PROCEEDINGS
OF THE
NINETY EIGHTH SESSION OF THE

INDIAN SCIENCE CONGRESS

CHENNAI, 2011

PART II

SECTION OF
CHEMICAL SCIENCES

President **: Prof. Vinod K. Singh**

CONTENTS

98th Indian Science Congress

January 3-7, 2011, Chennai

I

PRESIDENTIAL ADDRESS

President **: Prof. Vinod K. Singh**

PRESIDENTIAL ADDRESS

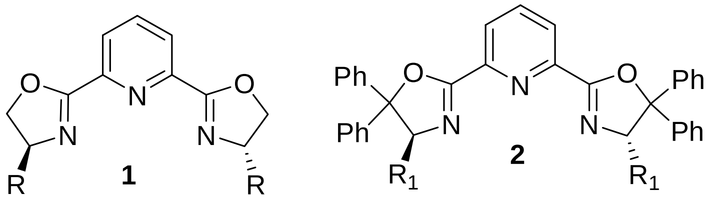
Enantioselective Reactions Catalyzed by Chiral Pybox-diph-Metal Complexes

President : Vinod K. Singh*

SECTION OF CHEMICAL SCIENCES

INTRODUCTION

The design, synthesis and tuning of a suitable chiral ligand around a metal center are important tasks for enantioselective reactions. Bisoxazoline ligands are one of the most important class of chiral ligands used in asymmetric catalysis because of their easy accessibility, modular nature and coordination with a wide range of metals.[1] Much effort has been made to the stereoelectronic modification of the bis(oxazoline) framework to create superior ligands. In 1989, Nishiyama first reported the tridentate *N*,*N*,*N*-type pyridine-bis(oxazoline) **1** (abbreviated as pybox) ligand for asymmetric catalysis (Fig. 1).[2] Since small changes in conformational and stereoelectronic properties of the chiral ligands can often lead to dramatic variation in catalytic efficiency, we have modified the pybox ligand **1** as pyridine 2,6-bis(5´,5´-diphenyloxazoline) (henceforth pybox-diph) **2** which has *gem*-diphenyl groups at C5 of the oxazoline rings (Fig. 1). We have successfully used the C_2-symmetric



2a: R_1 = *i*-Pr
2b: R_1 = *t*-Bu
2c: R_1 = Me
2d: R_1 = *s*-Bu
2e: R_1 = *i*-Bu
2f: R_1 = Ph
2g: R_1 = Bn

Fig. 1 Pybox and pybox-diph ligands.

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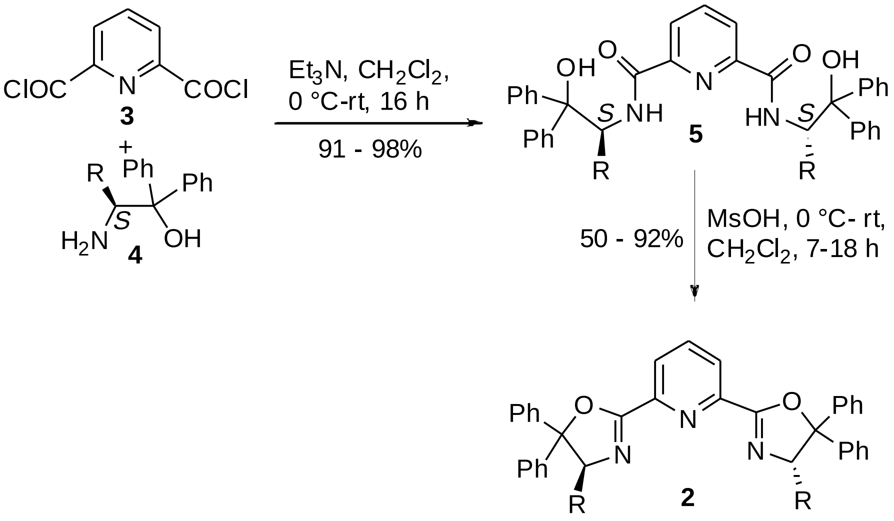
pybox-diph ligand in enantioselective allylic oxidation of olefins, one-pot three-component synthesis of propargylamines and Friedel-Crafts alkylation reactions. This manuscript provides an overview of some of the work done using pybox-diph ligand in our laboratory.

SYNTHESIS OF PYBOX-DIPH LIGAND

The pybox-diph ligands can be easily synthesized from pyridine 2,6-dicarbonyl chloride **3** and chiral *gem*-diphenyl β-aminoalcohol **4** in two steps. Pyridine 2,6-dicarbonyl chloride **3** reacts with chiral β-amino alcohols **4** to give bisamide **5**, followed by cyclisation of bisamide **5** to bis-oxazoline **2** by methanesulphonic acid. The ligand was purified by column chromatography followed by recrystallization from ether (Scheme 1).



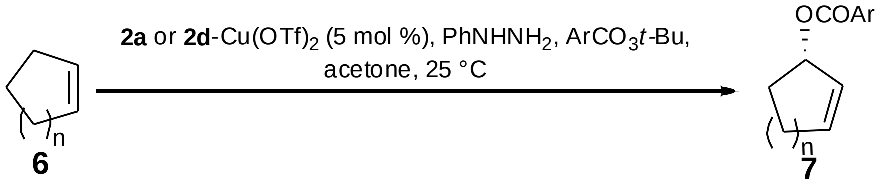
Scheme 1 Synthesis of pybox-diph ligands

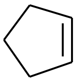
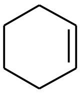
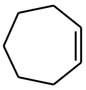
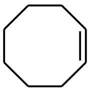
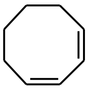
ENANTIOSELECTIVE ALLYLIC OXIDATION OF OLEFINS

The pybox-diph ligand was used in enantioselective allylic oxidation of olefins.[3a] It was demonstrated that Cu(I) species prepared by the reduction of Cu(II) with phenylhydrazine in acetone is more efficient than use of Cu(I) salt directly.[3b]

The reaction rate was very fast as compared to previous reported methods requiring several days for completion. The reaction proceeded smoothly with 5 mol % catalyst loading and gave the product in a maximum of 98% *ee* in the case of a cyclic substrate. A catalyst loading of as low as 1 mol % gave similar chemical

Table 1 Enantioselective allylic oxidation catalyzed by pybox-diph-Cu(II) complex



entry	Olefin	Ar	time		% yield		% *ee*	
			2a	**2d**	**2a**	**2d**	**2a**	**2d**
1		phenyl	3 h	20 h	76	75	70	65
2		*p*-nitrophenyl	13 h	6 h	47	42	62	58
3		*p*-methoxyphenyl	3 h	3 h	55	57	77	72
4		*o*-methoxyphenyl	4 h	4 h	71	74	80	80
5		phenyl	1 h	8 h	67	57	91	91
6		*p*-nitrophenyl	10 h	15 h	65	49	86	87
7		*p*-methoxyphenyl	2 h	5 h	60	61	93	92
8		*o*-methoxyphenyl	5 h	2 h	50	71	91	98
9		pentafluorophenyl	32 h	56 h	56	68	40	52
10		*p*-methoxyphenyl	96 h	18 h	45	45	91	94
11		*o*-methoxyphenyl	13 h	16 h	42	39	91	87
12		*p*-methoxyphenyl	21 h	19 h	31	42	96	90
13		*o*-methoxyphenyl	33 h	48 h	38	43	91	92
14		*p*-methoxyphenyl	29 h	15 h	49	50	95	96
15		*o*-methoxyphenyl	10 h	16 h	62	52	86	82

and optical yields but longer reaction times discouraged us to do the reaction at 1 mol % catalyst loading. Phenylhydrazine was used in the reaction for reducing the Cu(II) complex to Cu(I). We observed that the rate enhancement was much higher when the reaction was carried out in acetone. From experimental and EPR studies we have shown that phenylhydrazine and phenylhydrazone both were equally responsible for the rate enhancement, provided acetone was used as a solvent.[3c] We have shown that *gem*-diphenyl groups on the oxazoline rings are essential for high reaction rate and high enantioselectivity. The stereochemical outcome has been explained on the basis of the presumed transition state. The favoured transition state **TS1** was stabilized by the ð-ð stacking between the C5 aromatic ring of the oxazoline ring and the ester aromatic ring (Fig. 2). The fact that the presence of a *gem*-diphenyl group at C5 of the oxazoline ring is crucial for high enantioselectivity supports the ð-ð stacking.

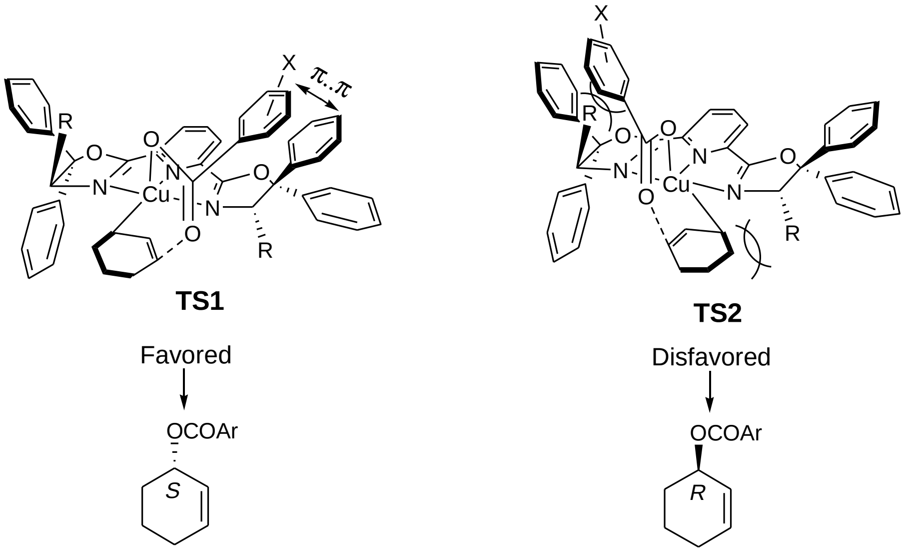


Fig. 2 Proposed transition state model for enantioselective allylic oxidation

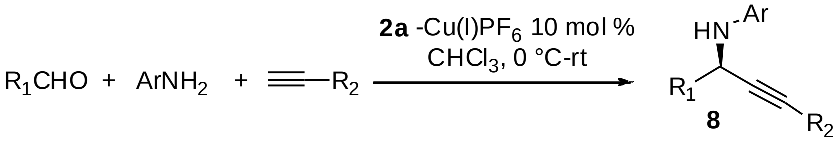
To further prove the ð-ð stacking in the transition state, a variety of *tert*-butyl peresters having different substituents on the aryl ring have been used. Surprisingly, electron-donating groups such as methoxy and alkyl group on the phenyl ring of the perester gave similar results as that of phenyl (Table 2, entries 5, 7 and 8), while pentafluoro substitution on the phenyl ring of the perester which is known to show strong ð-ð interaction with phenyl, has a detrimental effect on enantioselectivity as well as reaction rate (Table 2, entry 9). These anomalies can be rationalized using the fact that electron-withdrawing groups at the phenyl ring of the perester will show better ð-ð stacking. This additional attractive interaction stabilizes the disfavored transition state **TS2** overweighing the steric repulsion caused by the alkyl group on the chiral carbon, resulting in lowering the enantioselectivity (Fig. 2).[3d]

ENANTiOSELECTIVE ONE-POT THREE-COMPONENT SYNTHESIS OF PROPARGYLAMINES

The potential of the ip-pybox-diph ligand was further explored by its use in enantioselective one pot three component synthesis of propargylamines **8** (Table 3). The catalytic system works well in one-pot fashion with aldehydes, amines and terminal alkynes, and there is no need of preformed imine. 5-10 Mol % Cu(I)-

complex of ip-pybox-diph **2a** ligand turned out to be the best and a maximum of 99% enatioselectivity was obtained with excellent yields. Most of the substrates employed *viz*. aldehydes, anilines and terminal alkynes gave high enantioselectivity.

Table 3 Enantioselective one pot synthesis of propargylamine

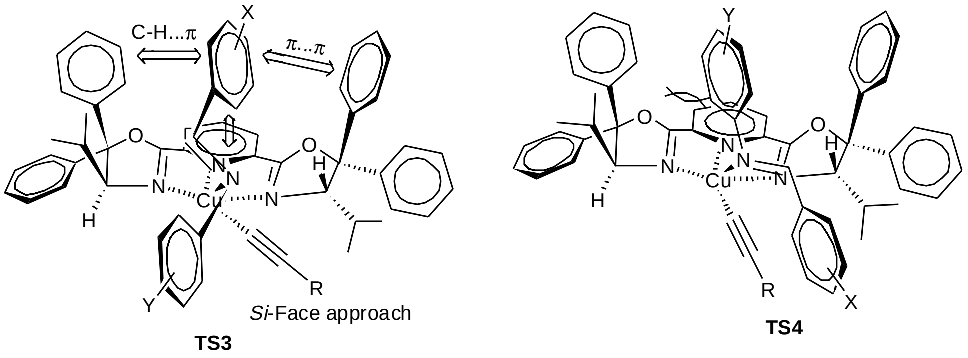


8

entry	R_1	Ar	R_2	time	yield (%)	*ee* (%)
1	Ph	Ph	Ph	12 h	98	96[a]
2	Ph	4-BrC_6H_4	Ph	24 h	98	96[a]
3	Ph	PMP	Ph	16 h	98	90
4	4-ClC_6H_4	PMP	Ph	28 h	91	90
5	2-ClC_6H_4	PMP	Ph	16 h	94	97
6	2,4-$Me_2C_6H_3$	PMP	Ph	18 h	97	99
7	Ph	PMP	4-$MeOC_6H_4$	20 h	96	93
8	Ph	PMP	4-BrC_6H_4	20 h	93	90
9	Ph	PMP	*n*-Bu	28 h	67	87

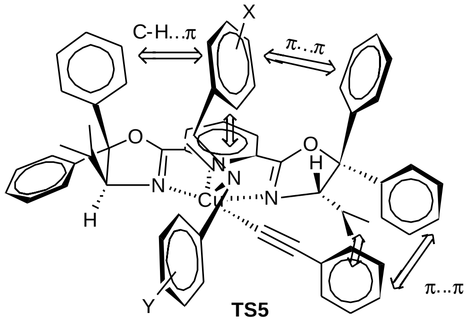
[a] 5 mol % catalyst was used.

The sense of asymmetric induction was explained by invoking transition-state assembly stabilized by three ð –interactions, two C-H…ð and one ð-ð interaction as shown in **TS3** (Fig. 3). Because of these three stabilizing interactions, the transition state becomes highly organized. The copper acetylide attacks the imine from the *si*-face to provide propargylamine. The *re*-face attack is disfavored because of the steric repulsion of the alkyl group on the chiral carbon of the oxazoline ring. Aromatic alkynes gave better results than aliphatic alkynes, which can be explained by considering one more C-H…ð interaction between the aromatic ring of the terminal alkynes with C–H of *i*-Pr group and a ð…ð interaction between aromatic rings of the terminal alkynes with the phenyl ring of *gem*-disubstituted pybox in transition state**TS5**.[4a]



Favored Transition State Assembly

Disfavored Transition State

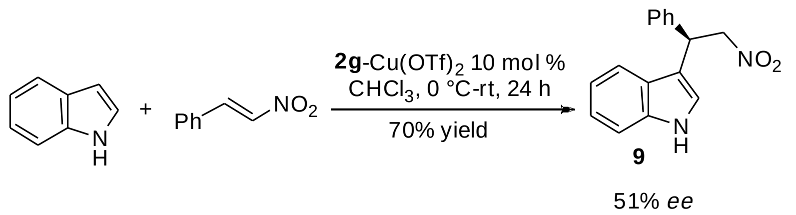


Si-Face approach

Fig. 3 Proposed transition state model of one pot synthesis of propargylamines.

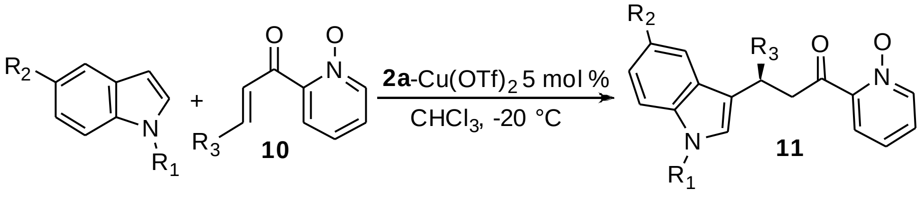
ENANTIOSELECTIVE FRIEDEL-CRAFTS REACTIONs

Recently, we have shown the application of pybox-diph ligand in enantioselective Friedel-Crafts alkylation reaction. The pybox-diph-Cu(II) complex was used in enantioselective Friedel-Crafts alkylation of indole with nitrostyrene. Among various substituted pybox-diph ligands, bn-pybox-diph (**2g**) gave the best result and the corresponding product **9** was obtained with 51% enantioselectivity (Scheme 2).[5a] Furhermore, the pybox-diph-metal complex was used in enantioselective indole alkylation with 2-enoylpyridine *N*-oxides **10**.[5b] The ip-pybox-diph-Cu(II) complex



Scheme 2 Enantioselective Friedel-Crafts reaction of indole with nitrostyrene.

Table 5 Enantioselective Friedel-Crafts Reaction of Indoles with various 2-Enoylpyridine-*N*-oxides



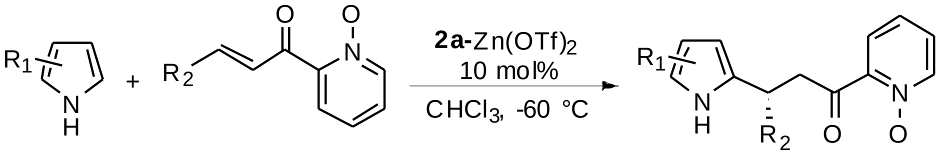
entry	R_1	R_2	R_3	time	yield (%)	*ee* (%)
1	H	H	Ph	15 min	97	99
2	H	F	Ph	1 h	97	97
3	H	OCH_3	Ph	15 min	98	95
4	CH_3	H	Ph	30 min	97	86
5	H	H	4-$CH_3OC_6H_4$	3 h	97	94
6	H	H	4-$NO_2C_6H_4$	15 min	95	99
7	H	H	3-$NO_2C_6H_4$	15 min	97	98
8	H	H	2-$NO_2C_6H_4$	15 min	96	97
9	H	H	1-naphthyl	2 h	83	89
10	H	H	2-furyl	3 h	97	87

was very efficient and gave the alkylated indoles **11** in excellent yields and enantioselectivities (up to 99% *ee*) (Table 5). The potential of catalytic system was proved by the cleavage of pyridine *N*-oxide ring of alkylated indole to give synthetically useful acid **15**[6] without any loss in enantioselectivity allowing further transformation (Scheme 3).

Furthermore, the use of pybox-diph ligand was extended to enantioselective Friedel-Crafts alkylation of pyrroles with 2-enoylpyridine *N*-oxides.[5c] We observed dialkylated product which was formed by dual Friedel-Crafts alkylation reaction at both the 2- and 5- positions of pyrrole along with the desired monoalkylated product **12** in the Cu(II)-pyboxdiph catalyzed pyrrole alkylation with 2-enoylpyridine *N*-oxide. The formation of dialkylated product was suppressed by a change in metal salt to $Zn(OTf)_2$.

The 10 mol % of ip-pybox-diph-Zn(II) complex catalyzed the pyrroles alkylation smoothly and gave the corresponding monoalkylated products with excellent yields and enantioselectivities. Our catalyst system offered substantial substrate scope and gave excellent results in all cases (Table 6). Even substituted pyrroles gave excellent enantioselectivities. The catalyst also worked well in enantioselective Friedel-Crafts reaction of 2-methoxyfuran and electron rich benzene derivatives.[5c]

Table 6 Enantioselective Friedel-Crafts Reaction of Pyrroles with various 2-enoylpyridine-*N*-oxides



12

entry	R_1	R_2	time	yield (%)	ee (%)
1	H	Ph	9 h	95	>99
2	1-CH_3	Ph	3 d	87	95[a]
3	2,4-diMe, 3-Ac	Ph	20 h	97	>99
4	H	4-F-C_6H_4	3 h	90	98
5	H	4-CH_3O-C_6H_4	18 h	54	99
6	H	4-NO_2-C_6H_4	3 h	96	85
7	H	3-NO_2-C_6H_4	3 h	99	98
8	H	2-NO_2-C_6H_4	5 h	98	97
9	H	1-naphthyl	9 h	71	99
10	H	2-furyl	18 h	82	95
11	H	cyclohexyl	12 h	76	94
12	H	*n*-pentyl	5 h	74	95

[a] Reaction was carried at -30 °C

CONCLUSIONS

We have introduced new types of tridentate *N,N,N*-type pyridine bis(oxazoline) ligands. These ligands have increased the ligand diversity for asymmetric synthesis. Metal complexes of these ligands gave impressive results in enantioselective allylic oxidation, one-pot three-component synthesis of propargylamine and Friedel-Crafts alkylation reaction of indoles and pyrroles. We have found that the *gem*-diphenyl substitutions at oxazoline rings are essential for getting high reaction rate and enantioselectivities. Efforts to extend the utility of these ligands in other enantioselective reactions are in progress in our laboratoty.

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January 3-7, 2011, Chennai

II

ABSTRACT OF PLATINUM JUBILEE LECTURE

PLATINUM JUBILEE LECTURE

Aromatics to Diterpene: Synthesis of (±)-Platencin

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Platensimycin **1** and platencin **2** (Figure), metabolites of *Streptomyces platensis*, have stimulated intense interest because of their unique molecular architecture and biological properties. Platensimycin **1** is active against *Staphylococcus aureus* by blocking fatty acid biosynthesis via inhibition of the enzyme FabF. Interestingly, platencin **2** inhibits action of both the enzymes FabH and FabF and therefore exhibits a broad range antibacterial activity. A formal total synthesis of platencin from a simple aromatic precursor will be presented. Transformation of aromatic compound into reactive spiroepoxycyclohexa-2,4-dienone and intramolecular cycloaddition are the key features of our methodology.

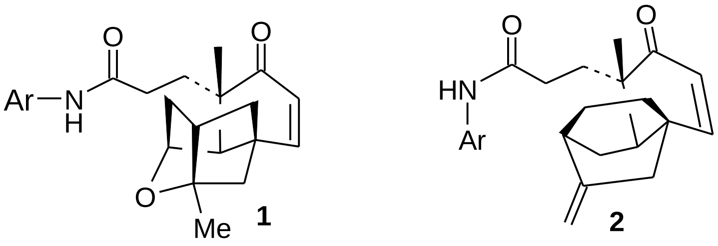

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Figure

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III

ABSTRACT OF AWARD LECTURE/YOUNG SCIENTIST AWARD PROGRAMME

YOUNG SCIENTIST AWARD PROGRAMME

Designing Receptor Molecules for Cation Sensing and Their Probable Application in Bio-imaging and Molecular Logic Operation

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The design of a chemosensor for selective recognition and sensing of cationic analyte is an area of significant importance. Among various cationic analytes, detection and recognition of Ca^{2+}, Mg^{2+}, Cu^{2+} and Hg^{2+} are of special significance owing to their participation in various physiological processes and environmental issues. The newly designed fluorescence-based receptor fragments have been used for selective recognition of these above referred metal ions. Use of some of these reagents towards bioimaging application in living cells also has been described. Further, it is shown that how novel fluorescent materials and supramolecular systems can be used to demonstrate the operating principle of Boolean logic gates at molecular level.

PROFESSOR R.C. MEHROTRA COMMEMORATION LECTURE

Single Molecule Magnets : Recent Advances

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Single-molecule magnets (SMMs) are molecules that can be magnetized in a magnetic field and which show slow relaxation when the magnetic field is removed. The magnetization occurs because there is a large energy barrier between the spin-up and the spin-down states. The magnetic order is within the molecules (single domain). The requirements for SMM behavior are (1) a very high spin state and (2) a large magnetic anisotropy. In contrast to classical nanomagnets obtained by a top-down approach SMMs represent a bottom-up approach. The potential applications of SMMs are vast. These include information processing, data storage, quantum computing, spintronics, biomedical applications (like MRI contrast agents) or magnetic refrigeration. One of the early compounds to have been studied as an SMM is the dodecanuclear mixed-valent manganese cage [MnIII/IV12O12(CH3CO2)16(H2O)4]1. This compound has an S = 10 ground state and shows slow relaxation of the magnetization. Further, this compound shows hysteresis; evidence of quantum tunneling was also observed. Subsequently, several multinuclear transition metal complexes have been investigated for their SMM behavior. More recently there have been examples of 3d-4f complexes that show SMM behavior 2.

In this talk we will present various synthetic strategies that are useful for assembling compounds that can be potential SMMs. In general the requirement that SMMs should have large ground state spin values suggests that multinuclear transition metal/lanthanide/transition metal-lanthanide complexes should be prepared. The strategies for assembling such complexes can be varied and use of multi-topic ligands is usually practiced. In addition, a philosophical divergence in terms of strategy can arise with an approach allowing nature to pick the best possible ensemble from a reaction milieu. On the other hand, reliable architectures can be ensured by specific design of ligands. The merits of these widely different methodologies will be presented with examples taken from the literature and from our work.

DOCTOR B.C. DEB MEMORIAL AWARD FOR SOIL/PHYSICAL CHEMISTRY

Impact of Organic Inputs on Soil Phosphorus Transformation Processes and Soil Test Maintenance Phosphorus Requirement

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Low native soil phosphorus (P) availability, coupled with low use efficiency of applied P (>25%) owing to its conversion into slowly cycling/recalcitrant pools, is a major constraint limiting crop productivity on most tropical soils of India. With emphasis on sustainable agriculture, attention has been increasingly turning to organic inputs (manures/crop residues) as a component of soil fertility management. Use of organic inputs may impact both biotic and abiotic P transformation processes in soils. Laboratory and field studies were made to investigate the role of organic inputs on P transformation processes in soils, P solubilization and soil test maintenance P requirement. The salient findings are presented briefly hereunder.

Crop residues effects on soil P transformation and availability in soil : Addition of soybean and wheat residues caused a net increase in labile P ($NaHCO_3$-P_i and -P_o) and moderately labile organic P (NaOH-P_o) at the expense of recalcitrant P (HCl-P) in Vertisol and both moderately labile NaOH-Pi and HCl-P in Alfisol. Crop residues suppressed P adsorption in soils as evidenced by decreased Langmuir b (adsorption maxima) and k (bonding energy constant). Consequently, standard P requirement was decreased by 17-33% for Vertisol and 24-43% for Alfisol. These results suggest that crop residues have potential to improve soil P fertility by lowering P sorption and redistributing P in favour of labile fractions and promoting accretion of organic P.

P solubilization from low-grade rockphosphates by soybean leaf litter : The decomposing soybean leaf litter (SLL - resulting from natural process of terminal defoliation in soybean) was found effective in solubilizing P to the extent of 20-26% from otherwise insoluble rockphosphates. A large portion (71-92%) of solubilized P was in organic P form. In the presence of SLL, low grade RPs were 46 - 74% as effective as fertilizer-P (SSP). Findings imply that soybean leaf litter can offer a natural opportunity for direct use of low-grade rockphosphates in the soybean based cropping systems.

Organic manure induced reduction in soil-test maintenance P requirement : A novel soil-test maintenance P fertilization technique for soil fertility maintenance and optimum crop yields under soybean-wheat system on Vertisol was developed by integrating relationships among soil-test values and rates of P addition and removal by crops. Soil test maintenance P rate was equal to crop P removal (24.1 kg ha^{-1}) if P was supplied as manure + fertilizer (1:1 P basis) and 1.4 times the P removal (36.1 kg ha^{-1}) when P was supplied as fertilizer alone. Results indicate that use of organic manure would reduce P requirement by 33% without sacrificing crop yields and thus reflect improved P use efficiency.

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IV

ABSTRACTS OF SYMPOSIUM/ INVITED LECTURES

PROCEEDINGS
OF THE
NINETY EIGHTH SESSION OF THE
INDIAN SCIENCE CONGRESS

CHENNAI, 2011

PART II (Abstracts of Symposium/Invited Lecture)

SECTION OF
CHEMICAL SCIENCES

President : **Prof. Vinod K. Singh**

INVITED LECTURES

1. NMR Conformational Analysis of *N*-linked Oligosaccharides by Paramagnetic Tagging

Takumi Yamaguchi[1], Sayoko Yamamoto[1,2], Mate Erdelyi[3]
Christian Griesinger[4] and Koichi Kato[1,2]
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Keywords : *N*-linked oligosaccharide, NMR, paramagnetic effect, lanthanide ion.

N-linked oligosaccharides, a major class of glycoprotein glycans, play crucial roles in a variety of biological events including protein quality control in cells. To determine 3D structures of *N*-linked oligosaccharides in solution is essential for understanding molecular basis of their various functions. Although NMR spectroscopy has a great potential in studying carbohydrate structures that have flexible properties, the insufficiency of conformational restraints of oligosaccharides provided by NOE data is the major limitation of traditional NMR methods. Hence, development of novel methodologies for NMR conformational analyses of *N*-glycans has been highly desirable.

We herein present an approach to provide additional distance and angular restraints based paramagnetic NMR data. Paramagnetic effects such as pseudocontact shift (PCS) induced by lanthanide ions offer long-distance information on conformations and dynamics of biological macromolecules. To apply this approach to analyses of carbohydrate conformations, an EDTA derivative as a lanthanide chelating-tag was covalently attached to the reducing end of the oligosaccharides. Upon complexation with paramagnetic lanthanide ions, the tagged sugar exhibited NMR spectral changes due to PCSs, thereby offering an opportunity to determine the spatial positions of the individual ^{1}H and ^{13}C nuclei with respect to the paramagnetic metal center. For example, the experimentally obtained PCS values of *N*, *N*'-diacetylchitobiose, which constitutes the common core structure shared among all *N*-glycans, were in excellent agreement with those back-calculated from a 3D structure model of this disaccharide. These data demonstrate that our paramagnetic tagging method can provide valuable conformational information of a variety of *N*-linked oligosaccharides.

2. New Organotitanium Reagents for Use in the Synthesis of Bioactive and Energy Harvesting Molecules

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In recent years, several new synthetic methods have been developed in this laboratory for applications in organic synthesis based on new routes to access boron, titanium, metal carbonyls and chiral reagents.[1-5] The organotitanium reagents, readily accessible via the reaction of $TiCl_4/R_3N$ reagent system, have been demonstrated for use in several organic transformations.

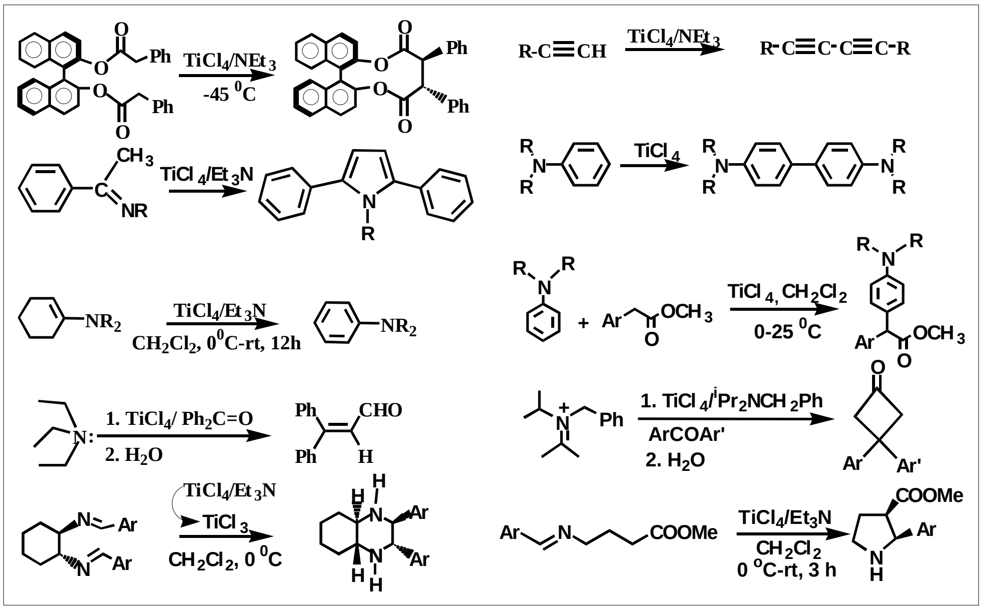

Fig. 1. Organic synthetic methods based on $TiCl_4/R_3N$ reagent system.

The titanium reagents prepared using the $TiCl_4/R_3N$ reagent system are also useful in the synthesis of certain bioactive organic skeletons and electron donor/ acceptor molecules with potential for applications in energy harvesting devices.[6-8] Salient features of these results will be presented.

3. New Fe-based oxyarsenide (LnOFeAs) superconductors

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There has been excitement in the field of superconductivity in designing new superconducting materials with high critical temperature (T_c) and high critical field (H_c). Recently a new class of oxypnictide (LnOFeAs, Ln = Rare-earth) superconductors [1] have been discovered which contains magnetic ions (Fe(II)), that normally destroys superconductivity. These superconductors show maximum T_c of 55 K [2] in Sm(O/F)FeAs which also shows very high value of critical field (H_{c2}) which is very important for high field applications like magnetic resonance imaging (MRI), magnetoencephalography, transportation (levitated trains), high energy particle research. LnOFeAs(Ln = Rare earth) crystallizes in the tetragonal ZrCuSiAs type structure (Space gp: *P*4/*nmm*) consisting of alternate Ln-O and Fe-As layers [3]. New superconductors with general formula AFe_2As_2 (A = Ca, Sr and Ba) have been designed containing multiple Fe-As layers per unit cell [4]. Our studies revolve around the substitution of ions at the rare earth, oxygen, iron and arsenic site. Here we describe our results [5-9] on these oxypnictide superconductors which lead to enhancement in T_c and H_{c2}. The talk focuses on the pnictide superconductors developed so far, their properties and the directions to follow for a better understanding of the nature of superconductivity in these materials.

4. Expanded Porphyrins: Syntheses and Applications as Third Order Nonlinear Optical Materials

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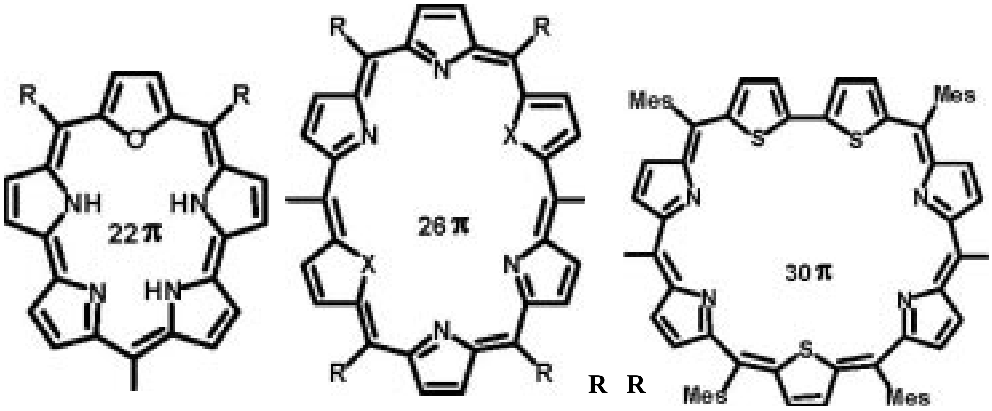
The design and synthesis of new molecules with large macroscopic optical nonlinearities represent an active research area in modern chemistry and material science. Such materials have potential applications in optoelectronic devices, two photon photodynamic therapy and holographic data storage systems. Currently, inorganic crystals such as LiNbO3, KH2PO4, KTiPO4 and semiconductor materials like GaAs and InSb are being used for such applications. However, to overcome the problems of low response time, magnitude of optical nonlinearity and molecular tailorability in Inorganic materials, search is on for organic NLO materials. Organic molecules with large conjugated ð-electrons exhibit bulk optical nonlinearity and are easy to process into thinfilms. In this talk, an overview of the design criteria for third order nonlinear response using organic molecules based on expanded porphyrin systems will be discussed. Specifically, the talk will address the following; (a) the design and synthesis of specific core-modified expanded porphyrins and fused porphyrins containing 22ð, 26 ð, 30 ð, 34 ð electrons in conjugation, (b) the third order nonlinear optical response measured by Two Photon Absorption (TPA) technique and (c) preliminary structure-function correlation.

