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# ABSTRACTS OF THE ACCEPTED RESEARCH PAPERS

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### SECTION OF PHYSICAL SCIENCES

### 1. Effect of conceptual teaching of modern mathematics on +2 students of Tribals and non-Tribals (Boys & Girls) of Jharkand State

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Conceptual teaching plays an important role in building the career and bright future of students. Ranchi, Bokaro and Jamshedpur of Jharkhand state are providing a good number of students to I.I.T the prestigious Technical Institutions of India. In this research paper I have performed the experiment of conceptual teaching of modern mathematics on +2 students of Jharkhand. After calculating the t-ratio of the two means, the Null hypothesis was proved to be true.

A random sample of 400 students, 200 Tribal's (100 boys and 100 girls) and 200 non-Tribals (100 boys and 100 girls) were taken to administer the test of modern Mathematics. A test of 100 questions containing all parts of modern Mathematics was prepared. Its reliability, validity and difficulty value was calculated. The test was administered on the above random sample. The mean of the two categories thus obtained, its t-ratio, chi-square test were calculated and was found that it is very useful and beneficial to compete the I.I.T examination.

# 2. Increasing use of metals like Arsenic, Mercury and Lead is warning for health and environment

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The distribution in the environment of metals like arsenic, mercury and lead has been a focus of scientific attention because of the potential health risks. Based on the important research findings and key policy development having occurred over past few years there is sufficient evidence of significant global adverse impacts of these metals and their compounds to warrant national and international action to reduce the risk to human health and the environment. It is critical and important that awareness programme is launched to educate the populations to the risk and impact of these metal and their compounds exposure in human's especially potentially vulnerable population as pregnant women, breast feeding women, the fetus new born and young children residing in the hot spot areas of the country.

# 3. Improved antimicrobial efficacy of *Murraya Koenigii* extract with silver nanoparticles

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The objective was to assess the antibacterial efficacy of the *Murraya Koenigi* leaves aqueous extract with and without AgNP (silver nanoparticles) using Minimum inhibitory Concentration (MIC) method. The MIC of original extract, ranged from 0.150-0.300mg/ml, was reduced to 0.075-0.150 mg/ml in the extract with nanoparticles. Thus, nanoparticles synthesized in the extract improved the antibacterial activity of original extract itself. Interestingly, the range was even lower than the reported MIC of the reference drug, Ciprofloxacin. Conclusively, the highest antibacterial efficacy was obtained in the extract with nanoparticles as compared to the original extract itself, nanoparticles in general and the reference drug.

### 4. Analysis of bulk modulus of periclase (MgO) at high temperatures

Rakesh Kumar<sup>1</sup> and Amar Kumar<sup>2</sup>

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<sup>2</sup>Department of Physics, K.R (P.G) College, Mathura-281001.

Tallon's model has been modified and used for the determination of bulk modulus for MgO in the temperature range 300-1800K. The concept of the modified Grüneisen parameter has been adopted to obtains an equation of state. The results are found to present close agreement with the experimental data and those reported by earlier workers.

### 5. Distribution and Uptake of Heavy metals (Cd, Pb and Zn) in Vegetable crops Grown in Sewage Irrigated Soils

Dinesh Mani, Niraj Kumar Patel, Vishv Kumar Mourya, Shailendra Kumar and Neeraj Pal Sheila Dhar Institute of Soil Science, Department of Chemistry, University of Allahabad, Allahabad- 211002.

Consumption of vegetable crops contaminated with heavy metals is a major food chain route for human exposure. In the present study, vegetables grown in the sewage and tap water irrigation are *Amaranthus* spp., *Spinacea oleracea* L. and *Beta vulgaris*. Distribution of heavy metals (Cd, Pb and Zn) was significantly higher in 100% sewage irrigated soil at all the four depths (0-15, 15-30, 30-45 and 45-60 cm), respectively. Cadmium, Lead and Zinc accumulation was found higher at the surface horizons and it decreased sharply with increasing depth in both tap and sewage irrigated soils. Extent of heavy metal build up in sewage irrigated soils was significant in both 0-15 and 15-30 cm depth. Higher uptake of Cd, Pb and Zn, were observed in the edible parts of all crops grown in 100% sewage water irrigated soils (T<sub>9</sub>) compared to that of crops grown on 100% tap water irrigated soils (T<sub>1</sub>). Sewage water irrigation has a great potential to contaminate the soil which may lead to the uptake of heavy metals in crop plants and may cause harmful effect on animals and plants. Results indicate that long-term and indiscriminate application of sewage water, which contains heavy metals may cause accumulation of heavy metals in surface and sub-surface soils and the build-up of heavy metals on soil profile may prove harmful not only to plants, but also to consumers of the harvested crops.

