guidelines for experimentalists for tailoring these novel copolymers with desired conduction properties.

**42. Density, Viscosity and Refractive Index of Binary Liquid Mixtures at 293.15, 298.15, 303.15 and 313.15K**

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**Keywords:** Viscosity, Refractive index, Associational behaviour, Ramaswamy and Anbananthan, (RS), Prigogine-Flory-Patterson (PEP), Density, McAllister.

Densities, Viscosities and refractive indices were measured for the binary liquid mixtures formed by formamide, N-methylacetamide, dimethylformamide and dimethylacetamide with acetonitrile at (T=293.15, 298.15, 303.15, 308.15 and 313.15) K and atmospheric pressure over the whole concentration range. Lorentz-Lorentz (L-L) relation, Prigogine-Flory-Patterson Model (PEP), model devised by Glinski and Ramaswamy and Anbananthan (RS) models were used to study the associational behaviour of weakly interacting liquids from viscosity and refractive index data. These non-associated and associated models were compared and also tested for different systems. The measured properties were fitted to Redlich-Kister polynomial relation to estimate the binary coefficients and standard errors. Furthermore, McAllister multi body interaction model was used to correlate the binary properties. Conclusively, viscosities and refractive indices of binary liquid mixture can be better understood from these models and interactions and association constant can be well predicted. The associated processes yield fair agreement between theory and experiment as compared to non-associated processes.

**43. Thermodynamics of equilibrium adsorption of antibiotics by clay minerals and humic acid-clay complexes**

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**Keywords:** Antibiotics, tetracycline, adsorption, montmorillonite, humic acid, thermodynamics, adsorption isotherms

The sorption interaction of three widely used tetracycline antibiotics, tetracycline (TC), chlortetracycline (CTC) and oxytetracycline (OTC), has been determined at three different temperatures from dilute solutions of montmorillonite, humic acid and humic acid-montmorillonite complex saturated with  $\text{Na}^+$ ,  $\text{Ca}^{2+}$  and  $\text{Al}^{3+}$  cations using batch equilibrium technique. The presence of humic acid enhanced the adsorption of antibiotics while rise in temperature decreases the adsorption. Adsorption isotherms were of 'L' type. The adsorption of antibiotics was in the order  $\text{OTC} > \text{CTC} > \text{TC}$ . The adsorption was maximum for Al-saturated complexes and followed the order  $\text{Al} > \text{Na} > \text{Ca}$ . The standard free energy changes ( $\Delta G^\circ$ ) for the adsorption reactions were negative, signifying a spontaneous reaction. The enthalpy changes ( $\Delta H^\circ$ ) calculated from the temperature coefficient of the equilibrium constant showed that process is exothermic. The adsorption of tetracyclines on adsorbents give rise to an entropy loss as antibiotics molecules adsorbed on surface had fewer translational and rotational degrees of freedom than antibiotics molecules in solution. Various studies e.g. IR and X-ray, as well as thermodynamic parameters and Freundlich adsorption isotherms revealed the existence of protonation or coordination (or both) between exchangeable cation and oxygen of  $>\text{C}=\text{O}$  group of antibiotics. The values of thermodynamic parameters indicated towards a partial physical adsorption.

**44. EFFECT OF PHYSICAL PROPERTIES OF FLYASH ON COMPRESSIVE STRENGTH OF CONCRETE**

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In recent years the construction industry has reduced its carbon footprint by increasing the use of flyash from Thermal Power Plants (TPP) in production of concrete. Fly ash has been widely used as a binder in concrete for many years. This paper presents an experimental investigation on the influence of particle size distribution, morphology and surface characteristics of flyash on the compressive strength, porosity, and pore size distribution of hardened concrete. The two properties of fly ash that are of most concern are the fineness and the extent of unburned carbon content. Both of these properties affect water demand of the concrete.

The effect of particle size of flyash was investigated. The fineness showed profound effect on the rate of strength development of concrete. Reactivity of flyash increased rapidly with the reduction of particle size, resulting in faster development of early strength.

The effect of the properties of fly ash on the water demand in concrete is influenced by the morphology of the fly ash, presence of unburned carbon and the size of spherical particles. Flyash particles of higher Blain's value reduced demand of water and improved workability of fly ash concrete because of the "ball bearing" effect. Higher carbon content, quantified by loss on ignition (LOI), increased water demand due to absorption of water. It is therefore concluded that the requirement of water for obtaining desired consistency of fresh concrete reduces if the flyash contains finer particles (Blain's value  $>350$  m<sup>2</sup>/Kg) and low carbon content ( $<6\%$  by weight).

Since the lower demand of water reduces water-binder ratio it produces hardened concrete of higher strength for specified content of cement. Conversely higher strength of concrete can be achieved with lesser cement content if the flyash of low carbon content and finer particles is used.

# **99<sup>th</sup> Indian Science Congress**

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