R' R'



R R

R' **σ_2 = 986 GM σ_2 = 24,000 GM σ2 = 68,400 GM**

5. Silver-Adenine Metallacycles

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Interaction of metal ions with nucleobases has implications for the understanding of nucleic acid structure and catalysis, medicinal action of metal-organic complexes at the nucleic acid level, and for the construction of coordination architectures. Our research is focused towards developing metalated nucleobase polymers for catalysis and for the construction of metal-nucleobase frameworks. Recent reports from our laboratory have described solid state structure of silver-adenine(purine) coordination motifs containing *N*-coordinated silver-adenine duplexes and metallamacrocyclic tetramers and a hexamer. In addition, we were also able to transfer solid state coordination structures on HOPG surface to reveal reproducible nanoscale patterns of metal-nucleobase frameworks.1a,b A decade of our research on metal-adenine interactions has recently been summarized in an Accounts article.1c

6. Luminescent Molecular Clusters of Noble Metals

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In this talk I shall present our most recent work on monolayer protected sub-nanometer clusters of gold and silver. All the clusters are molecule-like with well-defined absorption and emission features, spanning across the visible-near infrared window. In a few clusters, the emission is intense. In general, several clusters are prepared together by reduction of metal ions in presence of appropriate ligands and subsequently size separated by electrophoresis. We have also developed new methods for fast and efficient synthesis of clusters. All of these clusters are stable, highly water-soluble and can be made in the solid state. The clusters have been characterized by electrospray mass spectrometry which gives multiply charged species. Isotope patterns and theoretical mass spectra have been used to characterise the molecular composition. We have separated two distinct clusters, Au_8SG_8 and Ag_8MSA_8 where SG and MSA refer to the thiolate forms of glutathione and mercaptosuccinic acid, respectively. Functionalization of these clusters with various molecules and the kinetics of such functionalization will be discussed. Most recently, we have developed interfacial routes for the direct synthesis of some of these clusters. The synthesis of a diverse variety of clusters, their chemical stability and intense luminescence offer numerous applications in areas such as energy transfer, sensors, bio-labeling and drug delivery. Several of these applications are demonstrated.

7. Applications of the Baylis-Hillman Adducts : Towards Development of Novel Strategies for Synthesis of Indolizine, Maleimide and Maleic Anhydride Frameworks

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The Baylis-Hillman reaction is an atom-economical carbon-carbon bond forming reaction involving the coupling of á-position of activated alkenes with carbon electrophiles under the influence of a catalyst or catalytic system (most commonly a tertiary amine catalyst) to provide diverse classes of densely functionalized molecules. Applications of these multi-functional molecules, which are usually referred to as the Baylis-Hillman adducts, in various organic transformation methodologies have been well documented in the literature.[1-7] We have been working on various aspects of this fascinating reaction during the last twenty six years and contributed significantly to the growth of this reaction. This talk will present our recent endeavors[8-11] towards the development of useful strategies for synthesis of indolizine, maleimide and maleic anhydride frameworks of medicinal relevance using the Baylis-Hillman adducts.

8. Synergism in Organometallic Catalysis

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The 'synergism' between different components (metal and ligand) is being increasingly exploited in organometallic catalysis. Bimetallic catalysis is based on the premise that enhanced reaction rate and higher selectivity might emerge from the cooperative participation of two metal ions. Toward this goal, metal-metal singly-bonded dipalladium(I) and diruthenium(I) compounds have been used as catalysts in the cross-coupling and carbene-transfer reactions, respectively.[1] Further, Hieber's base reaction has been studied on a diruthenium(II) platform.[2] This talk would focus on the synergistic involvement of metals or of metal and (cooperating) ligand in the organometallic catalytic reactions.

9. Stereoselective Assembly of Diols and Triols by a Tandem Hydroboration-Suzuki Coupling Sequence

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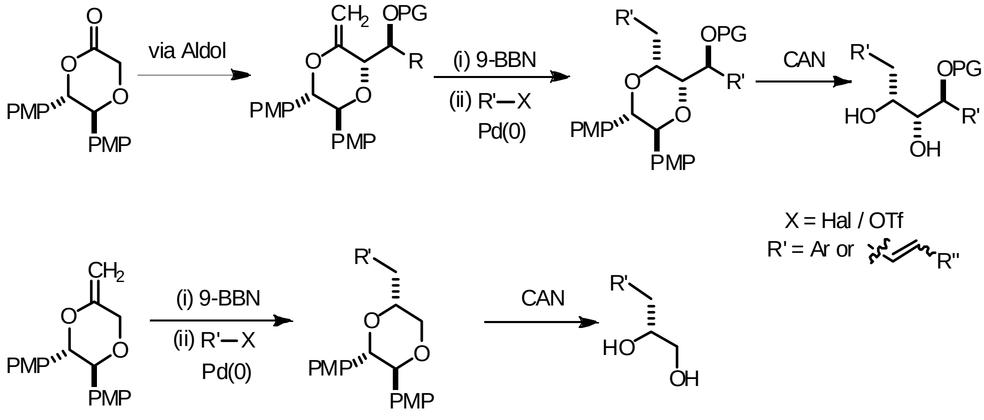

A new and easy alternative for the synthesis of complex *anti*-1,2-diols and 1,2,3-triols by a tandem hydroboration/Suzuki coupling sequence of a-alkoxy enol ethers has been developed. An easily available glycolate-based chiral oxapyrone has been employed. The simplicity of the tandem reaction, the easy preparation of both enantiomers of the Andrus' chiral oxapyrone, and a straightforward cleavage procedure complement other methods for the synthesis of highly functionalized diols. This methodology has already been successfully employed in the synthesis of complex natural products.

10. Desymmetrization of *meso* olefinic C=C *via* chiral ketalization : application in the total synthesis of natural products

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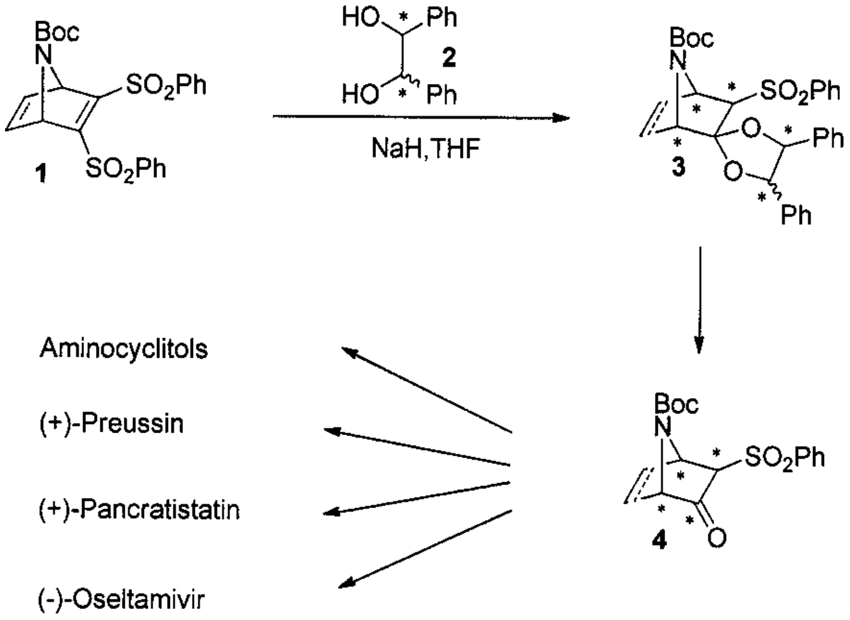
The enantioselective synthesis of chiral acetal has attracted considerable attention from organic chemist as they can be utilised as versatile precursor in the synthesis of optically pure compounds. We have developed an interesting strategy of desymmetrizing *meso* olefinic C=C via asymmetric ketalization for the synthesis of optically pure 7-aza-bicylco[2.2.1] heptane system. Asymmetric desymmetrization of *meso* olefinic moiety of **l** by reacting it with the equivalent amount of disodium salt of chiral diol **2** at 25°C furnishes optically pure ketal **3** in >99% *de.* Interestingly, desymmetrization is found to be temperature dependent and completely opposite stereoisomer of ketal **3** can be obtained if the reaction is performed at -100°C. Simple deketalization of **2** provides attractive strategy of obtaining 7-aza-bicylco[2.2.1] heptanone **4** in optically pure form. Bicyclic rigid structural framework of **4** along with suitably juxtaposed functionalities has rendered this molecule an attractive precursor in the synthesis of enantiomerically pure aminocyclitols, (+)- preussin, (+)- pancratistatin and (-)- oseltamivir.



Details of the concept and synthetic applications will be discussed.

11. Triggers, Switches and Glue for Nucleic Acids

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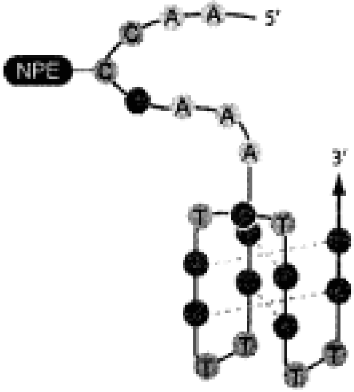
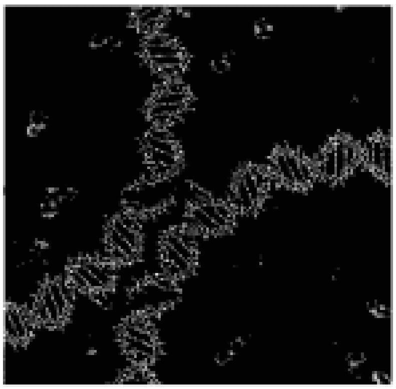
Our research focuses on engineering new properties into nucleic acids. In the first part we modify DNA and RNA to become light reactive. Specific aims are for example to regulate gene expression and control protein function with arbitrary choice of region, timing and extent in living systems. For this light is an ideal addressing mechanism since it can be generated and applied easily.[l] In most cases it is a highly specific and harmless trigger since only few cells react to light themselves and the wavelengths can be chosen so that unwanted phototoxic effects are avoided.

To make nucleic acids light-reactive we use photolabile groups (”cages”) to temporarily block the function. Using this approach we have shown that we can trigger transcription,[2] RNA interference[3] and aptamer activity with light.[4] The intrinsic properties of nucleic acids allow for quite different triggering strategies, addressing base pairing, conformation and antisense activity etc.

In the second part of our research we are interested in new interaction modules for DNA-based nanoarchitectures. Existing nanoarchitectures rely on polycatenation, or staple strands to build objects, since dsDNA is flexible, linear and has no significant tertiary interactions (unlike proteins). We have for example shown that DNA-binding polyamides can be arranged as ”DNA struts”[5] and ”anchors”[6] to glue large DNA-objects sequence-specifically together. We also introduced a new G-quadruplex-based interaction module which can be controlled via the addition of cations.[7] These studies have recently resulted in the construction of the first DNA rotaxane.[8]





12. Anna F. A. Pcacock,” Phillippa Ho, messize novel DNA binding metallopeptides, which may ultimatley to be monitored using a variety of speclmes”, Gemma Bullen”, Matthew

Berwick[a] and Vincent L. Pecoraro[b]

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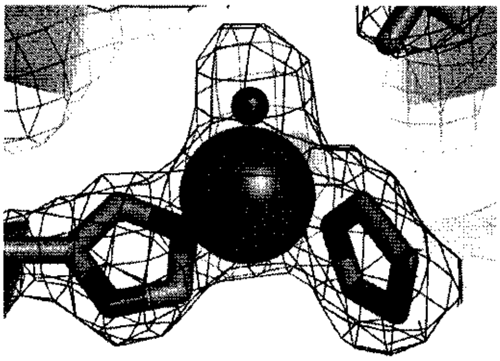
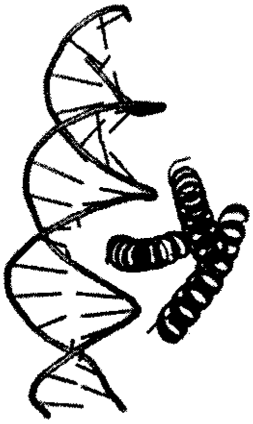
Keywords : *Peptide design, coordination chemistry, chemical biology*



De novo designed peptide constructs based on TRI, Ac-G(LKALEEK)$_4$G-NH2, and CoilSer, form amphipathic a-helices in solution and above ca. pH 4.5 these aggregate to form three-stranded coiled coils. These scaffolds provide a stable framework in the interiör of which we can design challenging metal binding sites by incorporating amino acids capable of binding to metal ions. Probing these systems using spectroscopic techniques as well as X-ray crystallography, permits their signatures to be compared with those obtained from biomolecules, offering important insight into metal ion biochemistry at the atomic level.



In addition to metal ions sites in the interiör, we have begun to exploit the exterior of these coiled coils for DNA binding. Key amino acids, thought to be responsible for DNA binding of the transcription factor GCN4, have been grafted onto the external surface of a three stranded coiled coil, providing a threefold symmetrical DNA binding motif, in which one a-helix at a time would be capable of interacting with the major groove of DNA. Furthermore, synthetic helix-loop-helix motifs, in which the a-helices are linked by artificial ”loops”, are being investigated for DNA binding.

98th Indian Science Congress

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V

ABSTRACTS OF ORAL/POSTER PRESENTATION

PROCEEDINGS
OF THE
NINETY EIGHTH SESSION OF THE
INDIAN SCIENCE CONGRESS

CHENNAI, 2011

PART II

SECTION OF CHEMICAL SCIENCES

President : **Prof. Vinod K. Singh**

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PROCEEDINGS
OF THE
NINETY EIGHTH SESSION OF THE
INDIAN SCIENCE CONGRESS

CHENNAI, 2011

PART II (Abstracts of Symposium/Invited Lecture)

SECTION OF
CHEMICAL SCIENCES

President : **Prof. Vinod K. Singh**

I. PHYSICAL CHEMISTRY

1. Kinetic Study of Thermal Degradation of Polyurethanes with Nonlinear Optical Chromophore

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Keywords : *Activation Energy, Copolymerization, Polyurethanes, TGA and Thermal degradation.*

In this work, a kinetic study on the thermal degradation of polyurethanes containing different feed concentration of 4-[bis(2-hydroxyethyl)amino]-4'-

nitroazobenzene as nonlinear optical chromophore (NLO) is presented, their degradation is also investigated using a conventional dynamic thermogravimetric analyzer (TGA) in air atmosphere at different heating rates i.e. 5, 10 and 20 °C min^{-1}. The activation energies of polyurethanes, which were synthesized by copolymerization of 4-[bis(2-hydroxyethyl)amino]-4'-nitroazobenzene and N-phenyldiethanolamine with 2,4-tolyenediisocyanate, are calculated using Kissinger, Friedman and Ozawa-Flynn-Wall methods. The values of activation energy thus obtained are directly proportional to the feed concentration of chromophore.The lower value of activation energy for polyurethane containing 100% chromophore feed concentration suggests its lower resistance to heat during its use in electro optic device applications.

2. Catalytic Effect of Bases in Enhancing the Flame Ratardancy Imparted by Guanidine Nitrate on Wood

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Keywords : *Wood, TG, LOI and flame retardancy.*

Wood, one of the flammable materials was treated with aqueous solution of guanidine nitrate in absence and presence of small amount of bases like N,N-Dimethylformamide, 4-Dimethylaminopyridine, Pyridine and Triethylamine. The weight gain percentage increase up to 33% by treating wood with guanidine nitrate. Further, the addition of small amount of bases in the treating solution, weight gain percentage increase up to 75%. To check flame retardancy, thermogravimetric (TG) analysis at 10 °C min^{-1} in nitrogen atmosphere and limiting oxygen index (LOI) was performed on all samples. The initial decomposition temperature of samples having bases is lower (222-225°C) than untreated (268°C) and sample treated with guanidine nitrate in absence of base (230°C). Limiting oxygen index and char yield calculated at 600°C for treated samples, are increasing from 21 to 30 and 11 to 26.3%, respectively.

3. Synthesis and Optical Characterization of Nano ZnS Phosphor

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Keywords : *Nanocrystalline, ZnS:Mn^{2+} phosphor, spectral properties, co-precipitation.*

Nanocrystalline ZnS phosphor doped with Mn^{2+} was prepared precipitating the zinc sulfide matrix with Mn^{2+} ions using potassium thiocarbonate that produced sulfide ions homogenously on hydrolysis in situ. The prepared material consisted nanocrystallinity. The phosphor obtained was characterized by X-ray diffraction (XRD) and field emission scanning electron microscope (FESEM). The phosphor under UV source produced orange luminescence due to the emission obtained by the transition $^4T_1 \rightarrow {}^6A_1$ of the Mn^{2+} ions present in the host lattice. The dependence of luminescence intensity on activator concentration and further effect of heat treatment on nanocrystallinity were also studied.

4. Preparation and Optical Characterization of Persistent Green Aluminate Phosphor

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Keywords : *Green phosphor; aluminate, persistent phosphor, optical properties.*

Europium doped aluminate phosphors were synthesized by a new combustion method. The synthesized phosphors were characterized and their optical properties

were studied. In the first step microwave technique was used for the combustion of prepared gel corresponding to the stoichiometric ratios of the metal nitrates, producing highly porous materials with fine particle size. In second step, doped Eu(III) was reduced to Eu(II) developing deep active centers of Eu(II) in the aluminate host lattice. Eu(II) activated phosphors showed the photo luminescence emission in the green region at 546 nm. Co-doping of Nd (III) and Dy (III) along Eu (II) enhanced after glow properties of these phosphors. The stoichiometric replacement of Sr^{2+} with Ba^{2+}, Ca^{2+}, Zn^{2+} and Mg^{2+} in $SrAl_2O_4:Eu^{2+}$ phosphor lattice was also investigated for their optical properties.

5. Synthesis and Optical Properties of Nano $(Y_{1-x}Eu_x)_{2-y}K_yO_{3-y}$ Phosphor

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Keywords : *Nano structure; phosphor; luminescence; optical properties.*

Gel combustion method has been utilized for the synthesis of europium-doped yttrium oxide red nano phosphor with the inclusion of alkali metal. Phosphor having the general formula $(Y_{1-x}Eu_x)_{2-y}K_yO_{3-y}$ where $0.005 \leq x \leq 0.1$ and K^+ is in the mole ratio 0.025 to 0.2 moles has been reported. Luminescence intensity of phosphor greatly enhanced with the inclusion of K^+ ions. The materials are soft with fine crystal size less than the 50 nm.

6. Kinetics of Oxidative Degradation of Tartaric Acid by Pyridiniumdichromate in Aqueous Perchloric Acid Media

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M. L. Sukhadia University, Udaipur-313 001

Keywords : *Kinetics, Oxidation, Tartaric acid, Pyridiniumdichromate.*

Oxidation of tartaric acid by pyridiniumdichromate (PDC) in perchloric acid medium has been studied. Active oxidizing species involved is protonated PDC. First order plot log (a-x) versus time is broken in two straight lines. Some induction period is also observed. Effect of concentration of substrate, PDC, $HClO_4$, Mn (II), Ce (III) and ionic strength has been investigated. Thermodynamic parameters have been evaluated. Energy of activation is 53.14 and 56.58 kJ mol^{-1} for two successive stages of oxidation. Entropy of activation is low and negative. Although the activation energy does not correspond to C-C bond breaking, but the reaction products indicate C-C bond breaking. Suitable mechanism has been proposed involving complex formation.

7. Ionic Liquids and Thermodynamics

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Keywords : *Ionic liquids; applications of ionic liquids; solution chemistry of ionic liquids.*

Modern room-temperature ionic liquids (RTILs) consisting of large and asymmetric organic cations and small inorganic anions exhibit a special class of recently developed liquids unifying the property of the liquid state and strong Coulomb interactions acting as the prevailing intermolecular interactions in the liquid state. Several selected examples of the most promising chemical and technical applications of ILs are presented, which underline the importanc e of thermophysical properties of ILs and their role of being particular solvents in catalytic and separation processes as well as in special fields of electrochemistry.

8. Excess Thermodynamic Properties for the System Ethanol + Tetrahydrofuran + Cyclohexane at 25°c

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A general picture of the excess thermodynamic properties G_m^1, H_m^E, S_m^E, $P_{p,m}^E$ and V_m^E for the ternary mixture ethanol + tetrahydrofuran + cyclohexane is presented and discussed. Emphasis is placed on the advantages for interpretation inherent in the contemporaneous observation of all these properties. The trend of the excess entropy and heat capacity reveals the nearly competitive behaviour of the two polar compounds with respect to the hydrocarbon in terms of order-disorder creation. Partial molar quantities of ethanol illustrate the phenomena associated with the presence of hydrogen bonds, while calculation of the Kirkwood-Buff integrals allows quantitative estimation of the local compositions. Lastly, some methods for predicting the thermodynamic properties of multicomponent mixtures are considered.

9. Synthesis and Characterization of Cadmium Oxide Nanoparticles in Reversed Micellar Media

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Keywords : *Reversed micellar synthesis, cadmium oxide nanoparticles, surfactant assisted synthesis.*

Cadmium oxide nanoparticles (NPs) were synthesized using reversed micelles as nanoreactors. The spherical shape of final product was confirmed by the SEM and characterized by FTIR and XRD. These studies concluded that the particle are almost spherical in shape and have an average size of 52-55 nm. The nanoparticles size is mainly controlled by the reverse micellar media.

10. Thermodynamic Studies of Molecular Interactions in Mixtures of o-toulidine with Pyridine and Picolines : Excess Molar Volumes, Excess Molar Enthalpies and Excess Isentropic Compressibilities

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Keywords : *Excess molar volumes V^E, Excess molar enthalpies, H^E, Excess isentropic compressibilities κ_S^E , Connectivity parameter of third degree of a molecule$^3\xi$, Interaction parameter, χ.*

Excess molar enthalpies, $H,^E$ densities, ñ and speeds of sound, u, data of o-toluidine (i) + pyridine or α-, α- or γ- picoline (j) binary mixtures have been measured over entire mole fraction range at 298.15K using 2-drop calorimeter and AntorPaar DSA -5000 The measured densities and speeds of sound data have been utilized to determine excess molar volumes, V^E and excess isentropic compressibilities, κ_S^E of the investigated mixtures. V^E, H^E and κ_S^E data of the studied mixtures have been analyzed in term of (i) Graph theory. Analysis of V^E data in terms of graph theory suggest that (i + j) mixtures are characterized by interaction between nitrogen and carbon atoms of pyridine or substituted pyridine (α-, β- or γ- picoline) with hydrogen atom and ð-electron cloud of aromatic ring of o-toluidine. The IR studies lend additional support to the proposed molecular entities in (i + j) mixtures. It has been observed that V^E, H^E and κ_S^E values predicted by Graph theory compare well with their corresponding experimental values.

11. Topological and Thermodynamic Studies for Binary Mixtures of 1, 4-Dioxane with Anilines at 308.15 K

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Keywords : *Excess molar volumes, V^E, Excess molar enthalpies, H^E Connectivity parameter of third degree, $^3\xi$, Interaction energy parameter, χ.*

Excess molar volumes, V^E and excess molar enthalpies, H^E data of 1,4-dioxane (1) + aniline or N-methyl aniline or o-toluidine (2) binary mixtures have been measured as a function of composition at 308.15K. The V^E and H^E data have been estimated by Graph theory. Analysis of V^E data in terms of Graph theory suggest that1, 4-dioxane or aniline or N-methyl aniline or o-toluidine are associated molecular entities and (1+2) binary mixtures are characterized by interactions between oxygen atom of 1, 4 dioxane and hydrogen atom of aniline or N-methylaniline or o-toulidine. The IR studied also support to this view point. It has been observed that V^E and H^E values predicted by Graph theory compare well their corresponding experimental values.

12. Estimation Of Theoretical Ultrasonic Velocity In The Liquid Systems (Glucose + α-amylase) at 298.15 K

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***Keywords* :** *Ultrasonic velocity, glucose, α-amylase.*

Various theoretical models have been applied to evaluate the sound velocity values at 298.15 K for the binary system of glucose with aqueous amylase and compared with the experimental values. The validity of Nomoto (NR), Van Deal-Vangeal (IMR), Impedance dependence relation (IDR), Collision factor theory (CFT) and Nutsch-Kuhnkies (NK) methods is checked and a comparative study of the above models is made. The non-ideal behavior of the systems is explained in terms of molecular interactions of the constituents of the mixture.

13. Thermodynamics of First Step of Dissociation of Biologically Active Molecules of Amino Acid (Alanine) in Mixed di-oxane-water Media and their Related Thermodynamic Quantities

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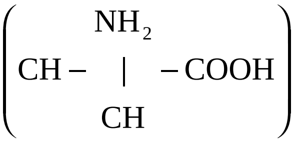
Keywords : *Alanine, Dioxane, Methanol, Deprotonation Constant Thermodynamic quantity.*

Deprotonation of alanine in aquo-organic solvent (dioxane-water system) apart from helping to understand the nature of ion-solvent interaction in this solvent is of some biological importance. They key to determination of various thermodynamic parameters associated with deprotonation of alanine  $\left(\begin{array}{c} \mathrm{NH_2} \\ \mathrm{CH-}\quad | \quad \mathrm{-COOH} \\ \mathrm{CH} \end{array}\right)$. In aquo-dioxane medium in the determination of pK values for the different stages of deprotonation.

pK for the first step of deprotonation of alanine in aquo-dioxane solution having 10, 20 and 30 per cent of dioxane by mass have been determined over the temperature range of 288.15 K to 318.15 K in steps of 10 K from e.m.f. measurement of the cells (C-1, C-2, C-3) respectively.

$$\text{Cell-1}\quad \mathrm{Pt, H_2}(g,\ 1\mathrm{atm})\left|\begin{array}{l} \text{Alanine, HCl,}\quad x\%\ \text{Dioxane,} \\ \quad m_1 \qquad m_2\ \ (100-x\%),\ \text{water} \end{array}, \mathrm{AgCl(s)}\right| \mathrm{Ag(s)} \quad \text{(C-1)}$$

$$\text{Cell-2}\quad \mathrm{Pt, H_2}(g,1\mathrm{atm})\left|\begin{array}{l} \text{Glycin, HCl,}\quad x\%\ \text{Dioxane,} \\ \quad m_1 \qquad m_2\ \ (100-x\%),\text{water} \end{array}, \mathrm{AHg_2SO_4(s)}\right| \mathrm{Hg(l)} \quad \text{(C-2)}$$

$$\text{Cell-3}\quad \mathrm{Pt, H_2}(g,\ 1\mathrm{atm})\left|\begin{array}{l} \text{Proline, HCl,}\quad x\%\ \text{Dioxane,} \\ \quad m_1 \qquad m_2\ \ (100-x\%),\ \text{water} \end{array}, \mathrm{Hg_2SO_4(s)}\right| \mathrm{Hg(l)} \quad \text{(C-3)}$$

The entire calculation was based on modified Davis equation which is advantage over other equation because the equation is very simple and accurate result.

We have also calculated transfer energetics give water to dioxane media in calculating thermodynamic parameters. They are

$$\Delta G^0_{transfer},\ \Delta S^0_{transfer} \text{ and } \Delta H^0_{transfer}$$

The first step of deprotonation constant over the calculated temperature and concentration range have been carefully measured after maintaining accuracy.

14. Use of Amido Black 10B–Tween-60-Ascorbic Acid System to Study Energy Efficiency of Photogalvanic Cell

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Keywords : *Amido black 10B; conversion efficiency; fill factor; ascorbic acid.*

Amido black 10B dye is used to sensitized photo-reaction with ascorbic acid. The Photogalvanic effect was studied in photogalvanic cell containing Amido black 10B- Ascorbic acid system. The phopotential and photocurrent generated by the cell were 996.0 μV and 420.0 μA, respectively. The effect of variation of different parameters like pH, temperature, light intensity, electrode area and diffusion length, on the electrical output of the cell were observed ed. Current-voltage characteristics of the cell and a mechanism for the generation of photocurrent in this photogalvanic cell in presence of Amido black 10B as a dye have also been studied. Efficiency of cell determined in terms of fill factor, conversion efficiency and storage capacity.

15. Comparative Study of Photogalvanic Effect in Photogalvanic Cell Containing Ethrosine Ammonium Lauryl Sulphate – EDTA System Using with and Without Sintered Filter

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Keywods : *Photogalvanic effect, Erythrosine, Ammonium Lauryl Sulphate, Fill factor, Conversion efficiency, Sintered Filter.*

Photogalvanic effect was studied in a photogalvanic cell containing Erythrosine as photosensitizer in Ammonium Lauryl Sulphate-EDTA system. At one time a sintered filter was used in H-cell between the diffusion lenth and another time sintered filtered is removed. In Erythrosine-ALS-EDTA system the photopotential and photocurrent using sintered filter were observed 688.0 mV and 95.0 μA respectively and without using sintered filter were observed as 641.0 mV and 90.0 ìA respectively. The conversion efficiency of the system using sintered filter was observed 03173%. Fill factor with sintered filter was determined as 0.50 and without filter it was observed as 0.46. The cell performance was observed 55.0 minutes in dark with sintered filter and 40.0 min. without sintered filter. The effects of different parameters on the electrical output of the cell were observed and current-voltage (i-V) characteristics of the cell were also studied with and without using sintered filter. The mechanism was proposed for the generation of photocurrent in photogalvanic cell.

16. Assessing the Ground Water Quality of Malpura Block (Tonk District, Rajasthan, India)

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Keywords : *Ground water, physico –chemical parameters, monsoon session, Hill–Piper trilinear diagram.*

The present Study was undertaken to assess the level of physico –chemical parameters of Ground water samples of Malpura Block in Tonk District, Rajasthan (India). Eighteen ground water samples were studied for selected water quality parameters such as pH, EC, TDS, calcium, magnesium, sodium, potassium, carbonate, bicarbonate, sulphate, chloride, fluoride and nitrate with the help of standard method of APHA during post monsoon session (October 2008-January 2009). From the observation it may inferred that the concentration of hydrogen ion (pH), F, Cl, Mg^{2+}, EC & TDS exceed permissible limit, but the value of Na^+, Ca^{2+}, NO_3, SO_4^{2-} & HCO_3^- were found within permissible limit as prescribed by WHO. From the Hill –Piper trilinear diagram it is observed that the majority of ground water is calcium-magnesium –chloride- sulphate type water.

17. Excess Molar Enthalpies and Excess Molar Gibbs Free Energy for Binary Mixtures of Tert-butyl Chloride with Cyclohexane or Benzene or Toluene at 298.15K

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Keywords : *Excess free energy, Excess molar enthalpy, Ideal associated model, Equilibrium constant, tert-butyl chloride.*

Molar excess enthalpy of mixing H_m^E the binary mixtures (tert-butyl chloride + cyclohexane, or + benzene, or + toluene) calorimetrically at 298.15 K. The excess Gibb's free energy of mixing G_m^E for tert-butyl chloride + cyclohexane, or + benzene, or + toluene mixtures at 298.15K were calculated by fitting the vapor pressure data to Redlich-Kister correlation according to Barker's method. Vapor pressure measurements have been done by a static method. The result has been analyzed in terms of Flory theory and Ideal associated model of non electrolytes. The ideal associated model which assumes the presence of AB type molecular species explains reasonably well the dependence of the excess enthalpy of these systems on the mole fraction of the components. The equilibrium constant for the reaction $A+B \rightleftharpoons AB$, along with the enthalpy of formation of AB molecular species, have also been calculated.

18. Excess Molar Enthalpies of Mixing of Sec- or Tert-butyl Chloride with Aromatic Hydrocarbons at the Temperature 308.15 K

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Keywords : *Excess molar enthalpy, sec-butyl chloride, tert- butyl chloride, aromatic hydrocarbon, Flory theory.*

Excess molar enthalpies of mixing for sec- or tert-butyl chloride + benzene or toluene or o- or m- or p- xylene have been determined experimentally as a function of mole fraction over the whole composition range at 308.15K. H_m^E is measured by a 2-drop calorimeter. The data have been analyzed qualitatively in terms of specific electron donor- acceptor type interactions and the interruption of the molecular order of the pure component in the mixture. The observed data of enthalpies of mixing for these binary mixtures are also analyzed in terms of Flory theory. The Flory theory gave poor agreement between experimental and calculated values.

19. Phytochemical Analysis of Fern & Fern-allies Growing Around Patna

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Keywords : *Phytochemistry, Fern &allies, Medicine, at Patna.*

Phytochemistry of Fern & its allies is one of the rapidly expanding areas in medical science. The origin of this science dates back to thousands of years ago, when the wild plants were used up as a source of medicine. Most of the Ferns & its allies were used for medicinal purposes by the early Greeks and Romans. Members of this group belong to non-flowering flora and recognized as first land plant migrated from aquatic habit to terrestrial habit.

During the course of evolution, Ferns adapted storage tendency, to accumulate amino acids, its derivatives and various types of secondary metabolites in its tissue systems, which are found fruitful in the treatment of various diseases. Natesh (2003) Ferns were used up as medicine in Unani system 2%, in Homeopath 14% in Ayurvedic system 30% and in folklore 100%. AIDS, HIV, Hepatitis-B, Cancer, Viral, Veineral, Wound, Cough, Cold, Rheumatism, Fever, Diarrhea, Epilepsy, Leprosy, Paralysis, Tumor, Snakebite, Asthma, Bronchitis so on are reported completely controlled by the Adianton, Adiantol, Isocontene. Marceline, Nefrolapine Pterine so on from Ferns & its allies. Adiantum, Azolla, Dryopters, Isoetes, Marsilea, Nefrolepis, Pteris are growing naturally at Patna, which requires attention of chemists and needs sustainable harvesting of this flora for future generations.

20. Effect of Iso-propanol on Kinetics of the Alkali-catalysed Hydrolysis of Ethyl –Iso –Valerate.

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Kinetic studies of alkaline hydrolysis of ethyl –iso-valerate in aqueous iso-Propanol medium of various compositions from 20 to 60% ($^{v}/_{v}$) of iso-Propanol at temperatures ranging from 20 to35^{0}c are reported. Rate constants and iso- composition activation energy (E_c) have been found to decrease with increasing proportion of organic co- solvent in the medium while iso-dielectric activation energy (E_D) has been found to increase with increasing dielectric constant. Decrease in rate has been explained on the basis of specific solvation phenomenon of amphoteric solvent.

21. Kinetics of Adsorption of Amaranth Dye on Steam Activated Pigmented Rice Husk Carbon

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Keywords : *Steam activated pigmented rice husk carbon, Amaranth dye, adsorption, adsorbent, colour.*

In the present work, kinetics of adsorption of Amaranth days on steam activated pigmented carbon prepared from rice husk (B. N. ORYZA SATIVA) was done Both pseudo first order and second order kinetics were applied to the adsorption of the dye on SAPRHC. It was seen that second order kinetics is followed by interactions between dye & SAPRHC. On the basis of the kinetics studies, the calculated rate constants showed that pseudo second-order model fit better to the experimental results. The rate constants calculated from the slopes of the best-fit

lines (coorelation coefficients were in the range of 0.896 to 0.978 with a mean value of R = 0.908) in all the cases was 4.6x10^{-3} min^{-1}. The values of Langmuir monolayer capacity (q_m), show the suitability of SAPRHC for high adsorption capacity of Amaranth dye on SAPRHC. The values of q_m are above 0.9 mg/g.

The results obtained indicate a potential use of SAPRHC for removing dyes like Amaranth dye from water.

22. Densities, Speeds of Sound, Viscosities and Refractive Indices of Binary Mixtures of 2-Octanol with 1,2-Dichlorobenzene, 1,3-Dichlorobenzene, and 1,2,4-Trichlorobenzene at *T* = (298.15, 303.15, and 308.15) K

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Keywords : *Densities, Viscosities, Excess molar properties, Halobenzenes, Alcohols.*

Densities, speeds of sound, viscosities, and refractive indices of binary mixtures of 2-octanol with 1,2-dichlorobenzene, 1,3-dichlorobenzene and 1,2,4-trichlorobenzene were measured over the entire range of composition from *T* = (298.15 to 308.15) K and at a pressure of 0.1 MPa. The experimental value of density was used to calculate the excess molar volumes of the binary liquid mixture. Excess molar volumes have been fitted to the Redlich–Kister polynomial equation to derive the binary coefficients and the standard errors between the experimental and the calculated quantities and have been used to discuss the presence of significant interactions between halobenzenes and alcohol molecules.

23. Partial Molar Volumes, Expansibilities and Compressibilities of Glyglyglyine in Aqueous Sucrose and Fructose Solutions between 288.15 to 308.15 K

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Keywords : *Glyglyglycine, Transfer functions, Saccharides, Adiabatic, Partial molar expansion.*

Apparent molar volumes (V_ϕ) and apparent molar adiabatic compressibilities ($K_{\phi,s}$) of triglycine (glyglyglycine) in aqueous and mixed aqueous solutions of fructose and sucrose (2, 4, and 6 mass %) have been determined at 288.15, 293.15, 298.15, 303.15, and 308.15 K. From these data, limiting partial molar volumes ($V_\phi{}^0$) and limiting partial molar adiabatic compressibilities ($K_{\phi,s}{}^0$) for glyglyglycine in aqueous sucrose and fructose solutions have been evaluated, together with the standard partial molar properties of transfer $\Delta_{tr}Y$ of the glyglyglycine from water to aqueous saccharides solutions. Transfer parameters have been interpreted in terms of solute-cosolute interactions on the basis of a cosphere overlap model. Pair and triplet interaction coefficients have also been calculated from transfer parameter data. The partial molar volume at infinite dilution ($V_\phi{}^0$) were used to obtain the partial molar expansion at infinite dilution, $E_2{}^0$, for glyglyglycine to examine the temperature dependence of such interactions.

24. Volumetric, Acoustic, and Viscometric Studies of Molecular Interactions in Binary Mixtures of Diethylene Glycol Monomethyl Ether with 1-Alkanols at Temperatures (293.15 - 308.15) K

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Keywords : *Binary Mixtures; Excess molar volumes; speed of sound; Isentropic compressibility.*

In this work densities ρ, speeds of sound *u*, and viscosities η, have been measured over the whole composition range for the binary mixtures of diethylene glycol monomethyl ether (DEGMME), $CH_3(OCH_2CH_2OH)_2OH$ with 1-hexanol, $CH_3(CH_2)5OH$, 1-octanol, $CH_3(CH_2)7OH$ and 1-decanol, $CH_3(CH_2)_9OH$ at 293.15, 298.15, 303.15 and 308.15 K along with the properties of the pure components. By using the experimental values of ρ, *u*, and η, excess molar volumes, V_m^E, deviations in viscosity, Δη, isentropic compressibilities κ_s, deviations in isentropic compressibilities $\Delta\kappa_s$, deviations of the speeds of sound Δ*u*, have been calculated.

25. Theoretical Investigation of Kinetics of CH_3OCH_2F (HFE-161) with OH Radical

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Keywords : *CH_3OCH_2F, Transition State Theory, Ab initio, Rate coefficients, Atmospheric lifetimes.*

Rate coefficients for the reaction of the hydroxyl radical with CH_3OCH_2F (hfe-161) were computed using Transition State Theory (TST) coupled with ab initio methods viz. MP2, G3MP2 and G3B3 theories in the temperature range of 200 and 400 K. Structures of the reactants in their Ground State (GS) and Transition State (TS) were optimized at MP2(FULL) and B3LYP level of theories. The potential energy surface was scanned at both the level of theories. Five different transition states were identified for each rotamer. Intrinsic Reaction Coordinates (IRC) calculations were performed to confirm the existence of all the transition states. The kinetic parameters due to all different transition states are reported in this paper. The rate coefficients for the title reaction were computed to be $k = (9\pm1.08) \times 10^{-13}$ exp [-(1713±33)/T] $cm^3 molecule^{-1} s^{-1}$ at MP2, $k = (7.36\pm0.42) \times 10^{-13}$ exp [-(198±16)/T] $cm^3 molecule^{-1} s^{-1}$ at G3MP2 and $k = (5.36\pm1.57) \times 10^{-13}$ Exp [-(412±81)/T] $cm^3 molecule^{-1} s^{-1}$at G3B3 theories**.** The atmospheric lifetimes of CH_3OCH_2F estimated at MP2, G3MP2 and G3B3 level of theories, to be 20, 0.1 and 0.3 years respectively.

26. QSAR Study and Molecular Modelling on Some 6-Benzyl Analouges of 1-[(2-hydroxyethoxy)methyl)]-6-(phenylthio)thymine(HEPT) : Potent and Selective Anti HIV-1 Agents

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Keywords : QSAR, Xeq, R, ☐, EC_{50}, Regression analysis, Molecular modelling

In clinical practice 6-Benzyl Analouges Of 1-[(2-hydroxyethoxy)methyl)]-6-(phenylthio) thymine (HEPT) have been extensively investigated as potent and selective anti HIV-1 agent for their ability to inhibit HIV-1 replication in MT-4 cells in submicromolar to nanomolar concentration range. In present work QSAR studies have been performed on a series of 16 HEPT analogues, with their biological activities $EC_{50,}$ CC_{50}, SI, one by one and molecular parameters, Equalised electronegativity (Xeq), Redundancy factor (R) and Topochemical index (□).

27. Sorption, Diffusion, and Permeation of Esters, Aldehydes, Ketones, and Aromatic Liquids into Tetrafluoroethylene/propylene at 30, 40, and 50°c

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Keywords : Sorption, Diffusion, Permeation

The coefficients of sorption, diffusion, and permeation for five organic esters, three aldehydes, one cyclic ketone, and three substituted aromatic liquids have been calculated for tetrafluoroethylene/propylene copolymer membranes at 30, 40, and 50°C with the sorption–gravimetric technique. With the sorption data, the concentration-independent diffusion coefficients have been calculated from Fick's diffusion equation. Analytical solutions of Fick's equation under suitable boundary conditions have been obtained so that the liquid concentration profiles in the polymeric membranes at different times and different depths of liquid penetration could be computed. Because of the linearly increasing trend of the diffusion coefficients with temperature, efforts have been made to estimate Arrhenius parameters. Experimental values and the computed quantities have been used to determine the membrane–solvent interactions and to propose suitable applications for the membranes under investigation in various situations.

28. Quality Aspect for VOD of Small Columns of Explosive Charge

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Explosives are now being used in wide scale for a variety of purpose. Only a few percent is being used for research and application purpose like space transport, medical etc.The main criteria for a chemical compound to be an explosive is that it should be in a unstable condition (by its spatial configuration) and on explosion the products should be much stable than the reactants. Normally the fuel is Carbon/Hydrogen, and the oxidizer is Oxygen/ Halogen. The striking feature of an explosive is that it is self sustained i.e. the fuel and oxidizers are already present in the explosive. For this reason explosives are often called as condensed explosives. The next striking factor is the speed of reaction. The reaction speed of TNT is in milliseconds hence the rate of production of energy (energy released per second) is much much higher than Coal, Petrol or Kerosene. This speed decides the usefulness of the explosive. Thus the deciding factor of an efficient explosive is: Amount of energy available in the explosive and the rate of release of the available energy when triggered. The various parameters to find these two factors are: Heat of explosion, Temperature and Pressure of explosion, Power index, Rate of burning, Velocity of Detonation (VOD) and Detonation pressure. Most of the explosives contain the elements C, H, N, O.In general the formula is $C_aH_bN_cO_d$.Here the oxygen or simply the Oxygen balance matters for the effectiveness of the explosive: e.g. For nitro glycerin Oxygen balance is + 3.5%, For RDX it is -22% and For TNT it is -74%. If the Oxygen balance = 0, it is referred as the most desirable or ideal condition. Any deviation to the (+) ve or (-) ve side will result in a comparatively lower heat of explosion and thus a lower performance. In space application the quality of the explosive is an important factor. Mainly two indicators are measured for the performance of explosives, they are: Detonation velocity and pressure.

Explosive velocity, also known as detonation velocity, is the velocity at which the shock wave front travels through a detonated explosive. Explosive velocities are always faster than the local speed of sound in the material. As we know that the VOD is the only measurable magnitude related to an explosive that can be given a number with certainty, it is easy to comprehend why it has been overemphasized as an indication of explosive strength. VOD is a function of the explosive configuration, charge diameter and confinement. Charge diameter and confinement are generic environment variables for any given blast. The same explosive in different environments will result in different VODs. Rather than strength, VOD gives an idea of the relative indication of the energy partitioning between shock and heave. The higher the VOD, the higher the shock component in relation to the total energy. While low VOD explosives will shift the energy partition towards a higher proportion of heave. In any case, the VOD should have to be measured with a confinement in order to be meaningful.

29. Densities and Ultrasonic Speeds of Binary Mixtures of Decan-1-ol with Cyclohexane and its Derivatives at 308.15 K

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Keywords : decan-1-ol + cyclohexane and its derivatives; Excess molar volumes; Excess molar isentropic compressibility

Densities, ρ, and ultrasonic speeds, u, of binary mixtures of decan-1-ol with cyclohexane, cyclohexanone, cyclohexylamine have been measured over the entire range of composition at 308.15 K and at a pressure of 0.1 MPa. The experimental values of densities were used to calculate the excess molar volumes of the binary liquid mixtures. Excess molar volumes and excess molar isentropic compressibility have been fitted to the Redlich-Kister polynomial equation to derive the binary coefficients, and the standard errors between the experimental and the calculated quantities.

30. Evaluation of the Coumarin Hydroxamates as Better hdac Inhibitor class through Descriptor Analysis and Binding Energy Calculations

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Keywords : Cancer, coumarin, HDAC-inhibitors, SBDD ligands, molecular descriptors, binding energy, ADME, docking.

Inhibitors of histone deacetylase (HDACi) proteins such as suberoylanilide hydroxamic acid (SAHA) have emerged as effective therapeutic anti-cancer agents. Here, we have designed 185 hydroxamic acid derivative inhibitors using an emerging Structure Based Drug Design approach (SBDD).

The physicochemical properties including Lipinski's rule of thumb for the SBDD ligands were analyzed using Molinspiration and Osiris property explorer. Pharmacokinetic properties for the designed ligands were profiled with ADME/Tox web which satisfied only 28 compounds. GRIP Docking studies were carried out using Vlife Molecular Design Suite 3.5 software for the suitable ligands. The stability of the docked complexes was determined by the binding free energy using MMFF force field calculation. However, seven docked complexes successively satisfied all the studies and seem to be a promising potent inhibitor against HDAC8.

31. Novel Synthetic Strategies and Characterization for Sulphur Frameworks

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Keywords : benzo[b]thiophene-2,3-dione; Friedal Craft's reaction; Chalcones; Cycloaddition 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 intermediates have been synthesized by employing a facile synthetic pathway. These intermediates are precursors for chalcones through which a variety of heterocycles of medicinal relevance have been prepared by cycloaddition reactions with alkenes. A brief account of our recent efforts towards developing novel synthetic strategies for the synthesis of new sulphur heterocycles will be presented.

32. Theoretical Studies on [2+2] *vs* [3+2]-Photocycloadditions of 6-Amino-2-(3-Thienoyl)-1,4-Benzoquinone)

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Keywords : 1,4-benzoquinone; [3+2]/[2+2] Photocycoadditons; DFT-B3LYP; CASSCF; Intramolecular H-shifting

Biradiacals or biradicaloid species derived from quinones present fascinating chemistry. Photochemical [2+2]-and [3+2]-cycloaddition reactions of quinones present useful pathways for preparing four membered and five membered rings respectively. Over the years our research program has revolved around developing novel quinones and understanding their cycloaddition reactions. DFT-B3LYP and CASSCF calculations have been performed using 6-31G* basis set to study photocycloaddition reactions of model quinone, 6-amino-2-(3-thienoyl)-1,4-benzoquinone, with ethylene. The calculated parameters of biradicals and transition states have also been compared with ground state parameters to completely elucidate the reaction mechanism of [2+2] and [3+2] photocycloaddition reactions. Preference for a particular cycloaddition pathway is ascertained by the relative stability between initially formed triplet biradical and another triplet biradical formed by hydrogen shift.

33. Isentropic Compressibilities Changes of Mixing of Tetrahydropyran and Aromatic Hydrocarbons Ternary Mixtures at 308.15 K

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Keywords : *Aromatic hydrocarbons, connectivity parameter of third degree, isentropic compressibilities. Speeds of sounds, tetrahydropyran.*

Speeds of sounds u_{ijk}, of Tetrahydropyran (THP) (i) + benzene (j) + toluene of o-of p-xylene (k); tetrahydrophyran (i) + toluene (j) + o- or p-xylene (k) ternary mixtures have been measured over entire mole fraction range of 308.15 kg and atmospheric pressure. The speeds of sounds data have been employed to predict isentropic compressibilitis. $(K_s)_{iik}$ and isentropic compressibilities changes of mixing. $(K_S^E)_{iik}$. The $(K_S^E)_{iik}$ values for the investigated mixtures are correlated with Redlich-Kister equation to estimate ternary adjustable parameters and standard deviations. The Moelwyn-Huggins concept (M.L. Huggins, Polymer, 12 389(371) of interaction between the surfaces of components of binary mixtures has been extended to predict isentropic compressibilities changes of mixing of ternary mixtures by employing the concept of connectivity parameters of third degree of a molecule (which in turn depends on its topology). It has been observed that $(K_S^E)_{iik}$ values predicted by Moelwyn-Huggins concept compare well with their corresponding experimental values.

34. Thermodynamic Contribution in Binary Organic Alloys and Compounds

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Keywords : *Organic alloys, phase diagram, mixing function and excess function.*

The organic substances have recently been attracting the attention in connection with searches of new charge transfer material in polymer matrix for various electronic devices. In present article 8-hydroxyquinoline (HQ)-4-chlorobenzoic acid (CBA) system has been under taken to study the thermodynamic contribution in the system in terms of mixing and excess functions. The negative value of molar free energy of mixing (ΔG^M) of alloys at 0.810 and 0.895 mole fraction of CBA suggests that the mixing is these case is spontaneous. The integral molar enthalpy of mixing value corresponds to the value of excess integral molar free energy of the system favors the regularity in the binary solutions. The positive value of excess free energy (g^E) for all the eutectic, noneutectic alloys addition compound suggest an association of weaker nature between unlike molecules and of stronger nature between like molecules.

35. Spectrophotometric Method for the Determination of Hydrochlorothiazide in Bulk and Dosage form by Using Polymeric Surfactant

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Keywords : *Ammonium metavanadate V(V), polymeric surfactants, Spectrophotometer, mechanism, oxidation.*

Hydrochlorothiazide (HCTZ) is widely prescribed diuretic, used in congestive heart failure and hypertension. In this work a validated spectrophotometric method has been described for the assay of HCTZ in bulk and commercial dosage forms. The method is based on the oxidation of drug by ammonium metavanadate [V(V)]. The V(V) is reduced, so the solution becomes green colored complex which absorbs maximally at 365 nm, Beer’s law obeyed in the concentration range with molar absorbtivity and Sendell’s sensitivity absorbance unit, respectively. The various experimental parameters were optimized. The method has been successfully applied for the quantitation of the drug in commercial dosage forms.

36. Volumetric and Compressibility Properties of Water as a Solute in Propylene Carbonate and Tetramethyl Urea Solutions at 298.15K

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The experimental measurements of the speed of sound and density in binary solutions of Propylene carbonate and Tetramethyl urea as solvents and water as the solute in the concentration range of 0.02 mol kg^1 to 1 mol kg^1 at 298.15 K are reported. The data are used to obtain the isentropic compressibility (β_S) of solutions. The apparent molar volume ($\square_V$) and compressibility ($\square_K$) of water at different concentrations of water are evaluated. The data of limiting partial molar volume (ϕ_K^0) and compressibility (ϕ_V^0) and concentration variation of apparent quantities are examined to study the effect due to water-solvent and water-water interactions. It has been observed that there is a loss of volume as well as of compressibility of liquid water molecules in transferring them from the pure liquid state to a non-aqueous solvent. The data are compared with similar data obtained for water in alcohols, glycols and other apolar solvents like dioxane, acetonitrile, dimethylformamide. A possible interpretation has been advanced on the basis of H-bonding characteristics and other structural details of the solvents and water to account for the effects due to water-water and water-solvent interactions.

37. Voltammetric Peak Separation of Dopamine and Uric Acid by using 2, 4-Dinitrophenylhydrazine Modified Glassy Carbon Electrode

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Key words : *Dopamine, Uric Acid, 2, 4-Dinitrophenylhydrazine, oxidation potential.*

Peak overlap voltammetry is a challenge for the quantitative analysis of electroactive species. Dopamine (DA), Ascorbic acid (AA) and Uric acid (UA) are these types of electroactive substances. They are typically challenging to be determined because of their similar peak potential. Modified electrodes are promising tool for the selective determination of such substances. In recent years there has been a great deal of interest in the development of various types of electrochemical sensors that exhibit increased selectivity and sensitivity. In this work we report a 2, 4-Dinitrophenylhydrazine (DNPH) modified GC electrode for selective determination of Dopamine and Uric acid. We observe here the response of cyclic voltammetry towards DA and UA using the modified electrode. The DNPH modified GC electrode found to shift the oxidation potential of DA from 270 mV (at bare electrode) to 455 mV (an anodic shift of 185 mV occurs). Similarly UA shows oxidation potential at -285 mV at modified electrode which is 1.08V apart from the oxidation potential (795 mV) at bare electrode. The curves were obtained at 125 μM concentration for DA and 225 μM concentrations for UA. Ascorbic acid shows no response to the modified electrode. The detection limit is 75 μM for DA and 25 μM for UA.

38. Zn^{2+} Ion Selective Fluorescent Sensor Derived from Benzil and Tryptophan

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Keywords : *Benzil, Tryptophan, Fluorescence, Photoinduced electron transfer,* Zn^{2+} *ions.*

A new fluorescent sensor derived from benzil and tryptophan is synthesized and characterized by ESIMS and FT-IR. In 1 : 1 methanol-water solution this sensor exhibit high selectivity for sensing aqueous Zn^{2+} ions with 10-fold enhancement in fluorescent intensity over a host of other metal ions such as Cd^{2+}, Cu^{2+}, Co^{2+}, Ni^{2+}, Fe^{2+}, Mn^{2+}, Mg^{2+}, Ca^{2+}, Ag^{+}, Hg^{2+}, and Pb^{2+}. The enhancement in fluorescent intensity can be explained on the basis of Photoinduced electron transfer mechanism due to the binding of Zn^{2+} ions. This sensor was found to determine Zn^{2+} ion within experimental error for commercial tablets containing zinc.

39. To Study the Optimum Conversion Efficiency in Photogalvanic Cells

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Keywords : *solar energy; conversion and storage; renewable energy; photogalvanic Cells.*

The solar energy is one of the most promising important and practically unlimited sources of renewable energy in since that the sun will last forever as far as human life on earth concerned. The solar energy is clean sources of energy which is low cost in exhaustive, harmless, hazard fee and does not add to the earth’s total heat burden. In this direction “to study the optimum conversion efficiency in photogalvanic Cells has been chosen to achieve the desired result to meet the existing challenge and put up in the front of new technique in solar energy conversion and storage.

40. Synthesis and Characterization of Tamarind Sulphosalicylic Acid [TSSA] Resin and its Application in Removal of Toxic Metal Ions from Industrial Wastewater

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Keywords : *TSSA resin; Ion exchange capacity; Distribution coefficient.*

A Tamarind Sulphosalicylic acid (TSSA) resin was synthesized. The TSSA resin was and characterized by FTIR, elemental and Thermogravimetric analysis. The TSSA resin was separate of toxic metal ions using column method .The distribution coefficient value of metal ions at different pH was also studied using batch equilibration method. The different factor affecting

metal ion adsorption on TSSA resin such as pH, treatment time, agitation speed and temperature were studied. The physical property of TSSA resin was also studied. The total ion exchange capacity was measured. The order of adsorption of different metal ions on TSSA resin was measured.

41. Determination of Balofloxacin in Human Plasma and Its Pharmacokinetic Study by Sensitive and Selective HPLC Method

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Keywords : *Balofloxacin, HPLC-UV,Validation, Human Plasma, Pharmacokinetic study.*

A simple and feasible high performance liquid chromatographic method with UV detection was developed and validated for the quantification of balofloxacin in human plasma. A simple liquid –liquid extraction method with high-throughput quantification was followed for sample preparation. The chromatographic separation was carried out in a cyano column (250×4.6 mm, 5 µm). The mobile phase was a mixture of 10 mM phosphate buffer (pH 3.0), acetronitle and methanol (70:15:15, v/v) at a flow rate of 1.0 ml/min. The UV detection was set at 295 nm. The extraction recovery of balofloxacin in plasma samples was more than 95 %. The calibration curve was linear for the concentration range of 10 to 1500 ng/mL. The inter-day and intra-day precision was within 10% relative standard deviation (R.S.D.). The method had also shown satisfactory accuracy (> 90%). The method had shown good sensitivity with a limit of detection (LOD) of 3 ng/mL. The method was validated according to the principles of the Food and Drug Administration (FDA) industry guidance. The developed and validated method is very simple, sensitive and economical in comparison to other established method. Thus this HPLC method has been used successfully applied to the pharmacokinetic study of balofloxacin in healthy human volunteers.

42. Studies in electrolytic conductance of aprepitant in non aqueous solvents at 310.15 K

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Keywords : *Electrolytic conductance, Molar conductance, Limiting molar conductance, relative permittivity, Onsagar equation, Walden constant.*

Electrical conductance of aprepitant (5-([2R,3S)-2-(®-1[3,5-bis(trifluoromethyl)phenyl] ethoxy)- 3-(4-flurophenyl)morpholino]methyl)-1H-1,2,4-triazol-3(2H)-one Formula: 23H21F7N4O3 AS No.170729-80-3 has been measured in methanol and ethanol in the vicinity of human body temperature 310.15 K. The conductance data has been treated on the basis of Debye Huckel Onsagar equation, Walden rule and the Fouss –Kraus assumptions.

43. Interaction of Small Aromatic Molecules : An *ab Initio* Studies on Benzene and Pyridine Molecules

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Keywords : *Molecular Structure, Quantum Chemistry, General Theory.*

The appropriate level of theories for studying weak stacking interaction of aromatic molecules has been an important aspect, since the high level methods have limitations for application to large molecules. The moderately accurate methods MP2/6-31+G(d,p) and MP2/6-31+G(df,p) are found feasible as demonstrated in stacking interactions of benzene and pyridine molecules.

44. Densities of Aluminum Ammonium Sulfate in Water and Water + N, N-DMF Mixed Solvent at T = (298.15, 303.15, 308.15, and 313.15) K

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Measurements of densities aluminum ammonium sulfate in water and water + (0 %, 5% 10 %, 15 % and 20%) N,N-dimethylforamide have been made as function of molality at T = (298.15, 303.15, 308.15, and 313.15) K and at atmospheric pressure. Density data have been used to calculate the partial molar volumes of aluminum ammonium sulfate. Partial molar volumes have been used to draw the conclusions regarding structure making or breaking behaviour of aluminum ammonium sulfate.

45. A Kinetic Study of the Solvating Power of Dipolar-protic Solvent on an Ion-dipolar Reaction : Alkali Catalysed Hydrolysis of Caproate Ester,

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Key words : *Solvating Power, Dipolar-aprotic, Iso-composition, Activation Parameters, Ion-Dipolar, Solvolysis, Enthalpy dominating, Entropy controlled.*

The kinetics of alkali catalysed hydrolysis of ethyl caproate was studied in water-EG media having varying concentration of EG (Dipolar-protic Solvent) at five different temperatures ranging from 20°C to 40°C.

Iso-composition activation energy of the reaction was found to decrease from 79.36 to 34.45 kJ/mole. The small but acceptable increase in ΔG^* values and nonlinear variation in ΔG^* values with mole% of EG in the reaction media are indication of specific solvation taking place in the process of activation.

From the evaluated values of iso-kinetic temperature i.e. 286.3, it is inferred that in water-EG media, there is weak but considerable solvent-solute interaction.

46. A Kinetic Study of the Solvent Effect on the Solvolysis of Heterocyclic Ester in Water-EG Media

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Key words : *Iso-dielectric, Iso-composition, Protic, Dipolar-aprotic, Activation Parameters, Desolvation, Solvolysis, Enthalpy dominating, Entropy controlled.*

The kinetics of alkali catalysed hydrolysis of ethyl nicotinate was studied in water-EG media having varying concentration of EG (Dipolar-protic Solvent) at five different temperatures ranging from 20^{o}C to 40^{o}C.

Iso-composition activation energy of the reaction was found to increase from 106.27 to 140.25 kJ/mole. The small but acceptable increase in ΔG^* values and non-linear variation of ΔG^*, ΔH^* and ΔS^* values with mole% of EG in the reaction media are indication of specific solvation taking place in the process of activation. The number of water molecules associated with the activated complex were found to decrease from 0.922 to 0.422 with increase in temperature from 20^{o}C to 40^{o}C and this indicates that the mechanistic path followed by the reaction is changed from unimolecular to bimolecular.

The evaluated value of iso-kinetic temperature 312.26 renders the sound proof for strong solvent-solute interaction in water-EG media.

47. A Kinetic Study of the Effect of Solvent on the Iso-dielectric Activation Energy and Solvent-Solute Interaction

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Keywords : *Iso-dielectric, Solvent-solute Interaction, Solvolysis, Specific Solvation, Mechanistic Pathwaya, Entropy, Inhibitor.*

The bulk dielectric constant of a particular solvent cannot be the same at different temperatures, rather it is appreciably affected by temperature. It is, therefore, necessary to evaluate the Iso-dielectric activation energy in such a way that effect due to change in bulk dielectric is reduced to minimum. The kinetic study of the solvent effect on the Iso-kinetic energy of acid catalysed hydrolysis of benzyl methanoate in water-propan-2-ol media reveals that with gradual increase in the organic content (propan-2-ol) of the reaction media or with gradual decrease in the dielectric constant of the reaction media, the Iso-dielectric activation energy has been found to decrease. From this, it is inferred that the transition state of the reaction is solvated whereas its initial state is desolvated.

The value of Iso-kinetic temperature, which comes to be 286, suggests that there is weak but considerable solvent-solute interaction in water-propan-2-ol media of the reaction.

48. Study of Kinetics and Mechanism of Solvolysis of a Heterocyclic Ester in Water-t-butanol Media

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Keywords : *Heterocyclic Ester, Activation Parameters, Iso-kinetic, Transition state, Barclay-Butler Rule, Enthalpy dominating, Entropy controlled.*

Solvent effect of tertiary butanol was studied on the Mechanistic pathway, Thermodynamiv Activation parameters, Activation energy and Iso-kinetic temperatures

of the alkali catalysed hydrolysis of Ethyl nicotinate in water-t-butanol media of varying composition ranging from 30% to 80% of t-butanol and at five different temperatures ranging from 20°C to 40°C.

The number of water molecules associated with the activated complex of the reaction were found to increase from 0.036 to 1.174 and from this, it is inferred that t-butanol acts as structure breaker of water converting its dense form into bulky form and it changes the mechanistic path way of the reaction from bimolecular to unimolecular.

With gradual addition of t-butanol to the reaction media, enthalpy of activation (ΔH^*) and entropy of activation (ΔS^*) were found decreasing with simultaneous increase in free energy of activation (ΔG^*). On the basis of this observation, it has been inferred that the entropy of activation depletes to greater extent than enthalpy of activation and initial state of the reaction is desolvated more than the transition state.

The Iso-composition activation energy values of the reaction were found to be depleted from 108.05 kJ/mole to 70.26 kJ/mole with increasing concentration of t-butanol in the reaction media. From this depletion, it has been confirmed that the initial state of the reaction is desolvated and its transition state is solvated.

49. Solvent Effect on the Mechanistic Pathways of Solvolysis of Ethyl Salicylate in Water-EG Media

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Keywords : *Mechanistic Pathway, Water cluster, Free water, Dipolar-aprotic, Viscous, Bulk dielectric, Transition state.*

The kinetic study of the solvent effect on the mechanism of alkali catalysed hydrolysis of ethyl salicylate has been carried out in water-EG media having varying concentration of ethylene glycol ranging from 30 to 80% (v/v) and at different temperatures ranging from 20 to 40^{o}C at interval of 5^{o}. Effect of change of concentration of the organic co-solvent of the reaction media (water-EG) was minutely observed and quantitatively reflected in terms of number of water molecules associated with the transition state of the reaction. On the basis of the number of water molecules associated with the activated complex of the reaction, it was inferred that alkali catalysed hydrolysis of salicylate ester follows $B_{AL}{}^2$ mechanistic path.

50. Studies on the Kinetics and Mechanism of the Solvolysis of Aromatic Formate in Water-EG Media

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Keywords : *Ion-dipolar, Aromatic formate, Activation Parameters, Solvolysis, Mechanistic Path, Iso-dielectric, Solvent-solute Interaction.*

The kinetics of acid catalysed solvolysis of Benzyl formate was studied in water-ethylene glycol media of varying composition ranging from 30 to 80% of ethylene glycol at different temperatures ranging from 20^{o}C to 40^{o}C.

The initial sharp decrease followed by slow but smooth depletion in the rate with gradual addition of the organic co-solvent in the reaction media and with increasing temperature of the reaction has been explained in the light of solvation or desolvation of initial and transition state to the different extent. The changes in the values of iso-composition and iso-dielectric activation energies of the reaction have been evaluated.

Enhancement in the values of free energy of activation, ΔG^*, with simultaneous decrease in enthalpy of activation, ΔH^*, and entropy of activation, ΔS^*, reveals that the specific solvation is taking place in the reaction media and the reaction is enthalpy dominating and entropy controlled.

Effects of ionic strength and [H^+] ion reveals that the reaction is of ion-dipole type and it follows $A_{AC}{}^2$ mechanism.

51. Studies on the KineticsA Kinetic Study of the Solvolysis of an Iso-butyrate Ester in Water-t-butanol Mmedia

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Keywords : *Solvolysis, Substituted Ester, Solvent Systems Solvent-Solute Interaction, Depletion, Specific Solvation, Uni and Bimolecular.*

The kinetics of alkali catalysed solvolysis of methyl isobutyrate (substituted ester) was studied in water-t-butanol media of varying composition ranging from 20 to 80% of t-butanol in the reaction media at different temperatures varying from 20 to 40^{o}C. The rate of the reaction was found to decrease with increasing proportion of the t-butanol at all the temperatures. It was observed that the values of activation energy (iso-composition) go on increasing with gradual addition of the organic co-solvent. For variation in rate and activation energy of the reaction, it is inferred that effect of change in dielectric constant values and selective solvation of reactants are responsible for depletion in rate while solvation and desolvation of the initial and the transition states respectively are the causes for enhancement in the values of iso-composition activation energy of the reaction.

From the decreasing number of water molecules from 1.678 to 0.355 with increasing temperature of the reaction, it is inferred that t-butanol changes its mechanistic path from unimolecular to bimolecular.

From the evaluated value of iso kinetic temperature (324.40) of the reaction, it is concluded that in this reaction media (water-t-butanol), there is appreciably strong solvent-solute interaction.

52. A Kinetic Study of Solvent Effect on the Solvolysis of Phthalate Ester in Water-t-butanol Solvent

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Keywords : *Depleting, Activation Parameter, Solvent-Solute Interaction, Iso-Kinetic Temperature, Specific Solvation, Stabilizer Operator.*

The kinetic study of the solvent effect of alkali catalysed hydrolysis of dimethyl phthalate was studied in water-t-butanol media having varying concentration of t-butanol (from 20 to 80% v/v). The rate of the reaction was found depleting with gradual addition of the organic content (t-butanol) of the reaction media. All the three thermodynamic activation parameters of the reaction were found to be enhanced simultaneously with the addition of more and more t-butanol in the reaction media. From the simultaneous enhancement in three thermodynamic parameters, it has been inferred that the said reaction is enthalpy dominating and entropy controlled. Ftom the plots of □H* against □S*, the isokinetic temperature of the reaction has been ealuated from the slope of the plot. The numerical value of its kinetic temperature of the reaction has been found to be 364.03. From the value of iso-kinetic temperature, which is greater than 300, it has been inferred that there is strong solvent-solute interaction in the reaction media in presence of t-butanol in it.

53. A Kinetic Study of Solvent Effect on the Activation Parametersand Solvent-solute Interaction in the Solvolysis Reactionof an Aromatic Ester

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Key words : *Activation parameter, Solvent-solute interaction, Solvolysis, Specific solvation, Iso-kinetic temperature, Co-solvent.*

The kinetic study of the alkali catalysed hydrolysis of ethyl salicylate (ion-dipolar) reaction was performed in water-EtOH media in order to highlight the solvent effect of ethyl alcohol on the thermodynamic activation parameters of the reaction and solvent-solute interaction in the reaction media. It was observed that the rate of reaction decreases with increase in the organic content (EtOH) in the reaction media. Out of the three thermodynamic activation parameters namely □H*, □G* and □S*, it was found that all of them increase with enhancement in the mole % of EtOH in the reaction media. From this observation, it was inferred that in the presence of organic co-solvent (EtOH) present in the reaction media (water-EtOH), the reaction (ion-Dipolar) is enthalpy dominating and entropy controlled. From the evaluated values of Iso-kinetic temperature which is 324, it is inferred that there is strong solvent-solute interaction for the alkali catalysed solvolysis reaction of ethyl salicylate in water-EtOH media.

54. A Kinetic Study of the Solvent Effect on the Solvolysis of Benzyl Methanoate in Water-MeOH Media

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Keywords : *Sharp and Smooth Depletion, Mechanism, Solvation, Iso-composition, Iso-dielectric, Iso-kinetic Temperature, Enhancement, Depletion, Interaction, Ion-Dipole Type.*

The kinetics of acidic solvolysis of Benzyl methanoate was studied in water-methyl alcohol media of varying composition ranging from 20 to 80% of MeOH at different temperatures (from 20^{O}C to 40^{O}C).

In the beginning, sharp decrease followed by slow depletion in the rate with gradual addition of the organic co-solvent in the reaction media and also with increasing temperature of the reaction has been explained in the light of solvation of initial and transition states to different extent. The changes in the values of iso-composition and iso-dielectric activation energies of the reaction have been explained in the light of solvation and desolvation of initial and transition states to different extent.

Enhancement in the numerical values of free energy of actication (ΔG^*) with simulatneous increase in the values of enthalpy of activation (ΔH^*) and entropy of activation (ΔS^*) of the reaction, reveals that methyl alcohol acts as enthalpy stimulator and entropy commander.

Effects of ionic strength and [H^+] ion have also been studied and it is inferred that the acid catalysed hydrolysis is of ion-dipole type and it follows $A_{AC}{}^2$ mechanistic path in water-MeOH media.

55. Ultrasonic Studies on Molecular Interaction of Saccharides in Aqueous Quanidine Hydrochloride Solutions at 298.15k

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Keywords : *Ultrasonic velocity, apparent molal compressibility, apparent molal volume and hydration number.*

Ultrasonic velocity (U), Viscosity (η) and density (ρ) of L-ascorbic acid, dextrose and sucrose in aqueous quanidine hydrochloride (0.3m) have been measured at 298.15k. The derived acoustical parameters namely adiabatic compressibility (β), apparent molal compressibility (φ_K) and apparent molal volume (φ_V) limiting apparent molal compressibilities (φ_K^0) and limiting apparent molal volume (φ_V^0) and their constants (S_k, S_V), Viscosity B coefficient and hydration number (n_H) have been computed from the experimental data. The results of these parameters have been explained on the basis of solute-solvent interaction and structure making tendency of the solutes in the solvents.

56. Synthesis of Cadmium (II) Selective Dioctyl Soium Sulfonsuccinate (Sodium bis (2-ethyhexyl) Sulfosuccinate –tin (IV) Phosphate New Hybrid Ion Exchanger

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Keywords : *Fibrous ion exchanger; Tin (IV) chloride; dioctyl sodium sulfonsuucinate tin (IV) phosphate, adsorption studies; environmental studies.*

The surfactant, dioctyl sodium sulfonsuucinate, based tin (IV) phosphate (AOT-SnP) fibroud ion exchanger has been synthesized and characterized by using different physicochemical methods. The characterization of the exchanger was performed by using IR, XRD, SEM and elemental analysis. The ion exchange property was studied by determining the ion exchange capacity, elution and concentration behavior of ion exchanger. The thermal behavior of exchanger was studied by performing ion exchange capacity at different temperatures. Adsorption studies on the synthesized material showed that it is highly selective for Cd(II), Zn(II) ions, therefore, the separations, of Cd(II), Zn(II) from other metal ions have been performed on its column and observed to be quite effective in presence of acid, alkali, alkaline eartyh and other transition metals.

57. Ultrasonic Velocity and Allied Parameters of Uni-univalent Mixed Electrolytes in Aqueous Solvent

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Keywords : *Ultrasonic velocities, inter-molecular free length, adiabatic compressibility, apparent molal compressibility, specific acoustic impedance and hydration number.*

Ultrasonic velocities of aqueous solutions of uni-uni valent mixed electrolytes have been measured at a constant frequenty of 10 MHz at 298.15 K. From the

ultrasonic velocity (u) and density (ñ) data of the aqueous solutions of these mixed electrolyte systems, the values of acoustic parameters – viz:adiabatic compressibility (β_{ad}) apparent molar compressibility (Φ_k), inter molecular free length (L_f), specific acoustic impedance (Z), hydraion number (H_n) and relativeassociatino constrant (R_A) have been obtained. The results of the study have been discussed in terms of ion-solvent and ion-ion interaction.

58. Studies of Photoacaustic Spectra and Optical Properties of Grafted Polycarbonate, Semicarbazide and Thiosemicarbazide

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Keywords : *Photoacoustic Spetroscopy, semicarbazide and Thiosemicarbazide.*

Photoacoustic (PA) of pure polycarbonate, grafted polycarbonate and its derivatives semicarbazide and thiosemicarbazide was recorded in the wavelength range of 200 to 800 nm, at a modulation frequenty 22Hz. The indigenous PA spectrometer used in the present study consist of 300 watt Xenon arc lamp, lockin amplifier, chopper, 1/8m monochromator controlled with spectra of grafted PC and its derivatives, Results revealed strong absorptions in the UV region. The absorption band in the case of PC compared to the corresponding bands in the PC. The FT-IR spectra of semicarbazide and thiosemicarbazide were also recorded. It was found that many peaks matched to each other, which shows that the semicarbazide and thiosemicarbazide have similar optical properties.

59. Solar Energy Conversion and Storage by Dye Sensitized Solar Cell

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Keywords : *Triton X-100, Rhodamine 6G, Fill Factor, Power Point, Conversion Efficiency.*

The effects of various parameters like pH, Diffusion length, electrode area and temperature on electrical output of the cell were observed and photogalvanic effect was studied in a photogalvanic cell containing TritonX-100 as surfactant, Rhodamine 6G as photosensitizer and Oxalic acid as reductant. The observed photopotential and photocurrent were 672.0 A and 165.0 μA, respectively. The observed conversion efficiency was 0.55% and the maximum output of cell was 57.06 μW. The photogalvanic cell can be used for 96 minutes in the dark and a mechanism has also been proposed for the generation of photocurrent in photogalvanic cell.

60. Excition Localization and Decomposition Dynamics In Cuprous Helide Nanocrystals

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Keywords : *Nanocrystals, Localized Luninescence.*

Excition, Localization and decomposition dynamics in cuprous halide nanocrystal is presented. We measured temporal charges of luminescence and absorption of excitons in CuCl nanocrystals embedded in Nacl or glass and CuBr nanocrystals embedded in glass. Both of the temporal charges for CuCl nanocrystals in NaCl agree well each other, and show two exponential decay.

Two decay time constants of ~100 ps and ~2 ns correspond to relaxation to the “Localized” state and radioactive recombination, respectively. In Cucl and cuBr nanocrystals in glass, the temporal changes of the differential transmission show two-exponential decay, and are different from the single exponential luminescerece decay. The decay time constant of the luminescence agrees with the fast decay time constant in the different transmission. This result shows persistent trapping of carriers, which is thought to be the origin of persistent spectal hole burning phenomena in nanocrystals.

61. Dye Sensitized Oxidationof 2-imidazolidinethione in Presence of Sodium Dodecylsulphate.

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The Dye sensitized photo oxidation of 2-imidazolidinethione (IT) in sodium dodecylsulphate (SDS) aqueous micellar solution gives 2-imidazolidine-2-yl-sulphinic acid as the primary product. The steady state rate expressions based on a likely mechanism have been derived. The data fit well into these equations showing both singlet oxygen and electron pathways. The relative efficiency of which depends upon the (IT). Higher quantum yields of product formation at high [SDS] are due to the increased efficiency of energy transfer/electron transfer processes in MB-$^3O_2$/ MB-IT pairs respectively. The effect of various kinetic parameters establishes the reaction to proceed through the participation of singlet oxygen. The ionic mechanism is suggested at higher IT concentration. Salt effect supports the stabilization of polar transition state/formation of dye rich micellar aggregates. The deactivation of triplet MB by dimeric dye species (MB2) has been postulated at higher [MB].

62. Influence of Aliphatic Chain Length on the Absorption and Fluorescence Spectral Characteristics of Norepinephrine, Epinephrine, Isoprenaline, Methyl Dopa, Terbutaline and Orciprenaline Drugs

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Influence of aliphatic chain length on the absorption and fluorescence spectral characteristics of norepinephrine, epinephrine, isoprenaline, methyldopa, terbutaline and orciprenaline has been investigated in different solvents, pH and β-cyclodextrin (β-CD). The inclusion processes are discussed by absorption, emission and semiempirical quantum mechanical calculations (DFT) methods. In solvents, the above drugs are not showing any significant absorption and emission spectral shifts.

The pH study reveals that, deprotonation takes place in the CHOH group and the longer wavelength emission at 450 nm is due to intramolecular proton transfer. All drugs gave one emission maximum in water (316 nm), whereas dual emission in β-CD (316 nm, 450 nm). β-CD study shows that (i) the above drugs are formed 1:1 inclusion complex, (ii) the shorter wavelength fluorescence intensity is regularly decreased and longer wavelength fluorescence intensity is increased, (iii) the aliphatic chain is present interior part and hydroxyl group is present hydrophilic part of the β-CD cavity and (iv) the absorption and emission spectral behavior of the drugs are different from DHBs indicate the inclusion process is different from the latter molecule.

63. Effects of Solvents, pH and β-Cyclodextrin on 2-Amino 3-Benzyloxypyridine

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Spectral characteristics of 2-amino 3-benzyloxy pyridine (2ABP) has been studied in solvents of different polarity, pH, β-cyclodextrin (β-CD) and compared with 2-amino pyridine (2AP). The inclusion complex of both aminopyridine (AP) molecules with β-CD are analysed by UV-visible, fluorimetry, FT-IR, ^{1}HNMR, SEM and DFT methods. The solvent studies shows no significant shift observed in absorption maxima between both AP molecules, but in the excited state a slight red shift is noticed in 2ABP than 2AP indicates addition of benzyloxy group in 2AP does not effectively increase the resonance interaction in 2ABP. The regular red shift observed in acidic pH solutions suggests intramolecular proton transfer (IPT) is present in both molecules. β-CD studies shows in pH ~7, 2ABP forms 1 : 2 inclusion complex from1:1 inclusion complex, however, in pH ~1 solutions 1 : 1 inclusion complex is formed. In pH ~7, a red shift is observed in 2ABP with lower β-CD concentration suggests aromatic ring encapsulated in the β-CD cavity and blue shift noticed at higher β-CD concentrations indicates pyridine ring encapsulated in the β-CD cavity.

64. Inclusion Complex Behavior of Aminobenzoic Acids with α-/β-cyclodextrins at Different pHs

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Spectral characteristics of 2-aminobenzoic acid (2ABA), 3-aminobenzoic acid (3ABA) acid and 4-aminobenzoic acid have been studied in α-/β-cyclodextrin at different pH. The inclusion complex of ABAs with α-/β-CD is analysed by UV-visible, fluorimetry, and CAChe - DFT method. Combining the results observed in the absorption, fluorescence emission and fluorescence excitation spectra; it is found that strong intramolecular hydrogen bonding (IHB) present in 2ABA. The above spectral studies show that ABAs forms a 1 : 1 inclusion complex with both CD, but in β-CD, the COOH group present in the cavity, whereas in α-CD aromatic ring present in the cavity. Binding constant and free energy change associated with inclusion process are calculated, these values suggested that the inclusion process proceeded simultaneously at 303 K and it is entropy driven process.

65. Intramolecular Charge Transfer Effects on 3,5-diaminobenzoic Acid

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Effect of solvents, buffer solutions of different pH and β-cyclodextrin on the absorption and fluorescence spectra of 3,5-diaminobenzoic acid (DABA) have been investigated. Effect of β-cyclodextrin on the absorption and fluorescence spectra of 3,5-dihydroxy benzoic acid (DHB) have been studied in pH~1, pH~7 and pH~10 buffer solutions. The solid inclusion complex of DABA with β-CD is discussed by UV–Vis, fluorimetry, semiempirical quantum calculations (DFT). The thermodynamic parameters of the inclusion process are also determined. (i) In solvents, the

observation of a large red shifted absorption and emission maxima even in non-polar solvents indicates ICT present in DABA molecule, (ii) DABA forms 1 : 1 complex with β-CD, (iii) proton transfer reactions in β-CD medium indicates, COOH group present in the hydrophilic part of the β-CD cavity whereas amino group present in the hydrophobic part of the β-CD cavity and (iv) Dual luminescence is observed in pH~1 and pH~7 solutions which shows that intramolecular charge transfer (ICT) is present in these pH. The above studies demonstrate that in DABA, an ICT interaction plays a significant role in β-CD aqueous/polar solvents.

66. First-order Hyperpolarizability Calculations and Structure Confirmation of O-chlorobenzoyl Chloride Based on Density Functional Theory Calculations

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Keywords : *Vibrational spectra; FT-IR and FT-Raman spectra; DFT calculation, first-order hyperpolarizability.*

The FT-IR and FT-Raman spectra of O-chlorobenzoyl chloride (OCBC) were recorded in the regions 4000-400 cm^{-1} and 3500-100 cm^{-1}. The fundamental vibrational frequencies and intensity of vibrational bands were evaluated using density functional theory (DFT) and standard B3LYP/6-311+G** basis set combination. The vibrational spectra were interpreted, with the aid of normal coordinate analysis based on a scaled quantum mechanical (SQM) force field. The infrared and Raman spectra were also predicted from the calculated intensities. Comparison of simulated spectra with the experimental spectra provides important information about the ability of the computational method to describe the vibrational modes. Unambiguous vibrational assignment of all the fundamentals was made using the total energy distribution (TED).Further, density functional theory (DFT) combined with quantum chemical calculations to determine the first-order hyperpolarizability.

67. Studies on the Outer-sphere Hexacyanoferrate(III) Oxidation of Aliphatic Aldehydes in Alkaline Medium

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Keywords : *Outer sphere reduction; reactivities; aliphatic aldehydes; hexacyanoferrate(III); kinetics and mechanism.*

The kinetics of the oxidation of aliphatic aldehydes by hexacyanoferrate(III) have been studied spectrophotometrically in alkaline medium. The most important iron(III) cyanide complex, $[Fe(CN)_6]^{3-}$, although a relatively mild oxidant, frequently used as an interceptor of free radicals. A unit order dependence of the reaction with respect to $[Fe(CN)_6]^{3-}$ and [aldehyde]. The rate of the reaction increases with increase in $[OH^-]$. The values of k_{obs} in the oxidation of aliphatic aledehydes in aqueous medium follow the order: $(CH_3)_2CH- > CH_3CH_2- > CH_3- > H-$. The rate constants correlate well with Taft's substituent constants with negative reaction constants. The reaction appears to be of outer-sphere type and occurs through the intermediate formation of free radicals. The products of oxidation were found to be the respective carboxylic acids in each case. Tentative reaction mechanism leading to the formation of oxidation products has been suggested.

68. Ice Crystals as Templates in Dissipative Convective Structures in Cross-linked Polysaccharide Hydrogels/Sponges

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Keywords : *Dissipative convective phenomenon, Polysaccharide gels.*

There is a substantive attention in the cross-linked polysaccharide hydrogels because of their diverse applications in drug delivery system, electronics, optics, molecular catalysis, sensors, actuators and tissue engineering. Ordered capillaries with patterned micropores were generated by dissipative convective process followed by unidirectional freezing of anisotropically ordered polysaccharide gels by ionic diffusion of metal ions. Different nanoparticles can easily be encapsulated into the gels with retention of the patterned complex microstructures. SEM, BET surface area, Rheology, Mechanical strength and FT-IR analysis were used to characterize the sponges.

69. Kinetic-spectrophotometric Determination of p-toluidine Based Upon its Periodate Oxidation Catalysed by Mn(II)

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The Mn(II) catalysed periodate oxidation of p-toluidine (TOL) in acetone-water medium is first order w.r.t. 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 4-methyl-1,2-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 TOL in the range 74.84 to 429.04 ìg/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.

70. Manganese(II) Catalyzed Periodate Oxidation of 2,6-dimethylaniline in Acetone-water Medium– a Kinetic and Mechanistic Study

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The Mn(II) catalysed reaction between 2,6-xylidine (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, $[IO_4^-] << [AMX]$, are in agreement with the rate law:

$$d[C]/dt = kK_3K_4K_w[Mn^{II}]\,[S]_0\,[IO_4^-]\,[H^+]\,/\{K_2\,K_w + (K_w + K_b\,K_2\,)[H^+] + K_b\,[H^+]^2\}$$

where kK_3K_4 is the empirical composite rate constant, K_w is ionic product of water, K_2 is acid dissociation constant of $H_4IO_6^-$ and K_b is base dissociation constant of AMX. $[S]_0$ represents the concentration of AMX which has been taken in excess. In agreement with the rate law the $1/k_{obs}$ versus $[H^+]$ profile passes through the minimum. The reaction products were subjected to solvent extraction, TLC, melting point, and spectroscopic studies and characterized as 2,6-dimethyl-*p*-benzoquinone. The values of thermodynamic parameters are: $Ea = 2.46$ kcal mol^{-1}, $A = 6.1 \times 10^6$ dm^3 mol^{-1} s^{-1}; $\Delta S^\# = -29.6$ cal mol^{-1} K^{-1}, $\Delta G^\# = 11.2$ kcal mol^{-1} and $\Delta H^\# = 1.84$ kcal mol^{-1}. Suitable mechanism has been proposed.

71. Voltammetric Study of ds-DNA-flutamide Interaction at Carbon Paste Electrode

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Keywords : *Flutamide, DNA-flutamide interaction, Modified Carbon paste electrode, DPV.*

Differential pulse voltammetry (DPV) has been used to develop an electro-analytical procedure for the determination of flutamide and evaluate its interaction with DNA immobilised on the carbon paste electrode (CPE) surface. In 0.3M phosphate buffer (pH7.0±0.01) as supporting electrolyte flutamide produced a well defined DPV peak at Ep= -0.75V vsSCE. The DPV study on the DNA-flutamide interaction clearly demonstrated that flutamide interacts preferentially with adenine and guanine groups in DNA. Thus, enabling to assign mechanism of action of the anticancer drug, flutamide. The developed method was successfully applied to the determination of flutamide in pharmaceutical formulations. The work has been supplemented by UV spectral study.

72. Nucleophilic Efficacy of Some Pyridinium Based Compounds for the Hydrolysis of *p*-nitrophenyl Acetate

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Keywords : *Pyridinium compounds,Nucleophilic reactivity, Hydrolysis, Oximes.*

Nucleophilic reactivity of some pyridinium based compounds with same alkyl chain length ($C_{12}H_{25}$) towards hydrolysis of *p*-nitrophenylacetate (PNPA) has been studied at *p*H 9.0 and temperature 27° C. The nucleophilic reactivity of newly synthesized pyridinium compounds was compared with commercially available pyridinium based compounds such as pralidoxime and dodecylpyridinium bromide (DPB). It was observed that with an increase in the concentration of these compounds there was an increase in the first order rate constant of the reaction. The apparent pK_a values of some compounds have also been determined spectrophotometrically. Among all the examined pyridinium compounds, functionalized pyridiniumoximes were found to be the most effective.

73. Physicochemical Properties of Cetyltributylphosphonium Bromide in the Presence of additives

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Keywords : *Monomeric Surfactants, Non-electrolyte, Thermodynamics of micellization, Effect of Additives.*

Physicochemical behavior of cetyltributylphosphonium bromide (CTBuPB) surfactants in presence of additives (urea, thiourea and sucrose) has been studied by conductometric measurement at 303-320 K. It was observed that the cmc and degree of micellar ionization (á) values increases with increasing concentration of non-electrolyte (urea, thiourea and sucrose). The standard free energy (ΔG°_{m}), enthalpy (ΔH°_{m}), and entropy (ΔS°_{m}), of micellization were determined using the temperature dependence of cmc. The dependence of these thermodynamic parameters on additives was determined. The free energy of micellization and enthalpy were found to be negative and show system is spontaneous.

74. Effects of Electrolytes on Micellar and Surface Properties of Some Cationic Surfactants

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Keywords : *Effect of electrolyte, micelle, cationic surfactant, cmc, surface properties.*

Micellar and surface properties of cationic surfactants i.e. cetyldiethylethanolammonium bromide (CDEABr) and tetrdecyldiethylethanolammonium bromide (TDEABr) in the presence of sodium halide (NaCl, NaBr and NaI) have been investigated by conductivity and surface tension measurements at 300 K. The critical micelle concentration (cmc) and interfacial parameters, such as the maximum surface excess (Γ_{max}), minimum area per molecule (A_{min}) and surface presence at the cmc (π_{cmc}) were computed from the surface tension data. The cmc and degree of micellar ionization (α) values were found to decrease with an increase concentration of salts and values decrease in the order NaCl < NaBr < NaI. Thermodynamic parameters, standard Gibbs free energy of micellization (ΔG°_{m}) and adsorption at air/water interfaces (ΔG°_{ads}) were also evaluated. The standard free energy of micellization values were obtained to be negative and show spontaneity.

II. ORGANIC CHEMISTRY

75. Synthesis, Spectral Characterization and Biological Evaluation of 4H-1, 4-benzothiazines

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

4H-1, 4-Benzothiazines are synthesized by condensation followed by oxidative cyclization of 2-aminobenzenethiols with β-diketones/β-ketoesters in presence of dimethylsulfoxide. Their antimicrobial activity has also been carried out. The structures of the synthesized compounds have been established by elemental analysis and spectroscopic data.

76. A New Acrlated 6-methoxyluteolin-7-O-B-D-Glucopyranoside from the roots of Anogeissus Latifolia (Wall)

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Anogeissus Latifolia (Wall) (N.O. Combretaceae) is known locally as DHAVA in Hindi and is distributed in the tropical and temperate regions of India. The roots of the plant are reported to possess important medicinal values.

The concentrated 95% ethanlic extract of the defatted, powdered roots was dissolved in water and separated into water soluble and water insoluble portions. The concentrated water soluble part was extracted successively with chloroform, ethyl acetate and acetone. Removal of solvent under reduced pressure from acetone extract yielded dark brown viscous mass, crystallized from chloroform : acetone (1:1). It gave the characteristic colour reactions of a flavonoid glycoside and analysed as $C_{13}H_{28}O_{14}M^{-}$ = 624, m.p. 258-60°C, ( )$_{D}$23-125° (in pyridine), and was identified as; 6-methoxyluteolin-7-)-(2”-O-p-coumaroyl)-B-D-glucopyranoside.

77. Synthesis of Quinolone Substituted Pyrazoles, Isoxazoles and Pyridines as Potential Blue Luminophors

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Keywords : *Dihydropyrazoles, Isoxazoles, Pyridines, Absorption and emission, Quantum yields, Heat of Formation, HOMO-LUMO energy*

Series of quinolone C_3-substituted pyrazolines, isoxazolines, pyridines and pyrimidines were synthesized in good yields by the cyclocondensation reactions of α,β-unsaturated ketones and hydrazines, hydroxylamine hydrochloride and dimedone respectively. The quinolone derivatives were synthesized and further studied for their photophysical properties. High absorption and quantum yield are found for N_1-phenyl and $C_{3,\ 4}$-dimethoxy substituents on phenyl ring. Energy optimization by PM3/PM6 methods showed high stability, suitable candidates to be use as future blue emitters and in the opto-electronic devices.

78. Synthesis of New Thieno [2,3-*d*] Pyrimidines, Thieno [3,2-*e*] Pyridines and Thieno [2,3-*d*][1,3] Oxazines

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Keywords : *Aminothiophene, Gewald reaction, Thienooxazines, Thienopyrimidines*

o-Aminothiophene dicarbonitrile on neat reaction with cyclic ketones in anhydrous $ZnCl_2$ yielded mixture of iminospirooxazine and fused amino pyridine

derivatives. Similarly, pyrimidine derivatives were obtained by the reaction of this intermediate with formic acid and DMF-DMA followed by hydrazine hydrate. The reaction on *o*-aminothiophene diamide at ambient temperature with cyclic ketones yielded spiropyrimidine as a sole product in quantitative yield. The regioselective pyrimidine and dihydro pyrimidine derivatives were also obtained by the reaction with aromatic aldehydes in presence of piperidine and molecular iodine respectively.

79. Synthesis of Nicotinonitrile Derivatives and Study of their Photophysical Properties

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Keywords : *Quinolone chalcone, Nicotinonitrile, Absorption and emission properties, Substituents effect*

A convenient route were successfully developed for the synthesis of novel nicotino nitrile derivatives by three component Dimroth reaction of chalcones, malononitrile and secondary heterocyclic amines, or sodium salt of alcohols. Nicotinonitrile derivatives obtained in excellent yields, their structures were established by spectroscopic techniques and elemental analyses. Synthesized nicotinonitriles were further studied for their photophysical properties.

80. New Bioactive Flavone Glycoside from *caesalpinia crista* Linn

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Caesalpinia crista Linn. belongs to family Leguminosae. It is commonly known as Karanjava or Karanju in Hindi. It is found throughout in India and most tropical countries. The juice of the leaves are useful in elephantiasis and small pox; destroy the bad odour due to perspiration. Its flower cures kapha and vata. The seeds are useful in treatment of colic, malaria, hydrocele, leprosy and skin diseases. The root-bark is useful in treatment of tumour and for removing placenta. The oil from the seeds is useful in convulsions and paralysis. The leaves and seeds after roasting with castor oil are applied externally to inflammatory swelling especially inflammed to piles, hydrocele, and orchitis with benefit. In the present paper we report the isolation and structural elucidation of a new compound A which has been isolated from the flowers of this plant. Compound A has been characterized as 3, 5, 3'-trihydroxy-6, 7, 4'-trimethoxy flavone-3-*O*-α-L-rhamnopyranosyl-3'-*O*-β-D-xylopyranosyl-(1→4)-*O*-β-D-galactopyranoside alongwith two known compounds Mearnsitrin (B) and Lyratin (C) by various colour reactions, chemical degradations and spectral analysis. These compounds were screened against various bacteria and fungi which showed good results.

81. A new flavone glycoside from *Tussilago farfara* (Linn.)

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Tussilago farfara (Linn.) belongs to the family Compositae. It is commonly known as ‘’Watapana’’ in Hindi. It is found throughout in India. It is a white, woolly, scapigerous herb, with a perennial rootstock. Its leaves are long-petioled, all radical, coming after the flowers, orbicular, cordate, toothed, 7.5-25 cm. broad, cobweb by, above, white tomentose beneath. Its leaf is used to remove ‘’ vata’’.

The roots and leaves are used in chronic bronchitis, asthma, chest complaints, inflammations. Its leaves are used for smoked like tobacco, as a domestic remedy for obstinate colds and coughs. It is used as expectorant and sudorific properties, also used in treatment of dyspepsia diarrhoea, rheumatism and nervous disorders. The present paper deals with isolation and identification of new flavone glycoside m.p. 246-248°C, m.f. $C_{32}H_{37}O_{19}$, $[M]^+$ 725 (FABMS) has been isolated the methanol soluble fraction of leaves of the *Tussilago farfara*(Linn.). Its structure was characterized as 3,5,7,4'-tetra- hydroxy flavone-3–O-β-D-glucopyranosyl (1→3) -O-β-D-xylopyranosyl-7-O-α-L-rhamnopyranoside, alongwith two known compounds Taxifolin (B) and Quercitrin (C) by various chemical degradations and spectral analysis.

82. Phytochemical Constituents from *Vernonia anthemintica* Willd

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Vernonia anthemintica Willd belongs to family Compositae. It is commonly known as Somraj or Kaliziri in Hindi. It is found throughout India. It is annual, robust, erect, leafy; stems 60-90 cm. high, branched, pubescent. Its seeds have sharp bitter taste. It is used in the treatment of asthma, kidney troubles, and hiccough. It is also applied in inflammatory swellings; remove blood from the liver, good for sores and itching of the eyes. The juice of leaf is given to cure phlegmatic discharges from the nostrils. The seeds are also used against some skin infections such as leucoderma and psoriasis. The present paper deals with isolation and characterization of three compounds; myricetin, quercetin and astragalin from seeds of *Vernonia anthelmintica* Willd by various colour reactions, chemical degradation and spectral analysis.

83. Condensed bridgehead nitrogen hetyerocyclic systems: synthesis of thiazolo [3,2-b]-s-triazole, isomeric thiazolo [2,3-c]-s-triazole, thiazolo [3,2-b]-s-triazole-5 (6*h)* -one, imidazolo [2,3-b]-1,3,4- thiadiazol-5-one, 1,3,4- oxadiazolo [3,2-a] -s-triazine-5,7 (6*h*)-dithione and 1,3,4-triazolo [3,2-b]-s-triazine-5,7 (6*h*)-dithione as antifungal agents

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Keywords : *Condensed bridgehead heterocycle, antifungal agents*

A new series of bridgehead nitrogen containing heterocycles like thiazolo [3,2-b]-s-triazole, isomeric thiazolo [2,3-c]-s-triazole, thiazolo [3,2-b] -s-triazole-5(6*H*)-one, imidazolo [2,3-b]-1,3,4-thiadiazol-5-one,1,3,4-oxadiazolo [3,2-a]-s-triazine-5,7(6*H*)-dithione and 1,3,4-triazolo [3,2-b]-s-triazine-5,7(6*H*)-dithione have been synthesized and compounds have been tested for their antimycotic potential against human pathogenic fungi. The structures of the compounds have been established with the help of elemental and spectral data (IR,PMR and Mass).

84. Synthesis of 3-{4'-(2", 4"-dichlorobenzyloxy)-phenyl}-4-amino-5-mercapto-1, 2, 4-triazole and its Derivatives as Antileishmanial and Antifungal Agents

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Keywords : *Triazole, triazolo-thiadiazole, triazolo-thiadiazine, antileishmanial agents, antifungal agents.*

3-{4'-(2",4"-Dichlorobenzyloxy)-phenyl}-4-amino-5-mercapto-1,2,4-triazole **1** was prepared by treating 4-(2",4"-chlorobenzyloxy)-benzoylhydrazine successively with alcoholic potassium hydroxide-carbon disulphide and hydrazine hydrate, which on reaction with hydrazine hydrate, phenyl hydrazine, carbon disulphide, benzoic acid, benzoin, phenacyl bromide, phenyl isothiocyanate, formic acid, chloroacetyl chloride, benzaldehyde and isatin gave condensed bridgehead heterocycles *i.e.* triazolo-thiadiazoles and triazolo-thiadiazines. Compounds **2-12** were tested for their antileishmanial potential against *Leishmania donovani* and for antimycotic potential against human pathogenic fungi. Pentamidine was taken as standard drug for antileishmanial activity and fluconazole for antifungal activity.

85. A Facile Method for the Synthesis of some Biorelevant *N*-lactosylated Thiosemicarbazones

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Key words : *Lactosyl isothiocyanate, thiosemicarbazide, thiosemicarbazones.*

Much of the cutting edges of synthetic medicinal and biological chemistry meet at the cross roads of sugar derivatives. Sugar isocyanates are important intermediate in the synthesis of various wide linked derivatives. Prompted by the aforesaid pharmaceutical activities, we aimed at developing a new approach for the synthesis of *N*-Lactosylated thiosemicarbazones, in order to study their antibacterial and antifungal activities.

A series of 4-hepta-O-acetyl-β-D-lactosyl-1-arylidine thiosemicarbazones have been synthesized by condensing hepta-O-acetyl-β-D-lactosyl thiosemicarbazide and aryl aldehydes. All the products obtained have been characterized by elemental and spectral studies.

86. Synthesis and Leptospirocidal Activity of Novel Series of N-Mannich bases of 3-(Phenylimino/44-chlorophenylimino)-2,3-dihydro-1-((N-substituted piperaziny)methyl)quinoxaline-2-(1H)-one

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Keywords : *Quinoxalines, Mannichbase, in-vitro leptospirocidal activity, in-vivo leptospirocidal activity*

A novel series of N-Mannich bases of (E)-3-(Phenylimino/4-chlorophenylimino)-2,3-dihydro-1-((N-substituted piperazinyl)methyl)quinoxaline-2-(1H)-one **4 a-f** and **5 a-f** were synthesized and evaluated Leptospirocidal screening against *Leptospiral interrogans.* The requisite **3a** and **3b** were obtained by Schiff reaction between quinoxaline-2, 3-dione 2 and aniline/*p*-chloroaniline. The Schiff bases underwent N-Mannich reaction with various substituted piperazines to yield title compounds. The synthesized compounds were evaluated *in-vitro* and *in-vivo* Leptospirocidal screening against *Leptospira interrogans*. The *in-vitro* activity was evaluated by microtitre plate method. The *in-vivo* activity was evaluated by MAT (Microscopic agglutination) testing. Biochemical and hematological studies were also carried out. Three compounds **5a, 5b** and **5c** displayed an encouraging Leptospirocidal effect.

87. Studies in the Antimicrobial Activity of S-triazines

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Keywords : *S-triazine, antimicrobial activity*

I-substituted-2thio(1H)-4-[(2-imino-4-thiobiureto-5-yl)guanyl]-6-sustituedamino-1-2-dihydro-s-triazines[1] [3a(i) to 3f(iv)] have veen obtained by the isomerisation of 2-sustitutedamino-4-(2-imino-4-thiobiureto-5-yl-carbamidino)-6-substitutedimino-1-3-5-thiadiazines [2a(i) to 2f(iv)] in presence of thanolic sodium bicarbonate solution, which have been obtained by basification of their hydrochlorides [1a(i) to 1f(iv)] which are synthesized by the interation of 1-formamidiono-3 –thioamido-N-substitutedformamidinothiocarbamides and N-aryl/alkylisocyanodichlorides. The latter were prepared initially by the condensation of N-aryl/alkylisothiocyanate and 1,3- Diformamidionothicarbamide. The structure of all these compounds was established on the basis of elemental analysis and IR and NMR spectral data. All the synthesized compounds have been screened for their antimicrobial activity against both gram-positive and gram-negative human pathogens.

88. 5-Substitutedarylidene-2-substututed aryl-4-oxo-1,3-thiazolidine Derivatives of Indole : A New Class of Biological Active Compounds

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Keywords : *Antitubercular, Thiazolidine, Indole, Conventional, Microwave irradiation.*

We report herein the synthesis and biological activity of a new kind of thiazolidine derivatives of indole. The reaction was carried out by both conventional and microwave methods. The chemical structures of all the synthesized compounds were deduced on the basis of FTIR, 1H-NMR, 13-C-NMR and FAB-Mass spectral and microanalytical data. All the synthesized compounds of series (5a-m) and (6a-m) were evaluated for their antitubercular activity against Microbacterium tuberculosis H37RV. Unexpectedly, some thiazolidine derivatives of indole displayed better activity.

89. Synthesis of some Novel *n*-glucosylated Isothiobiurets

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Keywords : *N-glucosides, aryl–S–benzyl isothiocarbamides, glucosyl isocyanate, isothiobiurets.*

Several 1-aryl – 5 - tetra – *O* – acetyl – β – glucosyl – 2 - *S* – benzyl – 2-isothiobiurets have been prepared by the interaction of aryl – *S* – benzyl isothiocarbamides and tetra – *O* – acetyl - β – glucosyl isocyanate. Non glucosidic isodithiobiurets and isothiobiurets are known to show anticonvulsant and hypnotic activities. While some sugar isothiobiurets and isodithiobiurets shows potential antimicrobial activities The structures of the newly synthesized compounds have been established on the basis of usual chemical transformations and IR, ^{1}HNMR and Mass spectral studies.

90. Synthesis and Antimicrobial Studies of Novel *N*-maltosyl 1,2,4-thiadizolidine-3-one Hydrochlorides

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Keywords : *Synthesis, Antimicrobial activity, Peracetylated maltosyl carbamides, Isothiocarbamoyl chloride, Peracetylated maltosyl thiadizolidine-3-one.*

A series novel of *N*-maltosylated 1,2,4 -thiadizolidine -3-one hydrochlorides possessing 1,2,4 –thiazolidine ring (substituted) were efficiently synthesized by oxidative cyclisation of peracetylated maltosyl carbamides with *N*-phenyl-*S*-chloro isothiocarbamoyl chloride. The synthesized compounds were structurally confirmed by analytical and spectral data and evaluated for their in vitro antimicrobial activities

using standard cup plate method against bacteria *E.coli*, *P. aeruginosa*, *P.vulgaris*, *S.aureus* and fungi *A.niger*, *C. albicans.*

91. Quantitative Structure Activity Relationship Studies on some Newly Synthesized Benzimidazole Derivatives using Phase Transfer Catalysis

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Keywords : *Phase transfer catalysis, Physicochemical parameters, Hydrophobic parameter, Quantitative structure-activity relationship (QSAR), 4,6-diphenyl-5[2-(2- methylprop1-enyl)-1H benzimidazole-1yl] pyrimidine-2-(5H)-thione*

A new series of 4,6-diphenyl-5[2-(2-methylprop1-enyl)-1H benzimidazole-1yl] pyrimidene-2-(5H)-thione derivatives [3a-q] has been synthesized and subjected to evaluate their antibacterial properties. All the synthesized compound of the series elicits, remarkable activity in comparison to standard drug (ampicillin). A number of descriptors were tested to adjudge a quantitative correlation between activity and structural features. However, significant correlations have emerged between activity and physicochemical parameters viz. polarizability parameter (MR) hydrophobic parameter (log P). Moreover, results are interpreted on the basis of multiple regression and cross-validation methodology.

92. Synthesis of new series of N-3-[-{2-(substitutedpheny1-4-oxo-5-(substitutedbenzylidene)-1,2-thiazolidine}-iminocarbamyl}-propy1-2-aminothiazole

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Key words : *synthesis, 2-aminothiazole, 4-oxo-thiazolidine.*

Tiazolidinone derivatives are playing an important role as widely exploited pharamcophore in medicinal chemistry having divers biological activity such as antimicrobial[1], antifungal2, herbicidal activities3, antiproliferative activity4, antinflammatory5, antiviral6, antidiabetic7, have been found to be associated with thiazolidinone derivatives. Substituted thiazolidine derivatives represent important key intermediates for the synthesis fo pharmacologically active drug. Thiazoles are amongst the most frequently encountered heterocycles in compounds of biological interest along with many other applications. They have been shown to possess abroad spectrum of biological activity depending on their particular structure antimicrobial8,9, antiinflammatory10, activities are observed in thiazole. Some synthetic thiazoles have exhibited a range of biological actities such as antibacterial11, antifungal12, antitumor13, antipsychotic13, anticonvulsants 15. Recently studies have shown the synthesis of some new thiazoles candidates as antimicrobial and anticancer agent. We have decided to synthesize a new series of N-3-[{2-substitutedphenyl-4-oxo-5-substituedbenzylidene-1,3-thiazolidine}-iminocarbamyl]-propyl-2-aminothiazole, compound 5(a-s). the starting material, 2-aminothiazole with 1-bromo-3-chloropropane undergoes electrophilic substitution reaction yielded N-(3-chloropropyl)-2-aminothiazoles, compound 1. The compound 1 on the reaction with urea afforded N-{3-(aminocarbmyl)-propyl}-2-aminothiazole, compound 2. the compound 2 on the reaction with several selected substituted benzaldehydes undergoes condensation reaction to afford N-{3-(substitutedbenzylidine-iminocarbamyl)-propyl} 2-aminothiazole, compound 3(a-s). The cycloaddtion reaction of thioglycolic acid with compound 3(a-s) in the presence of anhydrous $ZnCl_2$ gave new heterocyclic cmpunds N-3[-{2-(substitutedphyenyl-4-oxo-1,3-thiazolidine}- iminocarbamyl]-propyl-2-aminothiazole, compound 4(a-s). The compound 4(a-s) on treatment with various selected substituted benzaldehydes in the presence of C_2H_5ONa undergoes knoevenagel condensation reaction yielded compound 5(a-s). The structure compounds 1,2, 3(a-s), 4(a-s) and 5(a-s) were confirmed by IR, H NMR, 13 C NMR, FAB mass and chemical analysis.

93. Synthesis, Antimicrobial, Insecticidal and Anthelmintic Activity Studies of some New n-(5-methyl-1-(4-bromo phenyl-1,2,3-triazol-4-yl) Carbamic Acid Ester Derivatives.

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Keywords : *Synthesis, 1,2,3 Triazole, carbamic acid ester, antimicrobial activity, antifungal activity and anthelmintic activity*

The objective of the present study is to synthesize some new carbamic acid ester derivatives containing 1,2,3 triazole nucleus and to investigate the antimicrobial, insecticidal and anthelmintic activity of them. 5-methyl-1-(4-Bromophenyl)-1,2,3 triazole-4-carbonyl azide is used as a precursor to synthesize some biologically active alkyl/ aryl N-(5-methyl-1-(4-bromo phenyl)-1,2,3-triazol-4-yl), Carbamic acid ester derivatives. The IR and ^{1}HNMR spectral studies and elemental analysis confirmed the structures of these compounds. Several derivatives have been synthesized and screened for their antibacterial efficacy against *B. fragilis, B. vulgatus*, *F. oxysporum* and *T. viridae*, Insecticidal activity against *Periplaneta americana* and anthelmintic activity against *Pheretima Posthuma* (Indian adult earthworm).

94. An Expedient Synthesis, Spectral and Antimicrobial Study of *n*-maltosides

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Keywords : *Antimicrobial activity, maltosyl isothiocyanates, maltosyl aryl thiocarbamides maltosyl benzothiazolyl thiocarbamides, maltosyl alkyl thiocarbamates*

N-glycosides have gained increasing popularity as drug candidates. The current study was related to synthesis and antimicrobial activity of novel maltosyl

aryl thiocarbamides, maltosyl benzothiazolyl thiocarbamides and maltosyl alkyl thiocarbamates. A sequence of novel 1-hepta-*O*-benzoyl-β-D-maltosyl-3-aryl-thiocarbamides,1-hepta-*O*-benzoyl-β-D-maltosyl-3-substituted benzothiazolyl thiocarbamides and 1-hepta-*O*-benzoyl-β-D-maltosyl-O-alkyl thiocarbamates were synthesized by the interaction of hepta-*O*-benzoyl-β-D-maltosyl isothiocyanate with various aryl amines, 2-aminobenzothiazoles /substituted benzothiazoles and alcohols. IR, ^{1}H NMR, Mass spectral studies and elemental analyses evidenced the products obtained. The compounds synthesized were investigated for their antimicrobial activities against *Proteus vulgaries, Escherichia coli, Salmonella typhimurium, Staphylococcus aureus, Pseudomonas aeruginosa and Aspergillus niger.* Some of these tested compounds exhibit moderate and strongest inhibitory activity against the tested strains of bacteria and fungus.

95. Characterization and Identification of Oligosaccharides from Seeds Polysaccharide of *Acrocarpus fraxinifolius* Wight. Plant

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Keywords : *Oligosaccharides from Acrocarpus fraxinifolius Wight, seeds polysaccharide*

Acrocarpus fraxinifolius Wight. plant (Fabaceae) is known as *Mandania* and occurs in Garhwal region of Northern India. Seeds exhibited antimicrobial activities and Ayurvedic system of medicine. Seeds yielded a water soluble sugars as D-galactose and D-mannose in 1:3 molar ratio. Partial acid hydrolysis of seed polysaccharide over charcoal celite column and paper chromatography of hydolysate afforded three disaccharide and one trisaccharide. These oligosaccharides were purified separately and characterisol by its optical rotation, derivatives (disaccharides), D.P., reduction with sodium borohydride, acid hydrolysis and periodate oxidation studies. Oligosaccharides were characterized as : (I) α-D-galactopyranosyl-

(1→6)-O-α-D-mannopyranose (II) α-D-mannopyranosyl-(1→6)-O- α-D-mannopyranose (III) β-D-galactopyranosyl-(1→4)-O-β-D-mannopyranose and (IV) β-D-mannopyraonsyl-(1→4)-O-β-D-mannopyranosyl-(1→4)-O-β-D-mannopyranose. Oligosaccharides III & IV indicates that the main polymer chain is made up of D-galactose and D-mannose units which are joined through (1→4)-β-type while I & II supports the fact that branches of main chain consists double units of non-reducing D-galactose and D-mannose hexoses are glycosidically linked through (1→6)-α-type linkages at non-reducing terminal position of backbone. On the above finding the oligosaccharides resulted are fully favour for the support of polysaccharide structure for the seed galactomannan of *Acrocarpus fraxinifolius* Wight. plant.

96. A Practical and Efficient Method for the Synthesis fo 3,4,5,6,7,8-hexahydro-1-benzyl-isoquinolines via Bischler-Napieralski Reaction

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Keywords : *Bischler-Napieralski reaction: 3,4,5,6,7,8-hexahydro-1-benzyl isoquinolines; N-2- (I-cyclohexenyl) ethyl-1 – phenyl acetamides, trimethylsilyl iodide; trimethylisilyl chloride.*

A practical and efficient method has been achieved for the synthesis of key drug intermediate 3,4,5,6,7,8-hexahydro-1-benzyl isoquinoline derivatives by the Bischler-Napieralski type cyclization of non-activated N-2-(I-cyclohexenyl)ethyl-1-phenyl acetamides using in situ generated trimethylsilyl iodide (ITMS) from trimethylsilyl chloride (TMSCI) and potassium iodide in excellent yields. The products are the key intermediates for antitussive and analgesic drugs and their analogues.

97. Bio-ethanol Production Technology by Advanced Catalytic Reaction at Laboratory Scale using non Bio-catalyst from Cellulosic Feedstock

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Cellulose and hemicellulose are the two main reactants of higher composition in the ligonocellulosic feed that are required to be entreated for the production of ethanol, which is applicable for various alcoholic and biofuel standards. Cellulose treatment with biocatalyst and subsequent reactions that yield ethanol can be imitated through non bacterial catalysts at laboratory scale for the biofuel standard. These reactions (imitated laboratory scale production techniques) that assume the production of sugars and fatty acids as intermediates can be replaced with assumption of disaccharides production as intermediates and a proposed mechanism can be used with non-bacterial catalysts than enhance the reaction kinetics and produce ethanol at industrial scale. Similar to the prior technology in ethanol production, the suggested mechanism tried over also is a step wise multiple reaction. First reaction that involves the breakdown of polysaccharide cellulose into a disaccharide cellubiose is a catalytic reaction that mainly determines the rate of ethanol synthesis. This reaction is observed with normal acidulous catalysts and impressing optimization temperature and pressures over it. Besides the ionization stimulation available for the reactant molecules from acidulous substrates, it is observed that the rate is enhanced for times upon usage of an ionizing solvent for the entire hydrolysis reaction. Various ionizing catalytic solvents were observed and it has been observed yielding better conversion level at usage of complex ionizing compound especially with chlorine on the ionizing sphere of the complex. This has been tested by four carbon based coordinate compound with chlorine on the covalent side. The produced disaccharide is then processed with hydrogen iodide to give composition of fatty acids which can be pyrolysed to obtain smaller alcohols and Paraffins such as ethanol, methanol, butanol etc.,.

98. Insect Antifeedant Potent Tröger Bases

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Key words : *Chiral nitrogen compounds; Halogen substituted Tröger bases; Electrophilic substitution; Enantiomeric excess; Insect antifeedant activity*

A series of mono- and di- halogen substituted Tröger bases (chiral nitrogen compounds) are synthesized by substituted anilines and para formaldehyde in presence of anhydrous aluminium chloride catalyst. The product was resolved for getting (S, S + / R, R -) enantiomeric excess Tröger bases. The yields of the obtained Tröger bases are more than 35%. They are characterized by their physical constants, microanalysis and spectral (Uv-Vis, IR, NMR both ^{1}H and ^{13}C and Mass) data. Generally cyclic organic compounds contain one hetro atom with halogens they possess insect antifeedant activity. Based on this the author examine the antifeedant activity of the above synthesized Tröger bases. Dethlers and Caster leaf discs experimental method have been applied for evaluation of the insect antifeedant activity using 4th instar larvae such as *Caster semilooper* and *Achoea janata L.* The di- halogen substituted Tröger bases are most active against 4th instar larvae.

99. Microwave Assisted Bromomethylation of Aromatics : A Green Approach

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Keywords : *Microwave, Aromatics, Bromomethylation*

We report herein bromomethylation of aromatics material by microwave to yield bromo-methylation of aromatics, mediated by microwave to yield bromomethylated aromatic rings which are useful synthetic intermediates.

100. Curcumin Derived Heterocyclic Compounds Catalyzed by $SnCl_2.2H_2O$ under Microwave Irradiations and their Biological Activity

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Synthesis of curcumin heterocycles are disclosed using microwave irradiations in presence of $SnCl_2.2H_2O$. Method is very rapid, environment friendly, chief and high yield of the compounds are obtained. Catalyst used in experimental method is chief and easily available. All the synthesized compounds were characterized by their melting points, UV-visible, IR, ^1H-NMR and Mass spectra. Antibacterial and antifungal activity of the compound is evaluated by using some bacteria viz. *Pseudomonas aeuriginosa, Salmonella typhi, Escherichia coli* and *Staphylococcus aureus,* some fungi viz. *Aspergillus niger, Aspergillus flavus* and *Candida albicans.*

101. Synthesis of 1,2,4 - Trisubstituted 2- imidazolin-5- ones Condensed Pyrazolines

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Keywords : *imidazolines, pyrazolines, condensed ring systems*

Imidazolinones exhibit diverse biological properties. Pyrazolines are another important series of heterocyclic compounds associated with a wide range of pharmaceutical properties such as antidiabetic, analgesic, antifungal, antibacterial and anticonvulsant agents. Therefore, the compounds in which both the rings are fused must have these combined properties.1,2,4-trisubstituted-2-imidazolin-5-ones(I) are prepared from 4-arylidene-2-aryl-oxazol-5-ones by well known methods and treated with hydrazine and phenylhydrazine to obtain corresponding imidazolidinopyrazolines.

102. Eco-friendly Friedel-crafts Acylation of Aromatic Compounds

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Keywords : *Acylation, Green Chemistry, Lewis acids, Zinc Oxide*

A green alternative to the conventional Friedel-Crafts acylation reaction has been achieved by using inexpensive and non-toxic Zinc Oxide (ZnO) at room temperature. Acylations of arenes and ferrocenes were tried with acidchlorides and acidanhydrides as acylating agents in presence of different inorganic solids e.g., Zine Oxide, Alumina etc.

A simple, efficient and green procedure has been developed for mono-acylation of different arenas and ferrocenes with acidchlorides over Zinc Oxide in 2:1:2 molar ratio. Isolated mono-acylated aromatics and acylferrocenes were characterized by elemental and spectral (IR & NMR) data analysis. Recovered catalysts can also be reused without much loss of efficiency.

103. Synthetic Aspects of Novel Heterocyclic α-diones for Thiophenic Drugs

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Keywords : *Chalcones, [4+2] cycloadditions, Computational analysis, Spiropyrenes, Microwave, Sonochemical, Computational studies*

Heterocyclic compounds represent an important and integral class of organic compounds which are well recognized for their multifaceted biological properties and medicinal relevance. The chemistry of heterocyclic α-diones has been the

subject of considerable interest due to their versatile applications in organic synthesis. The results would be of immense importance to synthetic organic/ heterocyclic chemists, medicinal scientists, and biological scientists as well as in pharmaceutical industry. Benzo[b]thiophene-2,3-diones may act as building blocks for thiophenic drugs of industrial stand point. Our strategic work is based upon synthesis of models for thiophenic drugs *via* reactions of benzo[b]thiophene-2,3-diones with aromatic substrates. The work focuses on the reaction of benzo[b]thiophene-2,3-diones with aromatic and hetero aromatic amines and ketones as well as comparison of reactivities under conventional and microwave/ sonochemical methods. The stereochemical features and conformational behaviour of products as well as intermediates have been studied by Gaussian 03 suite of programs at B3LYP and CASSCF level. The results of our recent studies will be presented.

104. Comparative Study of Microwave Induced and Conventional Synthesis of Acetylated Sugar Isothiocyanates and Related Thiocarbamides

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Key words : *MORE, Conventional synthesis, Sugar isothiocyanates, Thiocarbamides.*

Owing to present environmental awareness, attempts are being made towards the evolution of environmentally benign processes using microwave induced organic reaction enhancement (MORE). MORE is simple, fast, clean, efficient and economical method for the synthesis of organic molecules. Microwave assisted organic reactions are rapidly becoming recognized as a valuable tool for facilitating a wide variety of transformations. To explore the variety of applications in carbohydrate chemistry, reactions have been carried out with microwave irradiation as activating agent. At the present time, microwave assisted carbohydrate chemistry is experiencing considerable growth and has potential to greatly improve the image of carbohydrate chemistry. Sugar isothiocyanates are the versatile reagent in the field of carbohydrate chemistry. In our laboratory, synthesis of acetylated sugar (glucose, galactose, lactose and maltose) isothiocyanates and related thiocar-

bamides has been reported by conventional methods. We herein synthesized acetylated sugar (glucose, galactose, lactose and maltose) isothiocyanates and related thiocarbamides under microwave irradiation.

105. Synthesis of Some Novel Benzoylated *N*-Glucosyl Carbamides and Carbamates

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Key words : *Glucosyl isocyanate, Amines, Alcohols, Carbamides, Carbamates*

Glucosyl carbamides and carbamates have several medicinal applications such as antitumor agents, antilukemic agents, antibacterial agents, antimetastatic compounds and many other ways. A series of some novel carbamides and carbamates derivatives were synthesized by condensation of Tetra-O-benzoyl-?-D-glucosyl isocyanate with several amines and alcohols respectively. The structure of these new N-glucosides has been established on the basis of usual chemical transformations and IR, ^{1}H NMR, and Mass spectral studies.

106. A Novel Ionic Liquid Mediated Synthesis of 2,3-Dihydro-1,5-Benzothiazepines Using Recyclable Catalyst Amberlyst-15®

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Keywords : *Ionic liquids, 1,5-Benzothiazepines, (E)-Chalcones, 2-Aminobenzenethiols, Amberlyst-15*

In this communication, we have attempted the synthesis of 1,5-benzothiazepines by reacting substituted 2-aminobenzenethiol with (*E*)-chalcone's/ (*E*)-4-oxo-4-phenylbut-2-enoic acid under nitrogen atmosphere at 60±2°C in ionic liquids, *viz.* [BMIM]BF_4/OTf/TFA in presence of Amberlyst-15. The progress of the reaction was monitored by TLC (on Merck Silica gel $60F_{254}$ aluminium sheets) using petroleum ether-ethyl acetate, 8:2. The product **3** was extracted and it was recrystalized by ethanol/chromatographed on a silica gel column (8'') to afforded 2,3-dihydro-1,5-benzothiazepines **3a-i** in good yields (67-92%).

107. A Facile Ionic Liquid Mediated Protocol for the Regioselective Synthesis of 1,5-Benzothiazepines

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Keywords : *Ionic liquids, benzothiazepines, regioselectivity, green chemistry, glycidate*

An efficient one step ionic liquid mediated green protocol for the regioselective synthesis of (±)-*cis*-2-(4-methoxy/benzyloxyphenyl)-3-hydroxy-2,3-dihydro-1,5-benzothiazepin-4-[5*H*]-ones has been developed from the reaction between 2-aminosubstituted benzenethiol and methyl- (±)-*trans*-3-(4-methoxy/ benzyloxyphenyl)glycidate under nitrogen atmosphere at 60±2°C. The ionic liquids used were 1-butyl-3-methylimidazolium bromide and 1-butyl-3-methylimidazolium hexafluorophosphate.

108. Synthesis and Antibacterial Activity of some Novel 4-(substituted sulfonamido) Benzoicacid Derivatives

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Key words : *antibacterial, MIC, PABA, sulfonamide, Vibrio parahaemolyticus*

Different 4-(substituted aromatic sulfonamido)benzoicacid derivatives were prepared by the reaction between p-aminobenzoicacid (PABA) and different substituted sulfonylchlorides in presence of aqueous base. All the compounds were characterized by UV, IR, ^{1}H NMR, ^{13}C NMR & Mass Spectrometry. Antibacterial activity of the title compounds were tested against 19 Gram –ve and 2 Gram +ve bacteria and the MIC values were determined by agar dilution method. Compound 4-(4-methoxyphenylsulfonamido)benzoic acid showed MIC value of 91.90 µgm/ml against *Vibrio parahaemolyticus*. The study concludes that further structural optimization of the lead compound may bring useful agent to treat infections caused by *Vibrio parahaemolyticus* effectively.

109. Synthesis and Biological activity Study of some New 2-(2’-(substituted phenyl -4-Thiazolinone-3-yl)-1’3’-Isoxazol-4-yl) Amino Pyridine Derivatives

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Keywords : *Pyridine, Isoxazoles, Thiazolodinones, antibacterial, antifungal, insecticidal activity*

Pyridine, a heterocyclic nucleus, played a pivotal role in the development of different medicinal agents and in the field of agrochemicals. Several pyridinylisoxazolythiazolidinones IV(a-k) have been prepared from pyridinylisoxazolylarylidines III(a-k) and tested for their antimicrobial and antifungal activity against different microorganism. The structure of compound III(a-k)and IV(a-k)have confirmed on the basis of their elemental and spectral such as IR, ^{1}HNMR and mass analyses etc.

110. Synthesis, Antibacterial and Antifungal Activity of some Pyrido Quinazolones

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Keywords : *Arylaldehyde, Vrea, P Aminobenzaic acid, PPA, Benzoin, antibacterial, Antifungle*

Alkylidenoarlideno bis ureas were synthesized by ureido-alkylation in the presence of alcohols, which on treatment with p-aminobenzoic acid results in 4-aryl-6-carbohylato – 1,2,3,4 tetra hydro quinazolines. Reaction of (II) with benzoin in presence of polyphosphoric acid yields, 4-aryl 8, 9 diphenyl 2-ox-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.

111. A New Concise Route to the Total Synthesis of Bacillamide I and its Analogues

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Keywords : *Bacillamide **I**; L-cysteine ethyl ester hydrochloride; pyruvaldehyde; 2-hydroxy- 4,6-dimethylpyrimidine.*

Bacillamide **I** is a new secondary metabolite isolated from marine bacterium *Bacillus species* SY-I during termination of blooms of *Cochlodinium polykrikoides*. It is the first compound which showed excellent selective algicidal activity against harmful dinoflagellates C*ochlodinium polykrikoides* without harming the useful microalgae e.g.: diatom, green algae and cyanobacteria. These *C. polykrikoides* are harmful dinoflagellates responsible for mass mortality of cultured fishes and

bivalves in coastal waters. Due to high selectivity exhibited by **1**, it might become a useful algicidal agent for regulating blooms of harmful dinoflagellate species. The structure of bacillamide **I** consist of a tryptamine and 2-acetyl-thiazole nuclei linked by an amide bond. Its first and only synthesis was given by Figueria *et al* in 2005. But the reported synthesis suffers from several drawbacks such as multistep reactions, formation of mixture of products and poor overall yield (~14%).

In the present study, bacillamide **I** was synthesized via a two step procedure. Initially, condensation of L-cysteine ethyl ester hydrochloride with pyruvaldehyde leading to the formation of key intermediate 2-acetyl-4-carbethoxy thiazole which further undergoes coupling with tryptamine in the presence of catalyst 2-hydroxy-4,6-dimethyl pyrimidine in solvent free conditions. Several analogues of bacillamide **I**, where acetyl group at position 2 of thiazole was replaced by alkyl/aryl/amino aryl group, were prepared by well known Hantzsch's thiazole synthesis. The final compounds were characterized by IR, ^{1}H and ^{13}C NMR and mass analysis.

112. Reaction of 2-hydrazino-4,6-dimethylpyrimidine and trifluoromethyl-β-diketones: Synthesis and Characterization of 5-trifluoromethyl-5-hydroxy-Δ^2-pyrazolines and isomeric 3/5-trifluoromethylpyrazoles

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Keywords : *Regioselectivity, Nucleophilicity, trifluoromethyl-β-diketones, 2-hydrazino-4,6- dimethylpyrimidine.*

Compounds containing pyrazole nucleus are extensively used as agro-chemicals and have found application in medicinal chemistry. Further, trifluoromethylpyrazoles have diverse biological properties associated with them because of increased lipophilicity due to the presence of trifluoromethyl group. Among the nitrogen containing heterocycles, pyrimidine derivatives too exhibit diverse pharmacological properties e.g. anti-HIV, anti-tubercular, antitumor, antineoplastic and anti-inflammatory. So, it was planned to synthesize various 1-(4,6-dimethylpyrimidin-2-yl)-5(3)-alkyl/aryl-3(5)-trifluoromethylpyrazoles and pyrazolines by the reaction of 2-hydrzino-4,6-dimethylpyrimidine with fluorinated β-diketones.

Reaction of trifluoromethyl-β-diketones with hydrazines may yield three products: 3-trifluoromethylpyrazoles, 5-hydroxy-5-trifluoromethylpyrazolines and their dehydrated products 5-trifluoromethylpyrazoles. It has been established by us earlier that the ratio of the three products depends not only on the relative nucleophilicity of NH and NH_2 of hydrazine but also on equilibrium ratio of the two enolic forms of β-diketones (which in turn depends upon the substituents present on β-diketones).

In the present study, the reaction of 2-hydrazino-4,6-dimethylpyrimidine and various alkyl/aryl-trifluoromethyl-β-diketones has been investigated. Reaction, when carried out in neutral conditions, afforded 5-hydroxy-5-trifluoromethylpyrazolines as the major product along with 3-trifluoromethylpyrazoles in accordance with the literature results. The ratio of products formed were analyzed by ^{1}H NMR of the crude reaction mixture. Their structures were established on the rigorous analysis of ^{1}H, ^{13}C and ^{19}F NMR spectral data. In acidic conditions, a change in regioselectivity was observed and 3-trifluoromethyl isomer was found to be major one. Also instead of getting 5-hydroxy-5-trifluoromehthylpyrazolines, we got corresponding 5-trifluoromethylpyrazoles.

113. Copper(II) Chloride Mediated Oxidative Cyclization of 2,3-Bis-(arylidenehydrazino)quinoxalines: An Efficient Synthesis of 3,10-Disubstituted-bis-1,2,4-triazolo[4,3-*a*][3',4'-*c*]quinoxalines

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Keywords : *Copper(II) chloride, oxidative cyclization, 2,3-bis-(arylidenehydrazino) quinoxalines, bis-1,2,4-triazolo[4,3-a][3',4'-c]quinoxalines*

The broad spectrum of pharmacological activities exhibited by several 1,2,4-triazoles fused with quinoxaline ring has placed them in an important class of medicinally potent compounds. They have been shown to be useful as antitumor, antimicrobial, antidepressants, anticonvulsants agents and as adenosine and benzodiazepine receptor antagonists. Synthesis of various 3,10-disubstituted-bis-1,2,4-triazolo[4,3-*a*][3',4'-*c*]quinoxalines has been reported by oxidative intramolecular cyclization of bis-arylidene derivatives of 2,3-dihydrazinoquinoxaline with four equivalents of copper(II) chloride in dimethylformamide in high yields. Remarkable properties of the present protocol are an efficient and general access towards the synthesis of bis-triazoloquinoxalines that could not be obtained by using iodobenzene diacetate as oxidizing agent, intriguing alternative to the literature protocols, commercially available nontoxic reagent and easy work-up. The title compounds have been characterized by the elemental analyses and spectral studies (IR, ^{1}H NMR).

114. A Novel and Efficient Approach for Regioselective Tosyloxylation of Some *ortho*-Substituted Phenolic Compounds using [Hydroxy(tosyloxy)iodo] benzene

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Keywords : *Hypervalent iodine reagents, [Hydroxy(tosyloxy)iodo]benzene, ortho-substituted phenols, regioselective tosylation.*

Some *o*-substituted phenols undergo regioselective tosyloxylation reactions with [hydroxy(tosyloxy)iodo]benzene (HTIB, Koser’s reagent) in dichloromethane to give the hitherto unknown 4-tosyloxy-2-substituted phenols. The results accomplished in this study reveal that the reaction of the various *o*-substituted phenols with HTIB is strongly affected by the nature and position of substituents at the *ortho* position of phenols. The oxidation of phenols that contain electron-withdrawing substituents at their *ortho* position leads to the *para* substituted product. In case, *para* position of the phenol is not free; the oxidation of the phenol gives corresponding *ortho* substituted product.

The conversion reported in the study demonstrates a unique application of HTIB in aromatic substitution.[3g] finally, noteworthy features of this study are: (i) Oxidation of *ortho* substituted phenols with one equivalent of HTIB offers a novel route for their regioselective tosyloxylation at *para* position. The tosyloxy derivatives 4-tosyloxy-2-substituted phenols & *o*-tosyloxy phenol derivative obtained from this study are hitherto unknown. (ii) In enolizable ketones, $COCH_3$ group which is prone to undergo ?-tosyloxylation remains intact under the reaction conditions. (iii) In case of *o*-hydroxybenzamide, $CONH_2$ group does not undergo Hoffmann reaction to produce the amine with HTIB, as reported earlier.

115. Solution phase photo-transformations of 3-allyloxy-6-chloro-2-(thiophen-3-yl) -4*H*-chromen-4-one: Solvent effects

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Keywords : *photo-irradiation, Dewar thiophene, chromenones*

Solution phase photo-irradiation of 6-chloro-3-alkoxy-4*H*-chromen-4-ones bearing thiophen-3-yl moiety at 2-position, furnished novel angular tetracyclic photoproducts originating from the Dewar thiophene generated *in situ* through valence bond isomerisation upon photoactivation of the thiophene ring tethered to chromenones is reported. Such type of behavior is observed for the first time in the chromenones having thiophene as a substituent. The Dewar thiophene functionality formed permits the 1,7-sigmatropic shift which otherwise not feasible. The product formation depended exclusively upon the nature of solvent used. The identification of the photoproducts was carried out by the rigorous analysis of their spectral data.

116. Photochemical re-organization of some 2-(5-methylthiophen-2-yl)-3-[(naphthalen-2-yl)methoxy]-4*H*-chromen-4-ones:Type-II process

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Keywords : *Type-II reaction, 1,4-biradical, thienylchromone, 1,5-sigmatropic shift*

Photo-irradiation of 2-(5-methylthiophen-2-yl)-3-[(naphthalen-2-yl)methoxy]-4*H*-chromen-4-ones yielded the fascinating angular tetracyclic products via cyclisation involving both 2-thienyl ring and naphthylmethoxy group via I,4-biradical generated in the Norrish type-II process where the naphthyl group exerted a significant effect on photoproduct formation and their distribution. The increase in electron density on chromenone moiety favors the dihydro product formation and also amounts to their decreased yields. The stereochemical dispositions of the products were determined by MM2 energy minimized programme and spectroscopic analysis.

117. TEAPI, a Convenient Oxidant for Fe(III) and Mn(III), Catalyzed Olefin and Alcohol Oxidation

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Keywords : *oxidation olefin, alcohol, TEAPI*

Development of synthetic analogy for biological processes had remained a topic of choice for many decades and is keeping researchers busy even today. Each newer insight in to biomemitics opens floodgates for further investigations, in this field. The fact that almost two third of biological processes are driven by oxidant provokes a special attention to biomimetic oxidations. Present work explores a low key oxidations. Tetraethyl ammonium periodate, (TEAPI) for Fe(III)

and Mn(III) catalyzed olefin and alcohol oxidations. Moderate to good yield of oxidation products were observed with this system, in ambient conditions.

Oxidation of cyclohexene, showed preference towards seconday oxidation, over epoxidation, secondary clcohols, gave moderate results.

Pinene, cholesteryl acetate, gave good results making TEAPI, a prospective oxidant for such reactions. A possible mechanism is also suggested.

118. Electro Organic Synthesis : A Green Protocol for the Synthesis of Bioactive 1, 3, 4-Oxadiazoles and Evaluation of their Antifungal Activity

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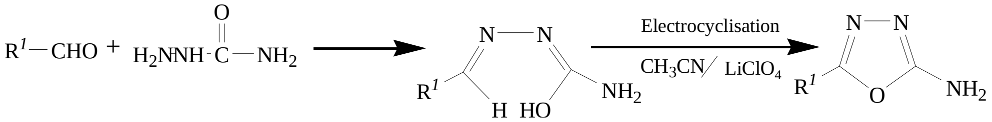
Keywords : *Electrocyclization, Controlled potential electrolysis, Semicarbazone Platinum anode, Oxadiazole, Cyclic Voltammeters, Antifungal activity, Green chemistry*

The oxidative electrocyclization of the semicarbazone into 5–substituted- 2–amino -1,3,4-oxadiazoles at platinum anode using acetonitrile as an organic solvent and lithium perchlorate as supporting electrolyte in an undivided cell. Newly synthesized compounds have been elucidated by elemental and spectral (IR, ^{1}H-NMR, ^{13}C-NMR, MS) analysis. The electrochemical synthesized compounds were screened for their fungicidal activity against *Alternaria solani*, *Fusarium oxisporum-udum* and *Aspergillus niger*. This is an environmentally friendly method in the field of electro organic reactions under controlled potential electrolysis, without use of toxic reagents.



Scheme

119. A New Method for the Synthesis of 4-Chloro,4'- Hydroxy Benzophenone.

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Keywords : *4-Chloro-4' Hydroxy Benzophenone, Friedel Craft Acylation, Phenol, 4 Chloro Benzotrichloride.*

A new method for the synthesis of 4- chloro,4'-hydroxy benzophenone by Friedel craft acylation of phenol with 4-chloro benzotrichloride as acylating agent in ethylene dichloride solvent using K10 Clay catalyst treated with acetonitrile solution of anhydrous ferric chloride and heated at 120^0C /550^0C respectively as green catalyst have been developed.

11.5 g of parachloro benzotrichloride in ethylene dichloride was added into a mix of 4.7 g of phenol and 1.0 g of K10 FeO-120^0C / K10 FeO-550^0C clay catalyst. in a four necked round bottom flask fitted with mechanical stirrer, addition funnel, water condenser & Thermometer pocket maintained below 10^oC in an ice bath. After the addition was completed the flask from ice bath was removed and kept on the heating mantle maintained at 80^oC and refluxed with constant stirring till five hours. The flask was cooled to room temperature and reaction mixture was filtered through G_2 sintered bed crucible to separate the catalyst. The catalyst was washed with EDC and the combined filtrate and washing was distilled and the residue obtained was dissolved in NaOH and acidified with HCl to pH 5.0 to reprecipitate the compound.

The compound was filtered and purified by column chromatography on silica gel column and mobile phase was benzene : ethyl acetate (80:20) and finally recrystallised in methanol. The yield of the product was 31.06% the melting point was $175\text{-}176^o$C. which was matched with the literature value. The structure was confirmed by I.R.,PMR and mass spectral data. The conversion of phenol was found to be 79.7% conformed by G.C.

120. Synthesis and Evaluation of some Novel 3-[5-phenyl-1,3,4-oxadiazole-2-yl]-2-styryl quinazoline-4(3h)-ones for Anti Bacterial Activity

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Key words : *4(3H)-quinazolinones, 1,3,4-oxadiazoles, antibacterial activity*

A series of novel 3-[5-phenyl-1,3,4-oxadiazole-2-yl]-2-styryl quinazoline-4(3H)-ones were synthesized and evaluated for antibacterial activity. The chemical structures of compounds have been characterized by IR, ^{1}H NMR and Mass spectral analysis. All the compounds were screened for antibacterial activity. Compounds with 4-methoxy **3b,** 4-chloro **3d,** and 4-isopropyl **3c** derivatives were markedly active against *E.coli and P. aureginosa.*

121. Synthesis and Characterization of Water-soluble Functional Biosupramolecular Systems

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Keywords : *Calixarene, Coumarin, Imidazole, Benzimidazole*

Calix(4)arenes[1-7] are believed to have a basket type of structure having the upper rim containing the para substituent in the original phenol while its lower rim contains the hydroxyl group. Calixarenes can be derivatized in the upper rim or at the lower rim depending upon the nature of R or the polar groups. Since our aim is to use Calixarenes as an organized medium, we have synthesized some known and some new Calixarene derivatives Calix-coumarin/Calix-imidazole/Calix-benz-imidazole analogs. These was purified by column chromatography over silica gel-

G using xylene-ethylacetate (6:4 v/v) as eluent and recrystallized from chloroform-methanol to give white crystalline compound and have examined their spectroscopic characteristics.

122. Synthesis of some Novel Perbenzoylated Lactosyl Carbamides

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Keywords : *Lactosyl isocyanate, aryl amines, lactosyl carbamides.*

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. *S*-and *N*-glycosylated derivatives and their utilities in medicinal chemistry have been extensively studied. They are also having applications in papers, textile and food industries. Several 1-hepta-*O*-benzoyl-?-lactosyl-3-aryl carbamides have been prepared by the interaction of hepta-*O*-benzoyl-?-lactosyl isocyanate and various aryl amines. The structures of the newly synthesized compounds have been established on the basis of elemental analysis, IR, ^{1}H NMR and Mass spectral analysis.

123. Phytochemical Investigation and Antibacterial Activity of Pod Extracts of Cassia obtusifolia Linn

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Keywords : *Antibacterial activity, Cassia obtusifolia, Fabaceae, Phytochemical, Urinary pathogens, Cup plate methods*

Phytochemical have played a vital role in the past and will continue to do so in the future. The source of many compounds used in modern medicine today can be traced down to plant origin. Various factions of Cassia obtusifolia pods have been studied for in vitro antibacterial activity against urinary pathogens. All fractions showed inhibitory activity against all test pathogens but maximum inhibition was seen with ethanol fraction.

124. Synthesis and Antibacterial activity of 6-(5^l – Substituted – 2^l – benzofuryl) – 4 – aryl – 4H – 2 – Oxopyrimidines.

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Key words : α, β-*Unsaturated ketones, benzofuran, oxopyrimidines.*

Various 2-acetyl – 5- substituted benzofurans and their subsequent transformation into benzofuran analogues of ?, ?. unsaturated ketenes by reaction with various 5 - substituted–5- hydroxyl benzaldehydes have been synthesized. These benzofuran analogues of ?,?. unsaturated ketones are further modified chemically into different nitrogen heterocyclic systems. In this connection weare reporting synthesis of oxopyrimidines coupled with various benzofurans. The structures of these compounds were established on the basis of elemental analysis and spectral studies. Screening of antibacterial activity of synthesized oxopyrimidines were also carried out by qualitative methods.

125. Organic Derivatives of Phosphorus as Pesticides

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Keywords : *O,O-diethylchlorothiophosphate, oxalic acid, succinic acid, glutaric acid, adipic acid, chenopodium amaranticolor.*

The reactions of O,O-diethylchlorothiophosphate with mercaptooxadiazols derived from dicarboxylic acids (oxalic, succinic, glutaric, adiphic) have been studied under inert atmosphere in the presence of pyridine and a variety of organophosphorous derivatives of types Li_1H_2, L_2H_2, L_3H_2, L_4H_2 have been isolated.

The spectral data of these organophosphorus derivatives are reported. All these derivatives were screened for their fungitoxic properties against two species of fungi, viz., *Aspergillus niger* and Helminthosporium oryzae. They show moderate fungi toxicity.

The viricidal activity of these derivatives were evaluated against cucumber mosaic virus using *Chenopodium amaranticolor* as the host plant. These organophosphorus derivatives show weak antiviral activities.

126. An Efficient Microwave Assisted One Pot Rigio and Stereoselective Synthesis of Novel Spiro Isoxazolidine Derivatives with α-chloro nitrones

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Microwave assisted 1,3 dipolar cycloaddition reaction of α-chloro nitrones with novel α-N-methyl/phenyl furan derivative afforded exclusively single

regioselective 5-spiro cycloadducts while same reactin with α-methylene-γ-butyrolactone afforded two diastereomeric 5-spiro isoxazolidines with high selectivity.

127. A c-methylated Flavonol Glycoside from *majorana hortensis* (moench.)

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Majorana hortensis (Moench.) belongs to family Labiatae, which is commonly known as Murwa in Hindi. It is extensively cultivated in India. It is reported to be useful in asthma, hysteria and paralysis. The present paper deals with the isolation and identification of a flavonol glycoside **A** m.p. 276-278 °C, $[M]^+$ 638, m.f. $C_{29}H_{34}O_{16}$ from the methanolic extract of the roots of this plant. Compound A was characterized as 6-C-methyl-3,5,7,4'-tetrahydroxy-3'-methoxyflavone-3-O-α-L-rhamnopyranosyl (1→2)–O- β-D-glucopyranos -ide, by various color reactions, chemical degradations and spectroscopic techniques.

128. Analysis of the Fixed Oil from *Artemisia vulgaris* Linn.

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Artemisia vulgaris[1,2] Linn. belongs to family Compositae. It is commonly known as "Dona" in Hindi. It is a found throughout the hilly regions of India, and

also found in Mount Abu in Rajasthan. The juice of this plant used in diseases of children. The herb is used as an emmenagogue, anthelmintic, stomachic and febrifuge. It also cures dysentery, chronic skin diseases, and also used in the spasmodic affections and treatment of inflammations blood. In the present paper we report Chemical examination of fatty acids from the seeds of this plant, which have been found to consist of Palmitic acid 63.64, Stearic acid 39.09, Linoleic acid 15.45 and Oleic acid 4.55%.

129. Antifungal Properties of Leaf Extracts of Melilotus Indica

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Key words : *Melilotus Indica, Antifungal Properties, Trichophyton Mentagrophytes, epidermophyton Floccosum, Aspergillus Flavus, Microsporum gypsum Rhizopus oryzae*

Antifungal activity of extract isolated from leaves of Melilotus Indica is being reported. The experiments were carried out using Filter Paper Disc Method as well as Serial Dilution Method. The activity was tested against various fungi, namely – Trichophyton Mentagrophytes, Epidermophyton Floccosum, Aspergillus Flavus, Microsporum gypsum and Rhizopus oryzae. The maximum inhibitory effects were shown by the compound against Epidermophyton Floccosum and the minimum inhibitory effects were found against Rhizopus oryzae.

130. Computational Investigations and Synthesis of 1-(4-methoxyphenyl)-4-methyl-3-(phenylamino) azetidin-2-one

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Staudinger reaction, (thermal [2+2] cycloaddition between imine and ketene) continues to be an important subject for computational studies in view of its synthetic value towards the synthesis of β-lactams and wide variety of other heterocyclic compounds of synthetic and medicinal interests. Staudinger reaction, discovered in 1919 consists of [2+2] cycloaddition of ketene and imine through a zwitterionic intermediate followed by cyclization to form ?-lactam ring. The paper accounts for the computation investigations of [2+2] cycloaddition between imine and ketene to afford 1-(4-methoxyphenyl)-4-methyl-3-(phenylamino)azetidin-2-one. The computation at semiempirical level using PM6 method has been performed to understand the reaction mechanism of Staudinger reaction i.e., [2 + 2] cycloaddition of imine to ketene. In addition, the effects of the substituents on products and reaction mechanism have also been investigated. Moreover, the synthesis of the target compound has been undertaken. A novel route was designed for the synthesis of 2-azetidinone incorporating Staudinger reaction strategy. The compounds were synthesized in excellent yields (64-76%) and the structures were established on the basis of consistent IR, 1H NMR, FAB-Mass and elemental analyses data. Their purity has been ascertained by chromatographic resolutions. Results of theoretical investigation have been found in accordance with experimental findings.

131. Green Chemical Synthesis of some Theophylline Derivatives

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Keywords : *Theophylline, Bromopropylphthalimide, antimicrobial activity*

Theophylline is a drug used to medications for the treatment of chronic asthma microwave irradiation has become a very useful tool in organic synthesis as Microwave technique can be used more efficiently for synthesis of organic compounds as compared to conventional reflux techniques. Theophylline is firstly converted to its sodium salt by using freshly cut small pieces of metallic sodium and then treated with bromoalkoxy phthalimide in DMF media, it results into phthalimide oxyallyl,theophylline this process was carried out in microwave oven. Progress of reactions was monitored by using TLC. These derivatives have been characterized by using FTIR spectra and all synthesized compounds have been screened in vitro for their antibacterial activity against E. coli, Bacillus subtilis, Pseudomonas alcaligens, Staphyllococcus aureus, Klebsiella pneumonia.

132. Silica Sulfuric Acid catalyzed solvent-free one-pot Synthesis of Biginelli Reaction

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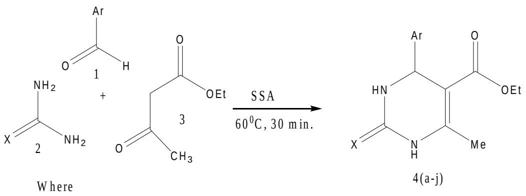
Keyword : *Silica Sulphuric Acid, aryl aldehyde, β-ketoester, urea and thiourea etc.*

Silica sulphuric acid catalyzed simple, one-pot, solvent-free, cost effective and environmentally benign process for the synthesis of dihydropyrimidones is described.



Where

X = O, S

133. Synthesis, Spectral Characterization and Biological Studies of 10*H*-Phenothiazine Sulfones

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Keywords : *10H-Phenothiazines, Smiles rearrangement, Sulfones, Antimicrobial activity.*

Synthesis of 10H-Phenothiazines was accomplished via Smiles rearrangement of formyl derivatives of diphenylsulfides. The latter were obtained by the formylation of the diphenylsulfides which in turn were obtain by the condensation of 2-Aminobenzenethiols with *o*-halonitrobenzenes in ethanolic sodium acetate solution. 10H-phenothiazine sulfones have been prepared by the oxidation of 10H-phenothiazine with 30% Hydrogen peroxide in glacial acetic acid. Their antimicrobial activity has also been carried out. The structure of the synthesized compounds have been established by elemental analysis and spectroscopic data.

134. Condensed Heterocycles from 5-aminopyrazoles

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Keywords : *Pyrazoles, Pyrazolopyrimidines*

Pyrazole compounds can provide privileged scaffolds for the generation of target compounds for drug discovery. Hence, the synthesis and study of pyrazolo-fused compounds have been of interest due to their wide variety of biological and pharmacological properties. The structural diversity and biological importance of pyridines and pyrimidines have made them attractive targets for

synthesis over many years. Robins and coworkers reported that certain 3-substituted pyrazolopyrimidines inhibits the metabolism schistosomiasis in snails .Pyrazolopyrimidines also have a wide spectrum of chemical & biological activity. The pyrazolopyrimidines are potent & selective Adenosine A_1–Receptor Antagonists. Pyrazoles have been found to be excellent precursors for the synthesis of condensed polyfunctionally substituted ring systems.

135. Facile Synthesis of Pyazolopyridine 3-carboxylates

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Tal-Niphad, Dist-Nashik, MS

Pyrazolo [3,4-b] pyridines as aza-analogues of indazoles are attractive targets in organic synthesis due to their significant biological activities, such as hypoglycemic [1], psychotropic [2] cytotoxic [3] or antiviral [4] activity. O-Amionaldehyde are the key intermediates for the synthesis of various biologically active heterocycles. The Friedlander condensation of o-aminoaldehyde with ketones furnished required tri and tetra cyclic pyraxolo [3,4-b] pyridine. The required starting material ethyl 4,5 – dihydro-5-oxo-1phyenyl-1H-carboxy late is prepared by esterification on ethyl 4, 5-dihydro-5-oxo-1-phenyl-1H-carboxylicacid. O-Aminoaldehyde the key starting compound was obtained by series of reactions including Vilsmeir-Haack formylation furnish o-chloroaldehyde which on SN^2 displacement of choride (CI^-) by azide ($-N_3$) yield 3 in 68%. This compounds on reduction with $Na_2S_2O_4$ gave two products o-aminoaldehyde in 80% and triazine-5-carboxylate in 20%, which were separated on column and were characterized by spectroscopic and analytical methods. Novel Friendlander condensation of o-aminoaldehyde with ketones, nitriles and esters containing active methylene were carried out in presence of piperidine offered fused pyridines in good yields.

136. Synthesis Characterization of Substituted Hydrazine Acetyl Arylidenes and Azetidinones and their Possible Biological Activities

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Keywords : *1,2,4-triazole, azetidinones, synthesis antimicrobial activity.*

3-mercapto-4-methyl-1,2,4-triazole was refluxed with chlorocetyl chloride to form [(1-chloro) acetyl]-3-mercapto-4-methyl-1,2,4-triazole. This product was refluxed with hydrazine hydrate (85%) to afforded [(1-hydrazino)acetyl]-3-mercapto-4-methyl-1,2,4-triazole. The hydrazine-acetyl product was treated with various substituted aldehydes to get [(arylidene hydrazino)-acetyl] 3-mercapto-4-methyl-1,2,4-triazole. These arylidene product was cyclised to [(2-oxo-3-chloro-4-aryl-azetidine) – (acetyl amino)] 3-mercapto-4-methyl-1,2,4-triazole. All the intermediates and title compounds were characterized by physical, chemical, analytical and spectral data. All the title compounds have been screened for their antimicrobial activities. Azetidinone compounds showed potent antimicrobial activity.

137. Silica Supported Sulphuric Acid Catalyzed Pechmann Condensation under Solvent free Condition using Grinding Technique

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Keywords : *Coumarins, Von Pechmann reaction, phenols, b-ketoesters, grinding technique*

Developing cleaner, safer, and environmentally friendly chemical processes is an important goal for chemists in both academia and industry. It is no longer acceptable in making products without being concerned about environmental pollution. Several strategies have been developed based on the idea that it is not only important what is produced but also how it is produced. To make the chemical processese ecofriendly many old reactions have been revised and carried out under solventless conditions , in supercritical fluids , in ionic liquids , in microemulsions , under high pressure, and by ultrasound and microwaves. Coumarins are an important class of naturally occurring oxygen heterocyclic compounds which are known to exhibit various pharmacological properties viz. antibacterial, antiviral, anticancer, anti HIV etc. They are also used as antioxidants and fragrances. *Herein we wish to report a* highly efficient, eco-friendly synthesis of coumarins via Pechmann condensation involving grinding of substituted phenols with â-ketoesters at room temperature using silica supported sulphuric acid catalyst in mortar and pestle under solvent free conditions.

138. A Facile Synthesis of Coumarin-3-carboxylic Acids by an Aqueous Grinding and MORE Technique

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Keywords : *3-Carboxycoumarins, 2-Hydroxybenzaldehyde, meldrum acid, Microwave Irradiation, grinding technique.*

A simple, efficient and green procedure for the synthesis of 3-carboxycoumarins (2-Oxo-2H-chromene-3-carboxylic acid) has been developed which involves the reaction of 2-Hydroxybenzaldehyde with meldrum acid (2,2-dimethyl-1,3-dioxan-4,6-dione) in moist conditions under grinding technique as well as microwave irradiations. The latter conditions are much more efficient in terms of time (3-5 min) as compared to grinding conditions.

139. Synthesis and Antimicrobial Studies of Thiazolo[2,3-b] benzo[h]quinazolines and their 2-arylidene Derivatives

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Keywords : *4-thiazolidinones, antimicrobial activity, heterocyclic system, etc.*

7-Methoxy-4-phenyl-3, 4, 5, 6-tetrahydrobenzo[h]quinzoline-2-thione (II), obtained by the condensation of 5-methoxy-2-benzylidenetetraline-1-one (I) with thiourea, on reaction with chloroacetic acid, α-bromopropionic acid and 1,2-dibromoethane furnishes compounds, III, IV and V and not their other possible isomers, VII, VIII, and IX, respectively. Arylidene thiazolidinones VI have been obtained by two routes. Compounds III-V represents a novel heterocyclic system. The structural assignments of III, IV and V are based on ^{1}H NMR, IR and mass spectral data. The condensed 4-thiazolidinones (III-V) and their 2-arylidene derivatives (VIa-c) were screened for antimicrobial activity and showed promising inhibition of *S. Typhi*, *S Aures* and *E. coli* bacteria.

140. Synthesis and Antimicrobial activity of some 5-substituted 2-phenyl-3-(6-aryl-3-cyano-2-substituted pyridin-4-yl)indoles and their Derivatives

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Keywords : *indole, pyridine, benzoxazine and antimicrobial activity.*

The precursor 3-(5’-substituted-2’-phenyl-1H-indol-3’-yl)-1-phenylprop-2-en-1-ones (**2a-i**) were prepared from indole-3-carboxyaldehydes (**1a-c**) and 4-substitutedacetophenones in presence of a base piperidine. Compounds (**2a-i**) subjected to cyclocondensation with ethylcyanoacetate in presence of ammonium acetate under thermal condition to afford 2-oxo-6-phenyl-4-(5’-substituted-2’phenyl-1H-indol-3'-yl)pyridine-3-carbonitriles (**3a-i**). These compounds when treated with ethylchloroacetate in acetone in presence of base yielded the corresponding esters ethyl 2-[3-cyano-6-(4-substituted phenyl)-4-(5’-sustituted-2’-phenyl-1H-indol-3’-yl) pyridine-2-yloxy] acetates (**4a-i**). Compound 4(a-i) on fusion with anthranilic acid at 130^0C afforded 6-(4-substituted phenyl)-2-[(4-oxo-4H-3, 1-benzoxazin-2-yl) methoxy]-4-(5’-substituted-2’-phenyl-1H- indol-3’-yl)nicotinonitriles (**5a-i**). Structures of all the newly synthesized compounds were confirmed by their IR, ^{1}H NMR and mass spectral data and elemental analysis. These compounds were screened for their antimicrobial activity.

141. Convenient Methods for the Reduction of Carbonyl and Nitro Compounds using $NaBH_4$-K-10 Montmorillonite System as Reducing Agent

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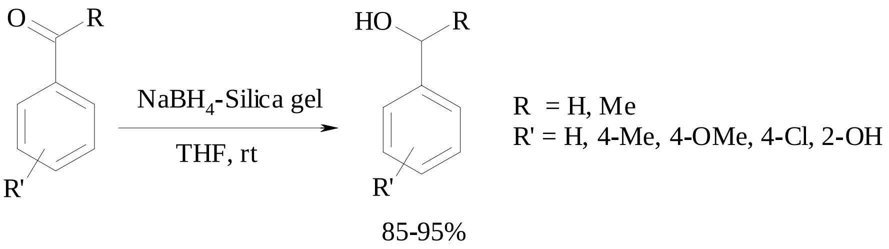
Reduction is one of the most fundamental and useful reactions in organic synthesis. Among the available reducing agents, sodium borohydride is the most widely used reagents in organic chemistry. It is certainly a reagent of choice for the reduction of organic functional groups, especially for the reduction of aldehydes and ketones. The carboxylic acids, esters, amides and nitriles are resistant towards

$NaBH_4$ under ambient conditions. Hereby we report a highly efficient, mild reduction methodology of reduction of carbonyl and nitro compounds with $NaBH_4$-K-10 Montmorillonite system in THF which gives the corresponding alcohols and amino compounds in 85-98% yields.



142. Efficient Synthesize of Tetra Substituted Pyrroles : A Green Approach

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Keywords : *pyrrole; solvent free; diaroylethylene, green approach*

Heterocyclic compounds have been in use in drugs as well pharmaceuticals due to their biological activity. This role of heterocycles in the drug industry has led organic chemists to make extensive efforts to synthesis novel heterocyclic compound involving simple and efficient methodology. We have found that diaroylethylenes as key intermediate for synthesizing a number of important heterocyclic compounds *viz.* chiral-bipyrroles,[1] furans, oxazines, pyrones etc. Pyrroles are being abundant in biological system, there are several synthetic methodologies reported in the literature using either metal catalysts or toxic solvents yielding low yield. Herein, we disclose a facile, one-pot, solvent and catalyst free route to synthesizing substituted pyrroles up to 98% yields at room temperature.

143. Comparative Studies on Conventional and Microwave Synthesis of Paracetamol

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Keywords : *Microwave synthesis, p-amino phenol, acetic anhydride*

Paracetamol (p-acetamidophen) has been synthesized using microwave irradiation and conventional heating method. Microwave technique can be used for more efficient synthesis of organic compounds as compared to conventional technique. Paracetamol has been synthesized in our laboratory by carrying-out a reaction between p-aminophenol and acetic anhydride inside a domestic microwave oven. Progress of the reaction monitored by TLC and product was characterized by its FTIR spectrum.

144. A New Pentacyclic Triterpene from *Limnophila indica*

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Keywords : *Limnophila indica, Scrophulariaceae,Triterpenoid*

Limnophila indica (Linn.) Druce (Scrophulariaceae) is a small aquatic herb, used widely in traditional Indian medicine in the treatment of various diseases like pestilent fever, dysentery, and elephantiasis; the plant has also been reported to possess immense anti-microbial activity. As a part of our continued work on the phytochemical investigation of *Limnophila* species, we wish to report herein the isolation and structural elucidation of a new pentacyclic triterpenoid constituent from the aerial parts and roots of *L. indica*. The isolate has been characterized as 3-oxo-olean-12(13),18(19)-dien-29a-carboxylic acid on the basis of detailed spectral studies including FT-IR, ^{1}H-NMR, ^{13}C-NMR, DEPT, HMQC and EIMS. Plant triterpenoids occupy a quite significant position among bioactive natural products as reported so far, and have contributed a lot in supplying useful and promising leads in drug discovery programmes.

145. Synthesis & Biological Activity of Some 2-Styrylquinazolin-4(3H)-ones

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Keyword : *Quinazolin-4(3H)-one, Thiophen-2-ethylamine, Styryl, semicarbazides, anti-microbial activity*

In an effort to discover new candidates with improved antimicrobial activities we synthesized and studied *in-vitro* antimicrobial activities of various series of 3-{(thiophen-2-yl)-ethyl}-2-(styryl)-quinazolin-4(3*H*)-one (3a-3g) (RDK-3a to 3g) and N^1-(substituted aryl)-N3-[3-{(3,4-dimethoxy phenyl-2-yl)-ethyl}-4(3H)-quinazolone-2-yl]-acetonyl semicarbazides (7a – 7j) (RDK-7a to RDK-7j). All the synthesized compound were characterized through FTIR, ^{1}H NMR, elemental analysis & screened against two Gram(+Ve) bacteria (*S. aureus*, *B. subtilis*), two Gram (-Ve) bacteria (*E. coli, S.typhi*) using the broth micro-dilution method.

146. Study of Analgesic & Anti-inflammatory Activity of some New Ditetrazoles

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Keyword : *Tetrazoles, 1,3,5-triazines, analgesic activity, anti-inflammatory activity.*

Tetrazole derivatives are reported to possess various biological activities such as anti -inflammatory, anti analgesic, anti-fungal, anti hypertensive, herbicidal, CNS stimulant activity etc., The biological activities of tetrazole are due to the two important reasons such as the tetrazole group is isostere with carboxylic group and its stability is higher than the acid function. Therefore continuous research is going on in this field to get more potent drugs. Triazines are a class of heterocyclic compound with wide spectrum of biological activities. The present paper deals with the study of analgesic and anti-inflammatory activity of some ditetrazoles derived from 1,3,5-triazines. The anti-inflammatory activity of the new compounds were carried out by Carragenan induced paw oedema method. The analgesic activity was carried out by Hot plate method and Tail flip method. Standard drugs were used for the comparing the results. The results of both the studies showed that the tetrazole compounds synthesized in our work possess fairly good analgesic and anti-inflammatory activity.

147. Synthetic Utility of Heterocyclic o-aminoaldehyde : Synthesis of Novel pyrazolo[3,4-*h*] [1,6]naphthyridine and Study of their Fluorescent Behavior

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Keywords : *O-aminoaldehyde, pyrazolo[3,4-h][1,6]naphthyridines, HOMO-LUMO, Absorption and Emission, Quantum yield*

From literature we noted remarkable biological activity of pyrazolonaphthyridine derivatives as anti-HSV-1 agents [1]. Moreover napthyridine derivatives were used as luminescence materials in molecular reorganization because of their planner structures [2]. Recently we have utilized heterocyclic orthoaminoaldehydes for annulations of benzonapthyridines ring on to quinoline [3]. Prompted with these reports, we have described synthesis of novel pyrazolonaphthyridine derivatives in this communication. Thus *Friedländer condensation* of 4-amino-3-(4-phenyl)-1-phenyl-1*H*-pyrazolo [3,4-*b*]pyridine-5-carbaldehyde (o-aminoaldehyde) with series of different cyclic ketones and 1,3-diketones yielded pyrazolonaphthyridines. The fluorescence spectroscopic properties of synthesized compounds have been studied and calculated their quantum yields.

148. Isolation of Meliacins from Chisocheton Paniculatus Hiern, their Chemical Transformations to New Limonoids and Screening for Antifungal Activity

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Keywords : *Meliaceae, limonoids, paniculatin, heterocycles, antifungal activity*

Paniculatin (**1**) (6α-acetoxyazadirone) and Paniculatol (**2**) (dihydroxycompound of 6α-acetoxyazadirone) are two naturally occurring meliacins have been isolated from the fruits and wood of *chisocheton paniculatus* Hiern. Chemical transformations of paniculatin and paniculatol gave 2-aminothiazolo [4,5-d] [1,2,20,21,22,23-hexahydro] paniculatin (**4a**), 2-aminothiazolo [4,5-d] [6α,7α -dihydroxy-1,2,20,21,22,23-hexahydro] paniculatin (**4b**), Dialdehyde (**5**), 3-hydroxy paniculatol (**6**), Dialdehyde **7**, 2-methyloxazolo [4,5-d][1,2,20,21,22,23-hexahydro] paniculatin (**9a**), 2-methyloxazolo [4,5-d][6α,7α–dihydroxy-1,2,20,21,22,23-hexahydro] paniculatin (**9b**). Antifungal activity of the above compounds and their derivatives are reported here. The structures of the new compounds have been elucidated on the basis of elemental analysis and spectral data.

149. Expedient Approach for Synthesis of Novel Indenothiophene Derivatives

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Keywords : *Indenothiophenes, Indenothienopyrimidines, Indenothienopyridines, 2-Amino-3-carbonitrile thiophene, 2-Amino-3-carboxamide indenothiophene, Gewald reaction*

Gewald reaction of 2-(1,2-dihydro-5,6-dimethoxyinden-3-ylidene) malanonitrile, elemental sulfur and catalytic amount of triethylamine furnish new synthon 2-amino-3-carbonitrile thiophene. Reaction of new 2-amino-3-carbinitrile with Conc. H_2SO_4 furnished expected 2-amino-3-carboxamide indenothiophene instead of 2-amino-3-carboxylic acid indenothiophene. Key intermediates 2-amino-3-carbinitrile and 2-amino-3-carboxamide were used for the synthesis of tetracyclic indenothienopyrimidine derivatives by cyclocondensation reaction with acid chlorides, amides; formic acid and hydrazine hydrate respectively. Neat reactions of 2-amino-3-carbinitrile with cyclic and aliphatic ketones in presence of anhydrous $ZnCl_2$ furnished pentacyclic and tetracyclic indenothienopyridine derivatives respectively in good yields. All new compounds were characterized by spectroscopic and analytical data.

150. Phosphorous Oxychloride ($POCl_3$) Catalysed Synthesis under Solvent Free Condition and Antimicrobial activity of 6-aryl-s-trizale-[3,4-b]-1,3,4-thiadiazole

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In the last few years there has been interest in the use of microwave heating in organic synthesis. The use of such non-conventional reaction condition reveals several features like short reaction time, case of work-up and selectivity.

The cyclization of 4-amino-5-mercapto-s-triazole **1** with different aromatic acid **2** using $POCl_3$ as a catalyst in solvent-free condition under microwave irradiation (2-3 min) gave 6-aryl-s-triazalo (3, 4-b) (1, 3, 4) thidiazoles 3a-f with improved yield is described here.

151. Synthesis of some Newer 2-Phenyliminothazolidinopyrazolines

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A large number of thiazolidines and pyrazolines are known for their biological properties. Therefore, it was considered worthwhile to synthesize some new thazolidonopyrazolines with substitutions in thiazolidine or pyrazoline ring. Thus 2-phenyl-thiazolidin-4-one and 2-phenylimino-3phenyl-seperated to yield the corresponding benzylidene derivaties 1 and 2 respectively. Both the benzylidene derivates when treated separately with hydrazine or substituted hydrazines gave their corresponding pyrazolines.

152. Chemical Constituents from the Stem of Cassia Marginata, Roxb. Hort

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Phhtochemical studies on the stem of Cassia marginata (Fem, Leguminosae, Subfam, Caeselpiniaceae) resulted in the isolation of the flavones glycoside : 5, 7-dihydroxy-6-methoxy-flabone-4’-O-α-L-rhamnoside along with kaempferol, kaempferide, rhein and β-sitosterol. The structure of all the isolated compounds were established on the basis of chemical and spectral analysis.

153. Biochemistry of Photosynthesis : A New Balanced Chemical Reaction

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Keywords : *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 the 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 (photo chemical) and “Dark Reaction” (Biochemical). Biochemical reactions are very much complicated being catalysed by various enzymes and the path of carbon is known 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 carbon dioxide react with twelve molecules of water in presence of chlorophyll and sunlight to give only one molecule of sugar (Carbohydrate), six molecule of water and six molecules of oxygen is being evolved in gaseous from. This is the accepted equation and also chemically 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 molecule of water is produced. As a Botanist teaching Chemistry of photosynthesis or more explicity photochemistry and photophysics or biochemistry and biphysics is certainly beyond one’s grasps but question raised by students at undergraduate level is still more rewarding. If the newly devised chemically well balanced equation is chemically accepted certainly it will be nice interaction between students and professor in the class room for better academic and scientific excellence at tertiary level of higher education.

154. Synthetic and Antimicrobial Studies of Azomethine Complexes of Pb (II)

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Key words : *Shiffbase IR.Spectra, Biological screening*

Metal chelates of salicylidine-o-aminobenzoic acid and salcylidine-o-aminothiophenol with lead (II) have been synthesized and characterized on the basis of elemental analysis , Infrared spectral studies, ligand and their metal chelates were also screened for their anti-bacterial and anti-fungal activity on Staphylococcus aureus (gram+ve) and E,Coli (gram-ve bacteria and Aspergillus niger and Candida Albicans fungi. Interesting results have been obtained in terms of increased activity of ligands on being coordinated with metal ion.

155. Selective O-methylation of Phenols with Dimethyl Carbonate in Ionic Liquids

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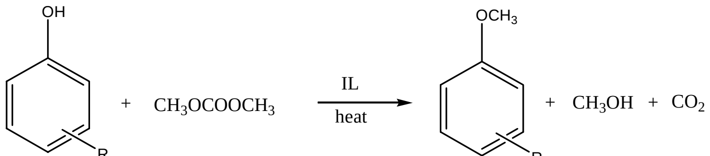
Keywords : *Ionic liquid, Arylmethyl ether, DMC, Phenol.*

Ionic liquids are efficient and environmentally friendly solvent cum catalyst for the synthesis of arylmethyl ethers from corresponding phenols. Arylmethyl ethers are starting material for the preparation of dyes, agrochemicals, fragrances and pesticides.

Dimethyl carbonate is a good alternative methylating reagent over other hazardous alkylating agents such as methyl halide, dimethyl sulphate. Arylmethyl ethers were also prepared from phenols and DMC by using the catalyst such as Tertiary amines or phosphines[1], nitrogen containing heterocyclic catalyst[2],pentaalkyl guanidines[3] etc.

Herein, we wish to report the synthesis of a new pyridinium based ionic liquid and by using this ionic liquids we have been able to synthesize the phenylmethyl ethers from phenol under environmentally benign condition and in high selectivity and yield. The phenylmethyl ethers were obtained in yield with 100% selectivity for the formation of the O-alkylated product over the other possible C-alkylated product. The reaction was carried out by simply heating of the reaction mixture and the same reaction was also carried out using microwave techniques. Selectivity for exclusive formation of O-methylated product was observed in case of nornal heating whereas under microwave condition both the O-methylated as well as the C-methylated products obtained. Product recovery and purification is simple and the ionic liquid could be recovered and reused.



Scheme 1

156. First Novel Silatrane Containing Exocyclic Methane Sulfonato Group

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Keywords : *Methane sulfonato silatrane, Pentacoordinated silicon, Hypervalent compound, Silatranes*

1-Methane sulfonato silatrane, $CH_3(O)_2SOSi(OCH_2CH_2)_3N$ has been synthesized in high yield by the reaction of 1- isothiocyanato silatrane with methyl methane sulfonate .This novel silatrane has been characterized by elemental analysis, infrared spectroscopy, ^1H, ^{13}C, ^{29}Si NMR spectroscopy and mass spectrometry. Semi-empirical quantum mechanical calculations were done to study the N?Si transannular bond length. The study revealed that the prepared silatrane is more stable than the parent silatrane.

157. Novel Synthesis of benzo[h][1,6]napthyridines Derivatives

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4-Amino-2-choloroquinoline-3-carbaldehyde were obtained by the three step synthesis. The key intermediate 4-Amino-2-(aryl) quinoline-3-carbaldehyde was synthesized by well-known Suzuki coupling of 4-Amino-2-chloroquinoline-3-carbaldehyde with substituted aryl boronic acid followed by Friedlander condensation of various ketones furnish arylbenzo[h][1,6]napthyridines in good yields. All the compunds were well characterized by analytical and spectroscopic methods.

158. Synthesis, Characterisation and Biological Activity of 3-arylidene bis Chromanones

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The 3-arylidene chroman-4-one moiety occupies a special place in the field of oxygen heterocyclics as this structural feature forms an integral part of many natural products and biologically active molecules. Some of them were reported to possess antimutagenic and anticlustogenic properties. These activities are supposed to originate from their antioxidant activities. Recently a Chromanone-12-oxocalanolide-A and its derivatives were reported to be having invitro antiviral activities against HIV and similar Immuno defeciency virus. Hence the synthesis of 3-arylidene chroman-4-ones becomes important to synthetic organic chemist. There are a few reports of their synthesis but no report so far on the synthesis of Bis-chromanones. Hence starting from simple starting materials several Bis-

Chromanones were synthesized making use of the Baylis-Hillman Reaction as an important step in the synthetic design.

159. Benzene extract Worked as anti-oxidant and Would Healing

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In the present study, the vacuum dried benzene extract of *Derris benthamii* leaves was evaluated for its wound healing property by incision and excision wound models. The extract was also investigated for its anti-oxidant activity by thin layer chromatography using β-carotene linoleate oxidation method. The extract exhibited significant wound healing properties and also possessed anti-oxidant activity. The wound healing property may be attributed to the anti-oxidant activity of the extract.

160. Study of Insecticidal nature of *Ocimum Americanum*

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Keywords : *Ocimum Americanum, Paradoxin, tribolium Confusum*

Different parts of *Ocimum Americanum* used as medicine since ancient time. Present work conducted to find out some other uses of *Ocimum Americanum.* It is found in present study that *Ocimum Americanum* has paradoxic nature and can be used as an insecticide for the beetles which destroy stored grain. Leaves extract of *Ocimum Americanum* reduced the survival rate of beetles and increase their mortality.

IV. ANALYTICAL CHEMISTRY

1. Removal of Fluoride from drinking water by Aluminum Hydroxide Gel & its Derivatives

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The batch sorption system using Aluminum Hydroxide Gel (HAG), HAG impregnated on cross linked guar (HAGG), starch (HASG) and micro crystalline cellulose (HACG) as adsorbents was investigated by removing fluoride ion from aqueous solutions. Effect of initial fluoride concentration, agitation time, adsorbent dose, pH, temperature, surfactants, and added ions, on the percentage fluoride removal, have been reported. The experimental data fitted well in the Freaundlich adsorption equation; the values of adsorption capacity, K, and intensity of adsorption, n have been reported. HAG & its derivatives showed promising results in the removal of fluoride from drinking water. The up-take of fluoride is rapid and proportionate in initial stages and decreases gradually while approaching equilibrium. The major part of total adsorption, nearly 80% of uptake at equilibrium takes in less than 15 minutes. The up-take of fluoride increases with the decrease in pH of water and the increase in [cationic surfactant], however it decreases with the increase in [anionic surfactant], nonionic surfactants have no effect. The pH of the system in all cases increases with the removal of fluoride indicating that the exchange of OH with F. The materials also solves waste disposal problem as these may be burnt after the use.

2. Acrylamide formation in Food during Thermal Processing

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The neurotoxic and carcinogenic compound, acrylamide found in heat processed food is mainly formed from an amino acid, asparagines and a reducing sugar through Maillard reactions. Higher temperature, low moisture conditions and frying time play a major role in its formation. Fried potato products, French fries, ready to eat breakfast cereals, baked foods and roasted coffee contribute most to acrylamide exposure. There are many harmful effects of acrylamide. It cause damage to nervous system in human and animals and is considered a reproductive toxin with mutagenic and carcinogenic properties in experimental mammalian in vitro and in vivo system.. The acrylamide formation can be reduced by various methods as By addition of acids, lowering the pH, in the presence of cation, microwave heating.

3. Characterisation of Polypropylene based Accurel® Hydrophobic support and its use for Selective Adsorption for Polyphenols

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Keywords : *Accurel® MP powder, Polypropylene, hydrophobic adsorption, microporous mesoporous, surfactant, phenolics*

Polypropylene based hydrophobic Accurel® MP powder with particle size ranges between 200-400 ìm was characterized for its use for selective adsorption for polyphenols. The pore distribution falls between microporous and mesoporous domains. During surfactant loading, a significant penetration of the surfactant molecules into the pores was found to occur. SEM of Accurel® reveals that it has a very regular microporous structure of typically 73% void volume with cells of 5-10µ connected by pores with 0.5-1.0µ diameter. The internal surface area (BET) of Accurel® was found 75-90 m^2/gm. The aforementioned facts and its hydrophobicity make it a unique adsorbent of all kinds of organic molecules. Here, it is recalled that in ICUMSA method for colour measurements; membrane filter of pore size of 0.45 ìm is recommended; such pore size of the membrane filter removes the colour bodies- colourants greater in size that of 0.5 ìm. Hence, Accurel$^{®}$powder (200-400 ìm) was found to be excellent adsorbent and is available commercially, hence, it could be used in sugar decolourisation in commercial scale for the removal of phenolics from cane juice.

4. A Simple and Rapid Reverse Phase High performance Liquid Chromatographic Method for the Estimation of Glycyrrhizic Acid from Roots of Glycyrrhiza Glabra

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Keywords : *glycyrrhizic acid, glycyrrhiza glabra, RP-HPLC-PDA.*

A simple reverse phase high performance liquid chromatographic method has been developed for the quantitation of glycyrrhizic acid from aqueous extract of roots of glycyrrhiza glabra using a photodiode array detector, a C18 column and 5.3 millimolar phosphate buffer and acetonitrile (65:35) as mobile phase. Good linearity was obtained in the working range of concentration (12.4 to124 µg/ml) with a correlation co-efficient of 0.999. The limit of detection and the limit of quantitation were 3.08 µg/ml and 10.27 µg/ml respectively. The method was validated under ICH guidelines. The developed method can be used for the routine analysis, stability testing and quantitation of glycyrrhizic acid from herbal preparations containing aqueous extracts of glycyrrhiza glabra.

5. Repulping of Waste paper Containing High Wet Strength with Natural Fruit Juices

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Dr. D.Y.Patil ACS Collge Pimpri Pune
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Key words : *Waste paper, Repulping, Slushing, Wet strength, Polyethylene glycol, Sodium hydroxide, Fruit pulp, Wetting agent*

Amongst the large varieties of waste papers available in market some waste paper do not easily disintegrate in water while others are repulped in water by maintaining a temperature of 40^0C – 50^0C in Paper Pulping machine. Waste paper such as toweling tissue, napkins, crepe tissues have 10-15%wet strength. They require chemicals for destroying wet strength of paper. Some papers have wet strength more than 30% due to which they do not slush in water easily. Such papers can be slushed by adding sodium hypochlorite, hydrogen peroxide combination. It has been observed that the polyethylene glycol helps in breaking wet strength in paper (Wet strength: - 30-35%) easily as compared to other chemicals.

The combination of Sodium hydroxide & Polyethylene glycol, gave the best results for the destruction of wet strength in paper whereas use of citrus fruit pulps gave the moderate results.

A comparative study of slushing of waste paper with Polyethylene glycol and fruit pulp under the similar conditions revealed that the waste paper (high wet strength) can be recycled more easily with the help of polyethylene glycol in alkaline conditions.

6. Simultaneous RP-HPLC Estimation of Escitalopram Oxalate and Clonazepam in Tablets

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Keywords : *Escitalopram oxalate, Clonazepam, RP-HPLC*

A new simple, precise, rapid, and accurate RP-HPLC method has been developed for the simultaneous estimation of escitalopram oxalate and clonazepam in tablets. The method was carried out on 5 µ C_8 (250x4.6 mm) column with a mobile phase consisting of acetonitrile : methanol : potassium dihydrogen orthophosphate buffer (pH 6.0, 55:20:25 v/v) at a flow rate of 1.0 ml/min with UV detection at 220nm over concentration ranges of 70-120 and 7-12 µg/ml respectively. The retention time of escitalopram oxalate and clonazepam were 12.36 and 19.07 min respectively. The developed method was validated and produced accurate and precise results for estimation of the two drugs.

7. Mitigating Membrane Fouling by understanding Feed Water Characteristics and Evaluating Coagulation Pretreatment

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Keywords : *Water treatment – membranes – fouling – natural organic matter – pretreatment - coagulation/flocculation*

In both, industrialized and developing countries, there is growing concern about the ability of traditional drinking water supply systems and existing technologies to cope with present and future demands and threats. Water supply in India faces opportunities as well as challenges promoting the application of advanced treatment technologies such as membrane filtration. Membranes are at the center stage these days when it comes to separation of materials and the use of membrane technology has been growing rapidly during the last few decades. This technology can improve drinking water quality and tackle pollutants of concern such as disinfection by-product precursors or trace organics. Membrane treatment of natural water (surface/sea water) to produce potable/process water and of wastewater for safe disposal is growing at a drastic rate owing to advantages like low energy consumption, no use of harsh chemicals, ease of use and maintenance. Hence it is seen as a sustainable step into the future.

Organic fouling has been identified as the most complicated problem facing MF/UF operations, due to its irreversible nature and difficulties with the cleaning procedure. It also initiates and supports bio-fouling of NF/RO as the organic foulants in the feed water are readily available as nutrients for microbial growth. So a clear understanding of the organic fouling is decisive for improving MF/UF operation performance; not only in the production of potable water from direct treatment of surface water, but also in the pre-treatment line prior to sea water reverse osmosis. Fouling on polymeric membranes is largely dependent on the nature and concentration of organic substances (TOC) in water. Different fractions of the organic matrix have fairly different fouling tendencies. This paper describes the steps involved in the development and validation of a laboratory-scale unit to obtain water samples with different DOC-fractions with a volume sufficiently high to carry out further experiments on polymeric membranes to test fouling potential and mechanism of organic fractions of different particle/molecular size in natural surface water, and additionally help evaluate use of pre-treatment by coagulation/ flocculation to curtail irreversible organic fouling and provide steady membrane performance. Results indicated that the fractions produced have fairly different fouling potentials on UF/MF submerged capillary polymeric membranes and the influence of coagulation pre-treatment on minimising fouling is also quite different for the different fraction

8. Isolation, Spectral Studies and Screening for the Anti-bacterial Efficiency of *cassia fistula linn*

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Keywords : *Cassia fistula, flower and pod extracts, spectral and antibacterial characterization*

Cassia fistula linn; a semi – wild Indian Labernum also known as the golden shower is widely used for its medicinal properties; its main property being that of a mild laxative suitable for children and pregnant women. This paper reviews the isolation of fistulic acid from the pods and flowers. The isolated fistulic acid was subjected to UV, FTIR spectral characterization to determine its purity and nature

of functional groups present in it. The antimicrobial sensitivity of plant extracts was observed using the well diffusion method by measuring the diameter of the growth inhibition zone of *cassia Fistula linn*. The ether and ethanolic extract of dried flowers and pods of *Cassia Fistula* investigated individually for *invitro* antibacterial activity by well diffusion method against *Escheria coli*, *Salmonella typhi, Shigella dysenteriae, Bacillus cereus* and *Psudomonas aeruginosa*.

9. Spectroscopic Studies on Prednisone Drug

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Keywords : *FTIR, prednisone, FT Raman, UV-Visible*

A drug product may become useless and even hazardous if it reacts with packaging material or decomposes because of improper storage. This may happen regardless of how well it is formulated or manufactured. Quality assurance plays a central role in determining the safely and efficacy of medicines. Modern spectroscopic techniques are sensitive tools for such purposes. In the present investigation infrared and Raman spectroscopic techniques are employed for identification and assignment of common functional groups [resent in some medicinally important compound, prednisone. It is used as an inflammation and also exerts main action on gluconeogenesis, glucogen deposition and protein and calcium metabolism. The internal standards ratio of the specific modes of the vibration in the IR spectra of the same stored in the suitable storage condition and exposed to environmental hazards are calculated. UV-Visible spectroscopic investigation on this compound also made to study the variation in the light absorption activity of ëmax of the drug with varying concentrations and at different storage conditions.

10. Water quality of Sagar City Lake

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Keywords : *Physiochemical parameters, water quality, Sagar City Lake*

This study consisted of the determination of the physiochemical properties of different types of untreated water in most polluted area of sager. The aim was to ascertain the quality of river water, ground water and pond water. Only the concentration of the chloride exceeded the permissible limits of the world Health Organization drinking water quality guidelines. The four out of five parts of ponds has very low dissolved oxygen content. On an average, the water in this area was slightly polluted. A simple pre-treatment is enough to make the water potable.

11. Determination of Atmospheric Concentration of Poly Aromatic Hydrocarbons by High Performance Liquid Chromatography

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Air borne particulate matter from the atmosphere of the city of Lucknow was collected on the filter paper which is made up of cellulose nitrate with quartz fibers. Poly aromatic hydrocarbons (PAHs) and associated with air borne particulate matter were extracted by Soxhlet procedure and analyzed by HPLC. The concentration of all the four zones were determined.

12. Analytical and Pharmacological Studies on Natural Origin Crocin and its Modified form as Nootropic Agent

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Keywords : *Crocus sativus; crocin; [Cro-(cys)$_2$] adduct; amperometry; nootropic agent, Alzheimer's disease.*

A new electroanalytical method has been developed for the quantitative determination of crocin in a sample of stigmata of saffron (***crocus sativus L.).***Crocin reacts with cysteine a polarographically active species in 1:2 ratio. Amperometric titration procedure has been developed for the quantitative determination of crocin in the sample of saffron. The observed results were found in good agreement with those determined by HPLC analysis. Extracted crocin and its 1:2 adduct with cysteine were characterized by FTIR spectral studies.

13. Novel Method for Treatment of Effluent from Dyeing Industry

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Keywords : *Column Chromatography, TLC, multilamp photoreactor.*

Present day scenario calls for more attention on pollution control, as the accumulation of hazardous chemicals into the environment have turned to show

their worst face now-a-days. In India more than thousands of dyeing industries are working in nook and corner, of which most of them are small scale industries and lack proper economical backup. Hence in populated country like India, hazardous effect of the effluent waste from these industries pose a threat to near by locality. Thus a search for more economical as well as efficient treatment method for effluents of these small scale dyeing industries is the aim of this work.

Sample was collected from nearby dyeing industry, which was then analyzed for its composition using column chromatography and TLC. Various components were then studied individually and their toxicity was analyzed. An advanced photo oxidation reactor using $TiO_{2,}$ which can effectively degrade their toxicity content, was experimentally verified and their effects on various parameters were studied and results were discussed. A fairly good output was obtained and the present investigation proves to be applicable both efficiently as well as economical.

14. Studies on Interaction between Cobalt (ii), Nickel (ii), Copper (ii), Aluminium (iii) and Iron (iii) with 3 (2- hydroxy- 5 chloro phenyl)-5-(4-methoxy phenyl) Isoxazoline at 0.1m ionic strenth p^h Metrically

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Keywords : *Metal complexes**,** 3-(2- Hydroxy- 5 chloro phenyl)-5-(4-methoxy phenyl) Isoxazoline, Stability constants**.***

The interaction of Cobalt(II),Nickel(II),Copper(II),Aluminium(III) and Iron(III) with 3-(2- Hydroxy- 5 chloro phenyl)-5-(4-methoxy phenyl) Isoxazoline have been investigated P^H metrically in 70 % DMF- Water mixture at 0.1M ionic strength at different temperatures.

The metal ions form 1:1 and 1:2 complexes with 3-(2- Hydroxy- 5 chloro phenyl)-5-(4-methoxy phenyl) Isoxazoline. The proton- ligand and metal-ligand stability constants have been determined by Irving –Rossotti's expression.

15. Resistance Response Models for Calcium Deficient Hydroxyapatite Gas Gensors

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Keywords : *Nano-CDHA, Gas sensors, Response model, Ethanol, Acetone, Ammonia.*

Considerable research into new type of gas sensors is underway to enhance the performance of traditional devices through nanotechnology. The use of Calcium Deficient Hydroxyapatite (CDHA) has proved a cleaner and safer alternative to gas detecting compounds. The synthesized compound has been characterized for the presence of nano-CDHA using X- Ray Diffraction, Fourier Transform Infra-Red Spectroscopy, Energy Dispersive X-ray Spectroscopy and Transmission Electron Microscope. From the resistivity obtained from nano-CDHA coated substrate on exposure to various gases, resistive response models have been developed.

16. Application of Periodate Oxidation of 2,4-xylidine for Nanogram Determination of Manganese(II)

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The Mn(II) catalysed periodate oxidation of 2,4-xylidine (XYL) in acetone-water medium is first order w.r.t. 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 is 3,5-dimethyl-1,2-benzoquinone. The effect of pH, dielectric constant of medium, ionic strength and free radical scavengers was studied to develop the conditions for nanogram determination of

Mn(II) in the range 0.54 to 345.22 ng/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.

17. Adsorption of As (III) from Aqueous Solution using Iron Acetate Coated Activated Alumina

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Keywords : *Iron acetate, activated alumina, adsorption, and arsenic.*

The present study describes the arsenite [As (III)] removal performance of Iron Acetate Coated Activated Alumina (IACAA) by batch sorption techniques. Surface morphology of IACAA before and after sorption of As (III) solution was characterised by SEM. Percentage adsorption was determined on IACAA as a function of pH, contact time and adsorbent dose. Batch study revealed that the best removal of As (III) was achieved at pH 7.4. The initial As (III) concentration (0.45 mg/L) came down to less than 0.01 mg/L at contact time 90 min with minimal dose of 1g/100mL. Both Langmuir and Freundlich adsorption isotherms were studied. R value predicts Langmuir isotherm (R=0.9910) is better mathematical fit than Freundlich isotherm (R=0.9865)

18. Estimation of Quercetin from Dried flowers of *nymphaea stellata*, Willd by Reverse-phase High Performance Liquid Chromatography

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Keyword : *Nymphaea stellata Willd; Quercetin; RP- HPLC., Quantitative estimation.*

A reversed-phase HPLC method has been developed and applied to determine quercetin content in hydroalcoholic extract of dried flowers of *Nymphaea stellata* Willd in a single analysis. The quercetin was analysed with a HiQ Sil C-18 column by isocratic elution using 0.01% (v/v) phosphoric acid– acetonitrile (60: 40 v/v) as the mobile phase. The flow rate was 1.2 ml min^{-1}, and detection was set at 380 nm. The recovery of the method was in the range of 99.00– 99.60 %, and all the compounds showed good linearity (r > 0.9880) in a relatively wide concentration range.

19. Development and Characterization of PMMA based Composite Materials for Gas Sensing Applications

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Keywords : *Polymer composite, PMMA, Ammonium dihydrogen phosphate, PMADP, gas sensor.*

Conductive particles when mixed with insulative polymers undergo modification in their electrical properties. Conductive polymer composites have various industrial applications. The composite prepared by mixing carbon black with PMMA has very good gas sensing applications. The gas sensors based on Carbon nanotube/polymer, ceramic and metal oxide composites such as epoxy, polyimide, PMMA / $BaTiO_3$ and SnO_2 have also been developed. In the present work, a new composite has been prepared by using PMMA and Ammonium dihydrogen phosphate (ADP). The PMMA/Ammonium dihydrogen phosphate (PMADP) composites PMADP 1 and PMADP 2 were characterized by using PXRD. The thick films of the composite on glass plates were prepared by using a spin coating unit at 9000rpm. The application of the thick film as gas sensors has been studied between 0 and 980 seconds. The experiment was carried out for different vapours at atmospheric temperature. The results show that the thick film of PMADP composite can function as a very good gas sensor.

III. INORGANIC CHEMISTRY

161. Synthesis, Spectral and Biological Studies of Some New Macrocyclic Complexes of Bivalent Metal Ions

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Keywords : *Characterization, biological studies, macrocyclic complexes.*

Six new macrocyclic complexes, viz.[{Bzo$_3$–[18]–pentaene N$_2$O$_2$}M(II)(H$_2$O)$_2$](Ac)$_2$, where : M^{+2} = Cu^{+2}, Co$^{+2,}$[{Bzo$_3$ –[18] – pentaene N$_2$O$_2$} Ni(II)(Ac)$_2$] and [{Bzo$_3$ – [20] – pentaene N$_2$O$_2$} M(II) (H$_2$O)$_2$] (Ac)$_{2,}$ where : M^{+2} = Cu^{+2}, Ni^{+2}, Co^{+2} have been synthesized by the reaction of *4,4'-butylenedioxodibanzaldehyde* and *o*-phenylenediamine / *p*-phenylenediamine in presence of metal salts by adopting template method and characterized by elemental analyses, I.R, ^{1}H- NMR, electronic spectral studies and magnetic moment values. The all compounds were screened for their biological studies against two bacteria *Staphylococcus aureus* (gram +ve) and *Escherichia coli* (gram -ve) bacteria and fungi *Aspergillus niger* and *Aspergillus flavus*. Macrocyclic complexes were found more active as compared to fragments.

162. Synthesis, Spectral Characterization and Antimicrobial Behavior of Heterobinuclear Complexes of Ni (II) Schiff Base and Alkali Metal Salt of Oxygen & Nitrogen Containing Organic Acids

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Keywords : *Hetrobinuclear alkali metal complexes, antimicrobial studies, MIC.*

The synthesis IR, UV-Vis spectral analysis, magnetic measurement, molar conductance measurements and biological studies of number of hetrobinuclear alkali metal complexes of Ni(II) of the Schiff base derived from the 1:2 refluxing of ethylenediamine and o-hydroxyacetophenone are reported. The low value of conductivity measurement shows non-electrolytic nature. The coordination of metal chelae takes place through the phenolic oxygen atom. The biological studies of some of the heterobinuclear complex are assayed and demonstrated a general inhibitory effect. The structure of the heterobinuclear alkali metal complex has been discussed on the basis of IR spectra, UV-Vis spectra and magnetic measurement. Binuclear nickel(II) complex of Schiff base have square planar geometry. There is no change in the stereochemistry of the Ni^2 in the adducts.

163. Estimation of Multiclass Pesticide Residues in Tamoto (*Lycopersicon Esculentum*) and Radish (*Raphanus Sativus*) Vegetables by Chromatographic Methods

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Keywords : *Estimation, Pesticides, Lycopersicon esculentum, Raphanus sativus, Chromatographic methods.*

Multiclass pesticide residues, viz. endosulphan, cypermethrin, monocrotophos and chlorpyriphos, have been estimated qualitatively and quantitatively in two vegetables tamoto (Lycopersicon esculentum) and radish (Raphanus sativus) by adopting gas liquid chromatographic and high performance liquid chromatographic methods. In the sample of tomato two pesticides endosulphan and cypermethrin and in radish four pesticides endosulphan, cypermethrin, monocrotophos and chlorpyriphos were found. The concentrations of the detected pesticides were determined from the area of the peaks.

164. Studies On Some Arylazo–Benzimidazole Mercury (Ii) Complexes

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Keywords : *Benzimidazole, ^1H NMR, pseudo transition element.*

Benzimidazole and its derivatives like 1H-2-(naphthyl á azo Benzimidazole (α-Na Benz) (II) and 1H-2-(arylazo benzimidazole (III) of the type HaaBzR, where R = H(a), $-CH_3$ (b), NO_2 (c) and OH(d) have been used up as ligands in preparation of complexes with an important pseudo transition element mercury(II). These complexes have been synthesized and characterized by their elemental analysis, infrared and ^1H NMR spectra. The stoichiometric ratios for the mercury (II) complexes have been suggested as (1 : 1), (1 : 2) or (2 : 1) with the contribution of coordinated water molecule and chloride ion in the complex formation. The probable structure for the mercury(II) complexes are also proposed.

165. Template Synthesis and Spectroscopic and Biological Studies of Macrocyclic Complexes Derived from Dimedone and Carbohydrazide

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Keywords : *Macrocyclic complexes; infrared; magnetic measurements; divalent metal salts; electronic spectra.*

A novel series of the complexes of the type $[M(TML)X_2]$ where TML is a tetradentate macrocyclic ligand; M=Co(II), Ni(II), Cu(II), Zn(II),; X=Cl^-, NO_3^-,

CH_3COO^-, Br^-have been synthesized by template condensation of dimedone and carbohydrazide in the methanolic medium. The complexes have been characterized by elemental analyses, conductance measurements, molecular weight determination, magnetic measurements, NMR, infrared and far infrared spectral studies. The low value of molar conductance indicates them to be non-electrolytes. All the complexes are supposed to have distorted octahedral geometry. The complexes were tested for their *in vitro* antibacterial activity. Some of the complexes showed satisfactory antibacterial activity.

166. Electronics Spectral Evidence of Intramolecular Inter – Ligand Interaction in the Mixed Ligand Complexes of Lanthanoid (III) Ions – Involving CDTA as Primary Ligand and Amino Acids as Secondary Ligands

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Keywords : *Oscillator strength, Judd-ofelt parameters, Racah parameters, nephelauxetic ratio, electronic spectra.*

Electronic spectral parameters viz. oscillator strengths (P) Judd-Ofelt parameters ($\tau\lambda$), the inter-electronic repulsion 'Racah' parameters (δE^k) and the nephelauxetic ratio ($\delta E^3 / \delta E^1$) values for the binary (ML) and mixed legend complexes (MAL) of some lanthanide (III) metal ions viz., Pr(III), Nd(III) and Er(III) involving cyclohexane diamine tetra acetic acid (CDTA) as primary legend and α – alanine, β – phenylalanine (β-phe) or tyrosine (tyr.) as secondary ligands have been evaluated at controlled pH-values in the pH-region of complexation (pH-region or complexation ascertained using SCOGS computer software), with a view to examine the possibility of intermolecular inter-ligand interaction in the mixed ligand complexes and also to observe variations in the spectral parameters as a result of inter-ligand interaction.

167. Macrocyclic Complexes of Trivalent Transition Metal Ions Derived from 1,2-diaminobenzene and 2,5-hexanedione.

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Keywords : *Trivalent salts; macrocyclic complexes; infrared spectra.*

A new series of the macrocyclic complexes of type $[M(C_{24}H_{28}N_4)X]X_2$, where M= Fe(III), Cr(III) and X = Cl^-, NO_3^-, CH_3COO^- has been synthesized by template condensation of 1, 2-diaminobenzene and 2, 5-hexanedione in the presence of trivalent metal ions. The complexes have been characterized with the help of elemental analyses, conductance measurements, electronic, NMR and infrared spectral studies. Electronic spectra along with magnetic moments suggest the five coordinate square pyramidal geometry for all the complexes. The molar conductance indicates them to be as 1:2 electrolytes.

168. Microwave Assisted Green Synthesis and Optical Properties of Silver Nanoparticles Stabilized by Polyvinyl Pyrolidone

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Keywords : *Silver nanoparticles; microwave irradiation; green synthesis; poly vinyl pyrolidone (PVP).*

In the present work silver nanoparticles are prepared by a simple green method. The silver nanoparticles prepared in this way are uniform and stable. Silver nanoparticles were prepared by the reduction of silver nitrate using glucose as

reducing agent and polyvinyl pyrolidone (PVP) was used as stabilizer. The resulting silver nanoparticles were characterized by transmission electron microscopy (TEM) and UV-Vis spectroscopy. TEM techniques showed the presence of silver nanoparticles with an average size of 11 nm. Various optimizing parameters such as effect of silver nitrate concentration, effect of glucose concentration and effect of microwave irradiation time, etc are also described.

169. Synthesis, Molecular Modelling and Spectroscopic Characterization of Nickel(II), Copper(II), Complexes of New 16-Membered Mixed-Donor Macrocyclic Schiff Base Ligand Incorporating a Pendant Alcohol Function

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Complexes of Cu(II) and Ni(II) are synthesized with 1,5- dioxo-9,10-diaza-3,ol-tribenzo-(7,6,10,11,14,15) peptadecane, a N_2O_2 macrocyclic ligand. The complexes are characterized by elemental analysis, molar conductance measurements, UV-VIS, IR, ^{1}HNMR, ^{13}C NMR, EPR and molecular modeling studies. All the complexes are non electrolyte in nature. So they may be formulated as [M(L)X] [where, M = Ni(II), Cu(II) and X = Cl^-, NO_3^-, CH_3COO^-]. On the basis of spectral studies, an distorted octahedral geometry has been assigned for Ni(II) complexes but a tetragonal geometry for Cu(II) complexes.

170. Corrosion Inhibition of Steel by Acid Extracts of Prosopis Juliflora

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Corrosion of steel in HCl, in H_2SO_4 and in HNO_3 solution at 299 + 2 k was studied by mass loss method in absence and presence of the acid extract of seeds,

leaves and bark of prosodies Juliflora (PJ). From the mass-loss data, it was concluded that the inhibition increased with increase in the concentration of the additives for the seeds in HCl. While in the case of leaves and bark, the corrosion rates were found to decrease with the increase in concentration of extract up to 0/ 2 % and then the reversal in trend of increase in concentration of 0.3 % to 0.5 %. In the case of in H_2SO_4 the inhibition increased with the increase in the concentration of the additives for seeds, leaves and bark.

171. Computational and Pulse Radiolytic Study of Homo- and Hetero-Metallic Derivatives of Binucleating Ligands

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Keywords : *Binucleating ligands, Oximes, Bulky boron ligands, Homo/Hetero-metallic complexes, Computational study, Pulse radiolytic study.*

The organometallic and coordination chemistries of oximes and boron ligands constitute an active area of research and act as a binucleating bridging unit to yield homo-and heterometallic complexes which can be potentially useful for the development of new materials. Generally, binucleating ligands are classified by the bridging groups that are used to assemble bimetallic complexes. Over the past one decade a new strategy of using “metal-oximates” or sterically encumbered boranes as ligands has emerged to synthesize various homo-/hetero-metal complexes with linear, triangular, butterfly, star-shaped molecules, as precursors for magnetic materials. Thus a number of Sn (IV) and Ge (IV) derivatives of these ligands have been synthesized and characterized by X-ray crystallography. Their properties and reactions have also been explored. The one-electron oxidation of oximes/metal derivatives by pulse radiolysis is currently being investigated and results will be presented.

172. Brij-35 Catalysis in the Oxidation of Amino Acids by Alkaline Hexacyanoferrate (III) Ions

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Keywords : *Critical micelle concentration, alanine, leucine, isoleucine, hexacyanoferrate(III).*

Surfactants are amphipathic molecules with both hydrophobic and hydrophilic properties. When these molecules are dissolved in water, they can achieve segregation of their hydrophobic portions from the solvent by self-aggregation. Aggregates of these surfactants, known as micelle, are responsible for altering the rates of organic reactions in aqueous surfactant solution. A wide variation in kinetic results, specially with variation in [hexacyanoferrate(III)] are reported. It was, therefore of interest to investigate the micellar effect on the oxidation of alanine, leucine and isoleucine by alkaline hexacyanoferrate(III), which shows most complications even in the absence of the surfactant or catalyst. The results of effect of non-ionic surfactant (brij-35) on the rate of oxidation alanine, leucine and isoleucine are reported here. The study shows that the rate of oxidation is strongly enhanced in presence of non-ionic micelle. The reaction follows a complex kinetics showing a first order dependence of rate with respect to both alkali and substrate concentrations. A suitable mechanism has been proposed and the kinetic data accounted for by the association/distribution of the substrate in micellar and aqueous pseudo phase. The binding parameters have also been evaluated.

173. Synthesis, Structure and Antimicrobial Effects of Some Co(II) and Cu(II) Complexes

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Keywords : *Antibacterial, antifungal, 2-imino, 4-thiobiuret, 4-aminoacetophenon, 1-acetonaphthone.*

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, FT-ir and FAB mass spectral studies. Synthesized complexes have been tested for the reactivity and substitution behavior. The Schiff base and metal complexes shows a good activity against the Gram-positive bacteria; *Bacillus subtilis, Staphylococcus aureus* and Gram-negative bacteria; *Escherichia coli, Pseudomonas aeruginosa; Candida albicans, Aspergillus niger, Aspergillus fumigatus* and *Fusarium oxysporum* fungal cultures.

174. Complexing Behaviour of 2-thiobenzimidazolyl Acetic Acid with Pd (II) & Pt (II)

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The growing interest of Pd (II) & Pt (II) complexes due to their catalytic behaviour and therapeutic properties tempted us to prepare and characterize some new complexes of Pd (II) & Pt (II) with 2-thiobenzimidazolyl acetic acid (TBZH). The complexes of Pd (II) & Pt (II) with TBZH of composition $M(TBZ)_2$ [$M=Pd^{+2}$ or Pt^{+2}], $M(LH)_2Cl_2$ [$M=Pd^{+2}$, Pt^{+2} and LH = TBZH] and [MLBCl] ($B=NH_3$ or Pyridine and $M=Pd^{+2}$ or Pt^{+2}) have been prepared and characterized. The ligand 2-thiobenzimidazolyl acetic acid (LH) co-ordinates as bidentate anionic ligand in complex [ML_2], unidentate S-donor neutral molecule in complex [$M(LH)_2Cl_2$] (M= Pd^{+2} or Pt^{+2}) and bidentate anionic co-ordinating molecule in [MLBCl] (M = Pd^{+2} or Pt^{+2} and B = Py or NH_3). The bonding of ligand and geometry of complexes have been suggested from the studies of UV and infrared spectral data. The corboxylate group õ(CO) vibration of ligand is raised to higher wave number in [MLBCl] and [ML_2] type of complexes suggesting absence of hydrogen bonding and co-ordinaton of carboxylic acid on deprotonation. The electrical conductance value

of $[M(LH)_2Cl_2]$ and [MLBCl] complexes displayed negligible electrical conductance in DMF suggesting co-ordination of chloride to metal in complexes. The UV spectral band positions of complexes are similar to square planar geometry of palladium (II) and platinum (II) complexes. The υ(C-S-C) of thioacetic acid part vibration suffers red shift indicating coordination of ligand through ether sulphur atom also in complexes. The carboxyl group υ(CO) vibration of ligand and the complex $[M(LH)_2Cl_2]$ observed as broad band at identical position supporting uncoordinated nature of (COOH).

175. Effect of Micronutrient on Inhibition Efficiency of Lactic Acid

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Formation of urinary stone is a function of several factors operating in the urinary tract. Three most important factors are (1) level of calculogenetic crystalloids in the urine (2) level of inhibitors of calculogenesis (3) Availability of a suitable nidus or matrix in the urinary tract. A disbalanced state state between the first two factors with crystalloid dominating would indicate the state of formation of stone.Sequestration by complexation would be most effective in inhibition the mineralisation of insoluble salt. In Urolilithiasis, it is the calcium ions that form stubborn insoluble minerals (phosphates, oxalates) and effective inhibitor has to be a good calcium complexing/ sequestering agent. Lactic acid was found to be good inhibitor in dissolution of urinary stone. Our primary aim is to find out the possibilities of dissolving urinary stone in the presence of micronutrients such as $FeSO_4.7H_2O$, $NiCl_2.6H_2O$, $CuCl_2.H_2O$, $ZnSO_4.7H_2O$, $MnCl_2.4H_2O$.

176. Characterization of Electrodeposited Zinc Oxide/ Tetrasulphonatedcopper Phthalocyanines (Zno/Ts-Cupc) Hybrid Films and Their Photoelectrochemical Properties

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Keywords : *Tetrasulphonatedmetal phthalocyanines, zinc oxide.*

Hybrid films of zinc oxide (ZnO) and tetrasulphonatedcopper phthalocyanine (Ts-CuPc) have been prepared by cathodic electro-deposition from aqueous O_2-saturated solutions of $ZnCl_2$ and Ts-CuPc. The Ts-CuPc content of the films can be varied in a wide range by variation of dye concentration in the electrodeposition bath – from single Ts-CuPc molecules embedded in compact crystalline ZnO to films based on an amorphous Ts-CuPc framework. With increasing dye content the colour of the films changes from light blue to deep blue. All films were characterized by XRD, SEM and AFM. Photo electro-chemical characteristics of the electrodes were studied by photo current spectra and by time-resolved photocurrent measurements in0.1M KCl electrolyte. At the same time, changes in the electrical and photoelectrical properties of the films are observed, enabling the tuning of these properties in view of optoelectronic applications.Theoretical calculations based on density functional theory (DFT) models were made to understand the optoelectronic properties of the hybrid films. Different parallel and perpendicular orientations were tested. For the most stable hybrid structure, total and projected densities of states of the system were obtained and the alignment of the levels observed.

177. Electrochemical Behavior of Complexes of Cd^{2+} with Bupropion Hydrochloride in Aqueous, Non-aqueous Binary Mixtures

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Keywords : *Polarography metal complexes, stability constant, thermodynamic parameters, Cd^{2+}, Bupropion hydrochloride.*

The complexation of Cd^{2+} with Bupropion hydrochloride was studied in aqueous and binary non-aqueous mixtures using DC polarographic technique at pH 7.30±0.01 and ionic strength μ = 1.0 M KCI at two temperatures 25^0C and 35^0C. The stiochiometry and stability constants of the complexes were determined by Deford-Hume method. Complexes formed were in 1:1, 1:2 ratios and the nature of electrode processes were reversible and diffusion controlled. The results show that the stability of the complexes depends on the nature and composition of the mixed solvents. The formation of the metal complexes was found to be spontaneous and exothermic in nature.

178. Chemistry of Zinc and its Hazardous Effects

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Keywords : *zinc finger, micronutrient and antioxidant.*

Zinc is one of the trace minerals which is required for huge range of bodily enzyme. Zn is a constituent of organic catalysis in the body. Zn as a micronutrient is being used indiscriminately in agricultural and husbandry practices and also in body foods and multivitamin supplements because Zn is nontoxic and promotes linear growth and body weight, however, in high concentration it can prove to be toxic. The copper supplement should be added with Zn supplement during pregnancy. It plays a vital role in physiological and metabolic process of many organisms; but excessive intake during the growth phase increases the growth hormone level in the blood and the level of glycosylated haemoglobin. In a zinc finger the Zn ion is tetrahedrally bonded to two cysteine and two histidine residues to form the zinc-finger domain.

179. Synthesis, Physico-chemical and Biological Properties of Some Mixed Ligand Complexes of Trivalent Lanthanides with 4[N-4’-Dimethylamino-Benzalidenne)Amino]Antipyrine Thiosemicarbazone and Pyridine.

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In the present studies, some seven and ten coordinated complexes of trivalent lanthanides derived from 4[N-(4’-dimethylaminobenzalidene)amino]antipyrine thiosemicarbazone (DMBAAPTS) and pyridine are reported with the general composition $LnX_3.n(DMABAAPTS).Py$ (Ln = La, Pr, Nd, Sm, Gd, Dy, Dy or Ho : X = NO_3 , n =1, X = NCS or ClO_4, n = 2, Py = pyridine). All the complexes were characterized by elemental analysis, molar mass, molar conductance, magnetic susceptibility, infrared and electronic spectral studies. The infrared studies suggest that the DMBAAPTS behaves as a neutral tridentate (N,N,S) while pyridine is coordinated to central metal ion *via* its lone N-atom. Perchlorate ions are not coordinated in coordination sphere, nitrates are bicovalently bonded, while isothiocyanate is coordinated through a strong N-atom. From electronic spectral data, nephelauxetic effect (β), covalence factor ($b^{1/2}$), Sinha parameter ($\delta\%$) and the covalence angular overlap parameter (η) have been calculated. Antibacterial and antifungal activities of the thiosemicarbazone and its Ln(III) complexes have been evaluated. Thermal stabilities of these complexes were also studied by TGA.

180. Synthesis and Characterisation of Boron Complexes with Schiff Bases Rearranged From Benzothiazolines

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Keywords : *Triisopropoxyborane; o-aminothiophenol; benzothiazolines; spectral studies.*

The present paper is a report on the synthesis of some new coordination compounds by the reactions of triisopropoxyborane with sulfur containing ligands. Ligands used in these reactions are benzothiazolines prepared by the reaction of p-tolualdehyde, 4-acetylbiphenyl, 9-anthraldehyde, 4-fluoroacetophenone and 2-acetylfluorene with o-aminothiophenol which on reaction with metal ion rearrange to Schiff bases. Characterization and structure elucidation of the complexes are achieved by elemental analysis, electronic, infrared, ^{1}H and ^{13}C NMR spectral studies. The potency of the synthesized compounds have been assessed by growth inhibiting potential of the complexes against variety of fungal and bacterial strains.

181. Synthesis, Characterization, Antimicrobial Activities, and Spectral Studies of Transition (II) Complexes with 1-(4-Chlorophenyl)-3-(4-fluoro/hydroxyphenyl) prop-2-en-1-thiosemicarbazone

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Keywords : *Characterization, Antimicrobial Activities, and Spectral Studies of Transition (II) Complexes.*

Fe, Co, and Cu complexes have been prepared by reacting metal chloride/ sulphate with 1-(4-chlorophenyl)-3-(4-fluoro/hydroxyphenyl) prop-2-en-1-Thiosemicarbazone. The transition complexes (5) were derived from the reaction between 1-(4-chlorophenyl)-3-(4-fluoro/hydroxyphenyl)prop-2-en-1-Thiosemicarbazone(4) with an aqoues solution of transition salt. Chalcone thiosemicarbazone ligands (4) was prepared by the reaction of1-(4-chlorophenyl)-3-(4-fluoro/hydroxyphenyl) prop-2-enone (chalcone) (3) with thiosemicarbazone in the presence of hot ethanol. All the transition-ligands 1:2 complexes have been isolated in the solid state, are stable in air, and characterized on the basis of their elemental and spectral data. Thiosemicarbazone ligands behave as bidentate ligands by coordinating through the Sulfur of the isocyanide group and nitrogen of the cyanide residue. The chalcone thiosemicarbazone ligands and their transition complexes have been screened for their IR, NMR, and antifungal and antibacterial studies.

182. Electrochemical Study of Zn^{+2} – Theophylline Complex

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Keywords : *Stability constant, thermodynamics parameters, Zn^{2+} -Theophylline system.*

The interaction between Theophylline and $Zn^{2+}$was investigated using direct current paleography. The polarographic technique was used to determine the stability constants and thermodynamics parameters such as enthalpy change (ΔH), free energy change (ΔG) and entropy change (ΔS) of Zn^{2+} complexes with Theophylline at pH-5 in 0.1 M acetate buffer. The study was carried out at two different temperatures 25° C and 35° C. Zn^{2+} - Theophylline complexes were formed in 1:1 and 1:2 ratios. The electrode processes were reversible and diffusion controlled.

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183. 3-Hydroxy-2-[1'-phenyl-3'-(4?-methoxy)-4'- pyrazoyl] – 4 - oxo- 4*H*-1-benzopyran as a Spectrophotometric Reagent for the Micro- determination of Tin

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Keywords : *tin, 3-hydroxy-2-[1'-phenyl-3'-(4''-methoxyphenyl)-4'-pyrazoyl]-4-oxo-4H-1-benzopyran, extraction, spectrophotometric.*

A simple, rapid, sensitive and selective spectrophotometric method for the determination of micro-amounts of tin has been worked out employing 3-hydroxy-2-[1'-phenyl-3'-(4''-methoxyphenyl)-4'-pyrazoyl]-4-oxo-4*H*-1-benzopyran as a complexing ligand in acidic medium. The complex is extractable into carbon tetrachloride and shows maximum absorbance at 424 nm. Beer’s law is obeyed in

the range 0.0 to 3.04 µg Sn(II)/ml with an optimum range of determination as found from Ringbom plot is 0.28-2.63 ppm. The molar absorptivity and Sandell's sensitivity of the complex are 4.87×10^4 L mol^{-1} cm^{-1} and 0.0024 µg Sn(II) /cm^2 at 424 nm respectively. The method is free from interference of large number of anions/complexing agents and cations. The method has been satisfactorily applied to the analysis of tin in various samples including tin can and gun metal.

184. Nanocrystalline Manganese Ferrite as a Redox Catalyst for Epoxidation of Styrene to Styrene Oxide

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Keywords : *Nanocrystalline Ferrite, Epoxidation, Styrene, Styrene Oxide.*

Slurry phase epoxidation of styrene to styrene oxide by hydrogen peroxide over nanocrystalline $MnFe_2O_4$ has been carried out. A maximum conversion of 92% with a selectivity of 90% towards styrene oxide was obtained at a temperature of 333 K. The catalyst performance is almost par with TS-1. The catalyst has been characterized by BET surface area measurement, XRD, Mössbauer, AFM, SEM and ESCA techniques. It is concluded that unlike TS-1 and Mn Salen complex $MnFe_2O_4$ catalysts does not form peroxo species and that lattice oxygen is involved in the redox mechanism.

185. An Innovative Experiment of Pedagogical Value to Determine Manganese Content by Volhards Method

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Keywords : *Chemistry education, Pedagogy, Manganese ore.*

As an alternative to the regular experiments dealing with analysis of an ore, experiment was developed based on volumetric analysis of some used-up consumer product. The determination of manganese from the electrolyte powder in a run-down dry cell by volhard's method is an alternative for analysis of pyrolusite ore. The experiment helps student to think about the relationship between the properties and composition of the material also. It may be successfully incorporated in the programme of practical for undergraduate or postgraduate students of analytical or inorganic chemistry.

186. Chemical Effect of Contact Glow Discharge Electrolysis Using $Fe(CN)_6^{4-}$ Ion as an Oxidisable Substrate

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Chemical yields of contact glow discharge electrolysis (CGDE) show strong deviations from faradaic behavior. The products are novel for normal electrolysis and yields significantly exceed the Faraday law value. Anodic CGDE gives rise to $Fe(CN)_6^{3-}$ in the anolyte in yields significantly exceeding the faradaic value besides the faradaic yield of O_2. The relative yield of $Fe(CN)_6^{3-}$ depends on the concentration of $Fe(CN)_6^{4-}$ and the quantity of electricity passed. A kinetic analysis of the variation of the initial differential yield of $Fe(CN)_6^{3-}$,G_0 ($Fe(CN)_6^{3-}$) with the concentration of $Fe(CN)_6^{4-}$ after applying certain approximations leads to an estimate of the generation of 12 moles of OH? Radicals in the liquid phase reaction zone of anodic CGDE for the passage of each mol electron of electricity.

187. Intercalation of $[Cr(C_2O_4)_3]_{3-}$ in Nickel-Aluminum Layered Double Hydroxide

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Keywords : *Ni-Al carbonate LDH, intercalation.*

A Nickel Aluminum carbonate LDH was synthesized by mixing $Ni(NO_3)_2.6H_2O$, $Al(NO_3)_3.9H_2O$, and a NaOH and Na_2CO_3 solution at PH 9. The suspension was centrifuged, washed and transferred into a Teflon-lined autoclave with 80 ml water and heated at 150^0C for 10hrs. The suspension was dried in an oven at 70 0C. The NiAlLDH was characterized by XRD, FTIR, SEM, EDX, DRS and TGA. [Cr(C2O4)3]3- was intercalated in the NiAlLDH by ion exchange process. This intercalated compound was characterized by XRD, FTIR, SEM, EDX, DRS and TGA. The TGA study of NiAl LDH shows two weight losses in the temperature ranges between 30^0C-240^0C and 240^0C-700^0C but in $[Cr(C_2O_4)_3]^{3-}$ intercalated NiAlLDH four weight losses in the temperature ranges between 30^0C-110^0C, 110^0C-240^0C, 240^0C-440^0C, 440^0C-700^0C were observed. The XRD study shows the basal spacing of NiAlLDH as 7.93Å and of $[Cr(C_2O_4)_3]^{3-}$ intercalated NiAlLDH as 8.14 Å. The SEM images shows the morphology of the LDH. The EDX, IR and TGA study confirms intercalation of $[Cr(C_2O_4)_3]^{3-}$ in NiAlLDH.

188. Synthesis, Structural Characterization and Thermal Studies of Co(II), Ni(II), Cu(II) and Zn(II) Complexes of Schiff Base Derived from 4-Amino-5-mercapto-3-methyl-1,2,4-triazole

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Keywords : *Synthesis, Schiff Bases, 1,2,4-triazole, Thermal study.*

Co(II), Ni(II), Cu(II) and Zn(II) Complexes of bidentate Schiff bases derived from the condensation of 4-Amino-5-mercapto-3-methyl-1,2,4-triazole with 5-Nitrofurfuraldehyde were synthesized and characterized by elemental analysis, magnetic, spectroscopic (IR, Electronic, ^{1}H NMR, ESR) and thermogravimetric analysis. A square planar geometry was suggested for Cu(II) and octahedral geometry proposed for Co(II), Ni(II) and Zn(II) complexes. TG curves indicated that the complexes decompose in two to three steps. The presence of coordinated water in metal complexes was confirmed by thermal and IR data of the complexes.

189. Trivalent Transition Metal Ion Directed Macro Cyclic Complexes Derived from 2, 6 – diaminopyridine Isatin

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Keywords : *Antibacterial, diaminopyridine isatin, MIC.*

New series of complexes of the type $[M(C_{26}H_{16}N)X]X_2$, where M = Cr(III), Mn(III), Fe(III) and X = Cl', $NO_3CH_3COO^-$ and CH_3COO^- for Mn(III) has been Synthesized by template condensation reaction of 2, 6-diaminopyridine and isatin in the presence of trivalent metal salts in methanolic medium. On the basis of various physic-chemical studies, a five coordinate square-pyramidal geometry for all of these complexes has been proposed. The complexes were also tested for in vitro antibacterial activities against some bacterial strains viz. staphylococcus aureus, Bacillus subtilis (Gram-positive), Escherichia coli Pseudomonas aeruginosa (Gram-negative. The MIC shown by the complexes were compared with MIC of standard antibiotics Ciprofloxacin.

190. Synthesis, Spectral and Antimicrobial Studies of Zinc(ii) Complexes with Schiff Bases Derived from 2-hydrazino-5-[substituted phenyl]-1,3,4-thiadiazoles

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Keywords : *Zn(II), Schiff bases, IR, ^1H NMR, ^{13}C 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-thiadiazoles and 2-

hydroxyacetophenone/ benzal-dehyde/ 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 pallescence*) by paper disc method.

191. Synthesis, Spectral Characterization and Antifungal Studies of Lanthanum (iii) and Praseodymium (iii) Complexes with Schiff Bases Derived from 3-substituted-4-amino-5-hydrazino-1,2,4-triazoles and Isatin

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Keywords : *Lanthanum(III), praseodymium(III), Schiff bases, IR, NMR, fungitoxicity.*

Lanthanum(III) and praseodymium(III) complexes of type $[Ln(L)Cl(H_2O)]$ (Ln= La(III) and Pr(III); LH_2= Schiff bases derived from 3-(phenyl/2-chlorophenyl/ 4-chloro phenyl/ 4-nitro phenyl)-4-amino-5-hydrazino-1,2,4-triazoles) have been synthesized and characterized by elemental analyses, molar conductance, magnetic moment and spectral (electronic, IR, ^1H and ^{13}C NMR) studies. The presence of coordinated water molecule in the complexes has been inferred from thermogravimetric analysis. For praseodymium(III) complexes, nephelauxetic ratio, covalency parameter and bonding parameter have been evaluated from electronic spectral data. The fungicidal activity of the ligands and their corresponding complexes has been evaluated against *Aspergillus niger* and *Helminthosporium oryzae* by the agar plate technique.

192. Boron Spirochelates Derived From Catechol And Arylazonapthols

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Keywords : *catechol, arylazonapthols, boron heterocyclic, tetra coordinated boron.*

The reaction of 2-isopropoxy-1, 3, 2-benzodioxaborole with arylazonapthols in molar ratio 1:1 in benzene gives boron heterocyclic of type [o-OC_6H_4O]B[$OC_{10}H_6$:NN(Ar)] (where Ar = C_6H_5,o-$CH_3C_6H_5$, p-$CH_3C_6H_4$, p-$CH_3OC_6H_4$, o-ClC_6H_4 and p-ClC_6H_5). The complexes are coloured monomeric nonvolatile solids soluble in common organic solvents and have been characterized by elemental analysis, IR and NMR (1H and 11B) spectral studies. The physicochemical studies give evidence for the monofunctional bidentate behaviour of the arylazo ligands and tertra coordination around the central boron atom.

193. Synthesis and Study of Zinc -μ - Oxo Aluminium Isopropoxeide Derivatives

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Keywords : *Bimetallic -μ - oxoisopropoxides, 1, 3- ketoamines, complication and hydrolysis.*

The reaction of bimetallic (Al (III) Zn (II) -μ –oxoisopropoxide Zn [OAl (‘OPr)2 with 1,3 - ketoamines in 1:2 molar ration in Benzene gave the product Zn OAl (‘OPr)2]2 with the replacement of two isopropoxy groups by the stiffs’ base. The formation of the compound was monitored by estimating the liberated isopropanol oxidimetrically. The products formed were characterized by elemental analysis and spectral studies. The complexes obtained were subjected to hydorlisis

and the products formed were dried dehydrated and subjected to thermal treatment. The analysis of these products gives evidence for the formation of mixed oxide ZnAlO2.

194. Synthesis and Studied of Palladium Arylazopyrazolone Complexes

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Keywords : *arylazopyrazolone, palladium, complexes, tetra-coordinated.*

Some new arylazopyrazolone complexes of palladium having the general formula $[ArNN:CC(C_6H_5)C:O]_2Pd$ (where Ar = C_6H_5, p-MeC_6H_4, p-MeOC_6H_4, p-BrC_6H_4, p-Cl C_6H_4 and p-FC_6H_4) have been prepared. The derivatives were synthesized by the reaction of sodium bis(dichloropalladate) with 1, 3-diphenyl-4-arylazo-5-pyrazolones. Charaterization of the complexes by elemental analysis and IR and ^{1}HNMR studies suggest N-O coordination of the arylazo ligands and the formation of tetra coordinated complexes with square planar geometry.

195. Dna Cleavage, Antimicrobial and Spectroscopic Studies of Lanthanide (Iii) Chloride Complexes of 2-(N-*O*-Hydroxyacetophenone)Amino-3-Carboxy Ethyl-4,5 Dimethylthiophene

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Keywords : *o-hydroxyacetophenone, lanthanides, IR, molar conductance, DNA.*

Complexes of a novel heterocyclic Schiff base have been prepared by the interaction of Ln(III) chloride (Ln=La, Ce, Pr, Nd, Sm and Gd) with 2-(*N*-*o*-hydroxyacetophenone)amino-3-carboxyethyl-4,5-dimethylthiophene in 1:1 molar ratio.

The ligand and metal complexes were characterized on the basis of elemental analyses, molar conductance, magnetic susceptibility data, UV-Visible, IR, FAB mass and ^{1}H NMR spectral studies. The spectral data revealed that the ligand has been coordinated to the metal ion in a neutral tridentate manner, through the ester carbonyl, azomethine nitrogen and phenolic oxygen. The ligand and the metal complexes were subjected to i*n vitro* antimicrobial activities by disc diffusion method. The metal complexes were found to be more active when compared to the ligand. The interaction of ligand and metal complexes with DNA was also investigated by gel electrophoresis technique.

196. Synthesis and Characterization of Mixed Ligand Complexes Derived from Benzofuran Schiff's Base and 2, 6-diaminopyridine

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Keywords : *Benzofuran Schiff's bases, Mixed ligand complexes, Spectral studies, Biological activity.*

The mixed ligand complexes of the type MLL'Cl$_2$, where M = Co (II), Ni (II), Cu (II), Zn (II), Cd (II) and Hg (II), L = primary ligand derived from reaction between benzofuran-2-carbohydrazide and 3, 4, 5-trimethoxybenzaldehyde (TMeOBFC) and L' = secondary ligand, 2, 6-diaminopyridine (2, 6-dap) has been synthesized. All the mixed ligand complexes have been characterized on the basis of analytical data, IR, UV-Vis, ^{1}H NMR, DART-MS and ESR spectral data and magnetic studies. The complexes are soluble in DMF and DMSO. The measured molar conductance values indicate that, the complexes are non-electrolytic in nature. Based on the above studies we have assigned the probable geometry for all the mixed ligand complexes. The antibacterial and antifungal activities of the ligands and their metal complexes have been screened against bacteria *Escherichia coli* and *Staphylococcus aureus* and against fungi *Aspergillus niger* and *Aspergillus flavus*.

197. Synthesis, Characterization, Electrochemical Properties and Antimicrobial studies of Co(II), Ni(II), Cu(II), Zn(II) and Fe(III) Complexes with Isatin Derivative

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Keywords : *Isatin; Benzaldehyde; Electrochemistry; Spectral characterization; Transition metals.*

Metal complexes of Zn(II), Co(II), Ni(II), Cu(II) and Fe(III) with Schiff base derived from benzaldehyde and isatin monohydrazone have been synthesized & characterized on the basis of elemental analyses, I R spectral, electronic spectra. The elemental analyses of the complexes confine to the stoichiometry of the type $ML_2.2NO_2$ [M= Zn(II), Co(II), Ni(II), Cu(II)] and and $[FeL_2.2NO_2] NO_2$. The redox properties of the complexes were extensively investigated by electrochemical method using cyclic voltammetry (CV). The Co(II) and Cu(II) complexes exhibited quasi-reversible single electron transfer process where as Zn(II) and Fe(III) complexes shown two redox peaks of quasi-reversible one electron transfer process. All the coloured complexes have been screened for their antimicrobial activity against fungi viz. A. niger, A. flavous, P. triticena, F. species & bacteria viz. E. coli, B. subtilis, S. typhi, S. aureus. The results of antimicrobial activity shows that metal complexes of bivalent metals have more potency towards experimental fungi & bacteria. It also shows that Cu(II) complex is more toxic against bacteria S. aureus.

198. Photocatalytic Degradation of Methyl Blue by Heterogeneous $PbSnO_3$ Photocatalyst Under Simulated Sunlight

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Keywords : *Green chemistry, Photocatalyst, photodegredation, Solid stare synthesis, Mineralization.*

Light induced photocatalyst $PbSnO_3$ was synthesized by green chemistry approach, with mechanochemical method. The synthesized catalyst was characterized by various analytical investigative techniques like UV-DRS, FTIR Spectroscopy, X-ray Diffraction, SEM and Energy Dispersive X-ray Spectroscopy etc. Avarage partical size of the catalyst by Scherer's formula is found to be 26.36nm. Photocatalytic activity of $PbSnO_3$ was studied by photodegredation of Methyl blue dye under stimulated sunlight. Complete mineralization of Methyl Blue was successfully achieved by $PbSnO_3$ p hotocatalyst. In present study, result obtained is evaluated and reported.

199. Kinetics Studies and Mechanism Evolution of the Methylation of Aniline Over $ZnFe_2O_4$ Catalyst

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Keywords : *Kinetics, Methylation, Zinc Ferrite, Ferrospinal, N-Methylaniline, N,N,di-Methylaniline.*

Kinetic investigation of the Vapour phase methylation of aniline with methanol has been carried out over $ZnFe_2O_4$ and temperature range 503-583 K. The partial pressures of Aniline and methanol were varied and rate were measured for the formation of N-Methylaniline & N,N,di-Methylaniline. The rate equation $R_A = k.\ K_M\ P_A P_M / (1+K_M (P_M)$ deduced, on the basis of adsorption of methanol and aniline in gas phase represented the data most satisfactorily. Catalyst characterization has been made by XRD, IR, Mössbauer spectroscopy, ammonia desorption and BET surface area measurements.

200. Metal Ion Chelation Chromatography on Alizarin Red S loaded Titanium Phosphate : Selective Separation of Cd^{++} and Pb^{++} from Some Transition Metal Ions

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Keywords : *Chelation Chromatography, Alizarin Red S, Titanium Phosphate, distribution coefficient, separation of metal ions,* Cd^{++} *and* Pb^{++}.

Titanium Phosphate, a cation exchanger, has been modified by adsorption of Alizarin Red S (ARS). Adsorption of several metal ions like Cr^{+++}, Mn^{++}, Fe^{+++}, Co^{++}, Ni^{++}, Cu^{++}, Zn^{++}, Cd^{++}, Hg^{++} and Pb^{++} on the modified ion exchanger from aqueous solutions at different pH (from 1-6) were studied to calculate their distribution coefficients. On the basis of distribution coefficients several binary separations of metal ions has been achieved on a chromatographic column packed with modified ARS-Titanium Phosphate using aqueous solutions at different pH as eluent. In addition to some binary separations selective separation of Cd^{++} and Pb^{++} from a mixture of several cations have been achieved.

201. Synthesis, Characterization and Biological Activity of Mixed Ligand Complexes of Cu (II) Containing Pyridine and Isoxazole Schiff Bases

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Keywords : *Isoxazole Schiff base, Pyridine, Cu(II) Complexes, Biological activity.*

A series of new mixed ligand Cu (II) complexes of Pyridineand Schiff bases derived from 3-amino-5-methyl isoxazole and substituted salicyaldehydes (MIIMP / CMMIIMP / EMIIMP / MEMIIMP / BMIIMP / MIIBD) have been synthesized. The complexes were characterized by Elemental analysis, IR, ESR, ^{13}C, ^{1}H-NMR, UV-VIS, Mass, Electronic spectra and Magnetic susceptibilities. Spectral data

shows that in these ternary metal complexes the Schiff bases and Pyridineact as bidentate coordinating to the metal ion through phenolic oxygen, imine nitrogen and with two nitrogen donor atoms respectively. The biological activities of Ternary metal Complexes have been screened against bacteria and fungi. Ternary metal complexes show more biological activity than the corresponding ligands.

202. Synthesis, Characterization and Oxidation of Alcohols by Nanocobalt(II) on Polymer-supported Schiff Base

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Keywords : *Nanoparticles, Schiff base, Polymer system, oxidation of alcohols, recyclability of catalyst.*

Nanocobalt particles have been anchored to the matrix of polystyrene through Schiff base. Chloromethylated polymer refluxed with ethylenediamine in round bottom flask, to this polymer system add calculated amount of salicylaldehyde refluxed in alcohol medium, resulted yellow solid called as polymer-supported Schiff base. Cobalt anchored to the above polymer-supported Schiff base by refluxing cobalt chloride in the presence of ethanol medium. The resulting catalysts were characterized by TEM, scanning electronic microscope (SEM), infrared, ^{1}H NMR. TEM image shows uniform diameter of 20-40nm and also found to be air and moisture stable.

Catalytic activity of Polymer-supported Schiff base Co(II) achieved by oxidation of aliphatic and aromatic alcohols in the presence of atmospheric oxygen. Aromatic alcohols were oxidized to the corresponding carboxylic acids and ketones in high yields, no oxidation was observed in the aromatic ring. Aliphatic alcohols undergo oxidation to the corresponding carboxylic acids and ketones in moderate to good yield. One of the main objectives of our study was to investigate the recycling and reuse of the catalyst. The catalyst could be reused up to four times while retaining it catalytic activity.

203. Characterization and Photo-luminescence Properties of Some $MLn_{2(1-x)}O_4$:$2xEu^{3+}$ or $2xTb^{3+}$ Systems (M = Ba or Sr, Ln = Gd or La)

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Keywords : *Phosphor material, Phosphor particles, Luminescent materials.*

$BaGd_2O_4$, $BaLa_2O_4$ and $SrLa_2O_4$ powders doped with different concentrations of Eu^{3+} or Tb^{3+} are prepared by combustion synthesis method and the samples were further heated to 500, 700 and 900 ºC to improve the crystallinity of the materials. The structure and morphology of materials have been examined by X-ray diffraction and scanning electron microscopy. It is remarkable that all the samples of $BaGd_2O_4$, $BaLa_2O_4$ and $SrLa_2O_4$ have similar morphology. These images exhibited homogeneous aggregates of varying shapes and sizes, which are composed of a large number of small elliptical shaped crystallites with an average diameter of about 0.5to 3.0 um. Photoluminescence for all materials increases with increase of temperature and found maximum for the samples heated to 900 ºC with 4 mole% doping of Eu^{3+} or Tb^{3+} ions. Luminescence is almost same all powders when doped with same concentration of Eu^{3+}.

204. Chemicals or Substances Two Reactions or Lessons are More

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Keywords : *Chemical Reactions, Metallic and Non-Metallic Oxides, Acids and Bases, Neutralization Reaction, Hardness of water.*

In this methods we take low (two) Chemicals and tell or teach more reactions or class room lessons. Suppose we introduce this method, we get low chemical expenditure and low air pollution.

In this method Magnesium and Sulpher are used. We get four types of Chemical Reactions (a) Chemical combination, (b) Chemical Decomposition (c) Chemical displacement (d) Double decomposition, Preparation of Metallic and Non-Metallic Oxides, Preparation of Acids and Bases, Neutralization reaction, Hardness of water, Deco lour reaction etc. are present.

205. Oxygen Activation at Room Temperature and Pressure of Parathion to Remove its Toxicity

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The organophosphorus insecticide parathion was selected as an analog for the chemical nerve agent, VX. Degradation of 0.44 mM parathion in a 10 mL aqueous solution containing 0.50 g granular zero valent iron (ZVI) under ambient air and pressure was complete after 4 h to the detection limit of GCFID. The degradation kinetics demonstrate the system to be pseudo-first-order with respect to parathion disappearance with a rate constant of 0.92 h^{-1}. The only non-polar organic intermediates detected were diethyl thiophosphat e and paraoxon, of which paraoxon is degraded to below the limit of detection of the GC-FID after 12 h.

206. Synthesis, Spectroscopic, Thermal and Antimicrobial Studies of Toluene-3,4-dithiolatoarsenic(III)/Antimony(III) Derivatives with Some Oxygen and/or Sulphur Donor Ligands

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The 1,1-dithiolato and 1,2-dithiolato ligands exhibit wide range of diversity in

their bonding and coordination patterns [1,2] as well as these ligands and their metal complexes have found their applications [3-5] in a number of ways like analytical reagents, in the productions of petroleum derivatives, for regeneration of cracking catalysts, lubricants oil additives, antiviral agents, antidotes, antimicrobial and as antitumor drugs.

In view of the above, recently we synthesized 1,2-dithiolato complexes by replacement reactions of toluene-3,4-dithiolatoarsenic(III)/ antimony(III) chloride and oxygen and/ or sulphur donor ligands like benzoic acid, thiobenzoic acid, acetic acid, thioacetic acid, phenol, thiophenol, sodium salicylate and thio glycolic acid in 1:1 molar ratio as well as disodium oxalate in 2:1 molar ratio in refluxing anhydrous benzene yielded toluene-3,4-dithiolatoarsenic(III)/ antimony(III) derivatives of the general formula $SC_6H_3(CH_3)SMR$ where M = As and Sb; R = $OOCC_6H_5$, $SOCC_6H_5$, $OOCCH_3$, $SOCCH_3$, OC_6H_5, SC_6H_5, $OOCC_6H_4(OH)$, SCH_2COOH and $SC_6H_3(CH_3)SMOOC\text{-}COOMS(CH_3)C_6H_3S$. These newly synthesized derivatives are yellow-brown solid/ liquid and soluble in common organic solvents like benzene, chloroform, dichloromethane, DMF, DMSO etc. These derivatives have been structurally characterized by melting point determination, molecular weight determination, elemental analysis (C, H, S and As/ Sb) and spectral {UV, IR and NMR (^{1}H and ^{13}C)}, SEM and thermal studies. Tentative structures for these new compounds have been proposed on the basis of the above studies. Last products of thermal decomposition studies (TGA, DTA & DSC) were found to be pure M_2S_3 which may be used in a number of ways [6]. Some of these complexes have been screened for their antimicrobial activities using the disc diffusion method. All the complexes have shown good activity as antibacterial and antifungal agents on some selected bacterial and fungal strains, which increased on increasing the concentration. Chloroamphenicol and terbinafin were used as standards for the comparison.

207. Mixed Ligand Complexes of Silver (i) Metal Chelates of Some Organic Acids with Quinaldinic Aaicd-n-oxide

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Keywords : *Mixed Ligand complex, Quinaldinic acid-N-oxide, Silver (I) metal chelates,*

infrared spectra.

Some noble mixed ligand complexes of silver (I) metal chelates of different organic acids with quinaldinic acid-N-oxide of type ML.HL', where M = Ag(I); L = deprotonated o-nitrophenol(ONP), 2,4-dinitrophenol(DNP), 2,4,6-trinitrophenol(TNP), 8-hydroxyquinoline (8HQ), 1-nitroso-2-nepthol(1N@N), o-amenobenzoic acid (OABA), o-nitrobenzoic acid (ONBA), 5,7-dinitro-8-hydroxyquinoline(DN8HQ), salicylic acid(SaIA) or acetylsalicylic acid(AcSaIA); HL' = quinaldinic acid –N-oxide have been synthesized and characterized by element analysis, conductivity measurement , infrared electronic absorption spectral data. The problem structure of the complexes proposed on the basis if spectral studies. The molar conductivity measurement shows these complexes are covalent nature. Infrared spectra indicates the presence of hydrogen bonding in these complexes, which may be one of the factors stabilizing them.

208. Complexes of Hydrazine Carboxylic Acid and Formyl Hydrazine Carboxylic Acid with Co(II), Ni(II), Mn(II) and Zn(II)

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Complexes of hydrazine carboxylic acid (Hhyc) and formyl hydrazine carboxylic acid (HCH=N–NH–COOH) abbreviated as (Hhyc) of Co(II), Mn(II), Ni(II) and Zn(II) of composition $M(hyc)_2$ $(NH_2–NH_2)$. $H_2SO_4.2H_2O$, M(fhyc) $(H_2O)_2SO_4$ and Zn(Hhyc) $(NH_2–NH_2)$ SO_4 $2H_2O$ have been prepared and characterized by u–v, i.r., magnetic susceptibility and derivatographic studies of complexes. From above studies polymeric structure is assigned to both $M(NH_2–NHCOO)_2N_2H_4$ H_2SO_4. $2H_2O$ and $M(CH_2{=}N–NHCOOH)_2$ $(H_2O)_2$ SO_4 type of complexes.

209. Synthesis, Spectral Characterization and Biological Aspects of Mononuclear Chromium(III) Complexes with Schiff Bases Derived from Sulpha Drugs

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Keywords : *Synthesis, spectral analyses, transition metal complexes, sulpha drugs.*

Keeping in view the chemotherapeutic value of sulpha drugs, Schiff base ligands have been synthesized and their reactions with chromium under complex formation are the subject of study in this paper. The Schiff bases used here are o-Vanillin sulphanilamide(oVSaH), o-Vanillinsulfamerazine(oVSmrzH), salicylaldehydesulfanilamide (SdSaH), salicylaldehy-desulfamerazine (SdSmrzH), 2-hydroxy-1-naphthaldehyde sulfanilamide (2hNSah), 2-hydroxy-1-naphthaldehydesulfamerazine (2hNSmrzH). Reactions of chromium(III) chloride with Schiff base ligands have been investigated and on the basis of elemental analysis, I.R., UV spectral studies, possible structures have been suggested for the resulting new compounds. The Schiff bases used in these studies are condensation products of sulpha drugs: sulphanilamide and sulphamerazine with o-vanillin, salicylaldehyde and 2-hydroxy-1-naphthaldehyde. The disappearance of phenolic proton upon complexation indicates coordination by phenolic oxygen (after deprotonation) and azomethine nitrogen respectively. The magnetic and spectral spectral studies indicate octahedral geometry for the resulting complexes.

210. Study of Copier (II) Complexes

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Keywords : *Square pyramidal, tetragonally distorted octahedral.*

1-(Phenylazo)-2 napthol (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)2 Ln where L = Secondary ligands like pyridine , picoline, H_2O and n = 0, 1 and 2. These complexes have been characterized by their element analysis, conductivity

measurement, magnetic moment at room temperature infrared spectra 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 π-bonds in chelate ring. The magnetic moment values reveal the mononuclear nature of the complexes while the their electronic spectra reveal the geometry of the complexes Cu(PAN)2 complex is found square planner while Cu)PAN)2 L and Cu(PAN)2 L2 are found square pyramidal and tetragonally distorted octahedral.

211. Synthesis, Spectroscopic, Biological Activity and DNA Cleavage Activity Studies of Benzofuran Schiff's Base with Some Transition Metals

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Keywords : *Benzofuran Schiff's base, Spectral studies, Metal complexes, Antimicrobial Studies and DNA cleavage studies.*

The new Schiff's base has been synthesized from benzofuran-2-carbohydrazide and 2-acetyl pyridine [BCAP]. The ligand act as bidentate by coordinating through carboxy oxygen and azomethine nitrogen atoms. The complexes of the type MLX_2, where M = Co (II), Ni (II), Cu (II), Zn (II), Cd (II) and Hg (II), L = [BCAP] and X = Cl_2 have prepared. Structures have been elucidated on the basis of elemental analysis, conductivity measurement, magnetic properties, spectral studies like IR, ^1H NMR, ESR and electronic spectral studies. On the basis of spectral characterization we proposed tentative structures for all these complexes. The antibacterial and

antifungal activities of the ligand and their metal complexes have been screened by MIC method. DNA cleavage studies have been carried out.

212. Synthesis, Spectral and Antifungal Studies of Some Medicinal Compounds of Cobalt(II) and Copper(II) of a Novel 18-membered Octaaza [N_8] Tetradentate Macrocyclic Ligand

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Keywords : *Macrocyclic, Octahedral, Spectroscopic, Anisotropic, Antifungal.*

The stereochemistry and coordination behavior of Co(II) and Cu(II) complexes of a novel 18- membered quadridentate macrocyclic ligand (3, 4, 12, 13- tetraphenyl-1, 2, 5, 6, 10, 11, 14, 15 – octaazacyclooctadecane - 7, 9, 16, 18 - tetraone-2, 4, 11, 13 – tetraene) have been investigated after their template synthesis. The synthesized macrocycles have been characterized by means of various physicochemical techniques viz. elemental analyses, magnetic, conductivity measurements, spectral (IR, electronic, mass and EPR) techniques. The structure of complexes has been determined with the help of spectroscopic as well as conductivity values and found to be six coordinated octahedral and tetragonal for Co(II) and Cu(II) respectively. The ligand was coordinated to the metal ion via the malonylhydrazide moiety's imine nitrogen in a tetradentate fashion. Molar conductance measurements revealed that reported macrocyclic complexes were non-ionic in nature. All the complexes have been screened for their *in vitro* antifungal activity against a no. of fungi isolated from plants. The compounds exhibit significant antifungal activity.

213. Synthesis, Structural and Biological Studies of Some Schiff Base and their 3-d Transitions Metal Complexes

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Keywords : *Transition Metal, Schiff base, O, N Donor, Thermal study, Biological activities.*

Some new Schiff base complexes of Cr(III), Co(II), Ni(II) and Cu(II)derived from 5- bromosalicylaldehyde with 2-amino-5-nitrothiazole (BSAN) and 4-dimethylamino-benzaldehyde with 2-amino-3-hydroxypyridine (MBAP) have been synthesized and characterized by element analysis, FT-IR, FAB-mass, Molar conductance, electronic spectra,1H-NMR, ESR, magnetic susceptibility and thermal analysis. The complexes exhibit coordination number 4 or 6. The complexes are coloured and stable in air. Analytical data revealed that all the complexes exhibit 1:2 (metal: ligand) ratio. IR data shows that the ligand coordinates eith the metal ions in a bidentate manner through the phenolic oxygen and azomethine nitrogen. The 1H-NMR spectral data indicates that the phenolic protons have been displaced during complexation. FAB-mass and thermal data show degradation pattern of the complexes. The thermal behaviour 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. The Schiff base and metal complexes shows a good activity against the Gram-positive bacteria; staphylococcus aureus and Gram-negative bacteria; Escherichia coli and fungi aspergillus niger and canadida albicans.

214. Synthesis and Solid-State Reaction Kinetics of Non-Isothermal Decomposition of VO(II), Fe(II) and Zn(II)-schiff Base Complexes

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Keywords : *Solid state, Reaction Kinetics, Complexes, Non-isothermal, Schiff base.*

Metal Complexes of Schiff base are studied extensively due to synthetic flexibility of these compounds and their selectively as well sensitivity towards the central metal atom. Comparatively, less reports are available on the thermal behaviour of Schiff base complexes of transition metals inspite of their diverse biological activities. In view of our interest in the study of the thermal coordination thermal behaviour f these ligands towards transition metals, we report herein synthesis, structure and non-isothermal kinetics of some Schiff base complexes.

Schiff base metal complexes derived from 2-thiophenecarboxylidine-4-anisidine

(TCA), 3.4-dihydroxy-5-nitrobenxylidine-2-amino-5-methylthiazole (DAT) and 3,4-dihydroxy-5- nitrobenxylidine-4-chloroaniline (DCA) have been synthesized and characterized by element analysis, molar conductance, electronic spectra, FT-IR and thermal analysis. The complexes are of general formulae: [Fe (TCA) 2. (H2O) 2].SO4.H2O; [Zn(DAT).(H2O)2].CI2.H2O and [VO (DCA)2.(H2O)2].SO4.2H2)O. the thermal behaviour 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 E*, Z and ÄS* have been calculated from the TG curves using coats-Redfern and P-N Methods.

215. Compuetr Analysis of Potentiometric Data of cu(II) Mixed Ligand Complexes

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Studies on computer analysis of the potentiometric data data obtained in the Cu(II)-L-aspartic acid (aspt)/iminodiacetic acid (imda)(A)-imidazole(imd), histamine(hista) and L-histidine (histi)(B) complexes showed the presence of CuAB and $CuAB_2$ types of species. In the both CuAB and $CuAB_2$ tenary species, aspt/imda primary ligands bind the metal in a terdentate manner and in the CuAB species imd, hista and histi secondary ligands are respectively uni, bi- and terdentate.The $CuAB_2$ species has been found to have higher stability than the CuAB species in the Cu(II)-aspt/imda(A)-imd(B) complexes . The two five membered chelate rings in the $CuAB_2$ species in the Cu(II)-imda(A)-imda(B)complexes are more favored than those present in the CuAB species in the complexes.

216. Density Functional Calculations of EPR Parameter Hyperfine Coupling Constants of [Cu $(CO)_3$] [Mn $(CN)_5NO]^{2-}$ $[Mn(CN)_4]^{2-}$ Transition Metal Complexes

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Keywords : *Density Functional Theory (DFT). Transition Metal Complexes, Hyperfine coupling constants.*

We have calculated the EPR spectral parameter hyperfine coupling constants of [Cu $(CO)_3$], [Mn $(CN)_5NO]^{2-}$ [Mn$(CN)_4]^{2-}$ transition metal complex using Density Functional Theory. For these calculations, BHPW91, B3LYP, B3PW91, BLYP, BPW91, BP86, BHP86 functionals have been used 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. We have also found that the performances of the different functionals for different transition metal complexes are not same. The performance of the functional BHP86 have been found better for [Cu $(CO)_3$], B3LYP for [Mn $(CN)_5NO]^{2-}$ and BHPW91 for [Mn$(CN)_4]^{2-}$ transition metal complexes . We have also observed that performance of BLYP functional is very poor for [Cu $(CO)_3$], BHPW91for [Mn $(CN)_5NO]^{2-}$ and BLYP for [Mn$(CN)_4]^{2-}$ transition metal complexes.

217. Mixed Ligands Complexes of AI (III) Metal Chelates of Some Organic Acids with Picolinic Acid & Oicolinic Acid-N-oxide

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Keywords : *Mixed ligands complexes, organic acids, picolinic acid, picolinic acid-N-oxide, infrared spectra.*

A Number of mixed ligands complexes if AI (III) metal chelates of some organic acids with picolinic acid and picolinic acid-N-oxide have been synthesized and characterized. These complexes have the general formula ML2L’, where M = AI (III), L = deprotonated o—nitrophenol(ONP), 2,4-dinitrophenol(DNP), 2,4,6,-trinitrophenol(TNP), 8-hydroxy-quinoline (8HQ) & 1-nitroso-2-naphthol(1N2N); L’ = deprotonated picolinic acid (PicA) or picolinic acid-N-oxide(PicO). Infrared spectral data suggest that HPicA or HPicO act as bidentate ligand and that the coordination has taken place through oxygen atom of the-COOH and oxygen atom of N-O moiety (in HPicO) or nitrogen atom of the pyridine ring (in HPicA). It also indicates the presence of hydrogen bonding in these complexes, which may be one of the factors stabilizing them.

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