# 6. A kinetic study of the solvent effect of DMSO on the solvolysis of the substituted aliphatic esters

### R.I.Singh

### Professor and Head, Department of Chemistry, V.K.S University, Ara, Bihar.

The specific rate constant values of the alkali catalysed solvolysis ester namely Iso-propyl acetate were found to decrease with gradual addition of DMSO in the water-DMSO reaction media of varying composition ranging from 20 to 80% of DMSO in the reaction media. The iso-composition activation energy ( $E_C$  or  $E_{exp}$ ) and iso-dielectric activation energy ( $E_D$ ) values of the reaction were found decreasing and increasing respectively with increasing the organic component of water-DMSO reaction media and with decrease in dielectric constant values of water-DMSO media. In the light of these findings, it has been concluded that the initial state of the reaction is desolvated and the transition state is solvated. It has also been inferred that in water-DMSO media, the mechanistic pathways of the reaction is changed from bimolecular to unimolecular. From depletion observed in  $\Delta H^*$  and  $\Delta S^*$  values with simultaneous enhancement in  $\Delta G^*$ value of the reaction, it has been inferred that the solvent dimethyl sulphoxide acts more as entropy controller than the enthalpy inhibitor.

### 7. Comparison of Security in Wireless Communication Network with a Focus on WiFi and WiMAX

Md.Alimul Haque, Shameemul Haque and N.K.Singh University Department of Physics, V.K.S.University, Ara-802301.

This paper discusses the comparison two of the latest wireless technologies, namely Wi-Fi and WiMAX technology. Security has become a primary concern in order to provide protected communication in Wireless environment. We know the basic concept of communication is sent the information from source node to destination node but in my view the communication is not sent the information but the amount of secure information which is sent from source node to destination node. The much anticipated technology for wireless broadband access, the WiFi and WiMAX are finally starting to be available in the market with the aim to provide high data rates and provide interoperability of vendor devices at the same time. These technologies are considered as the promising broadband access solutions for wireless MANs and LANs, respectively. The intent in this paper is to provide a comparison of these technologies as well as the benefits and risks involved in their implementation.

### 8. Prediction of ultrasonic velocity of some organic halides through QSAR analysis

Shraddha Srivastava, Amrita Dwivedi and A. K. Srivastava

#### Department of Chemistry, University of Allahabad, Allahabad – 211002.

A Quantitative Structure Activity Relationship (QSAR) study has been performed on twenty five organic halides to predict the ultrasonic velocity of titled compound. The possible descriptors

which we have calculated for the present series of compounds were selected for multiple linear regression (MLRA) analysis. Various regression models have been tested and the regression analysis data indicate that some of the descriptors provide valuable information to predict the ultrasonic velocity of these derivatives. The predictive ability of the model was cross validated by observation of the low residual activity values and appreciable cross-validated  $R^2$  values ( $R^2_{cv}$ ) obtained by leave one out (LOO) technique.

### 9. Journey of the Jodhpur city since its foundation through Water Impounding Structures

Shiv Singh Rathore and Suresh Chandra Mathur

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The Jodhpur city commenced its journey with a curse," Jodha! May your citadel ever suffer a scarcity of water!" by great harmit Cheeria Nathji in the year 1459 AD when foundation of Mehrangarh Fort of Jodhpur was laid down by Rao Jodha. From small town to now it is a second largest city in Rajasthan which is growing in the heart of the Thar Desert. The total area of Jodhpur is now 76 sq. km. (located between Latitudes 26°15" N to 26°20" N and Longitudes 73°E to 73°4"E) of which more than 60 percent is now urban area. The population explosion and expansion of city put pressure on civic services especially on supply of drinking water. However, it also proves that without water no city can grow especially in the arid zone. If we travel through history of the growth of the Jodhpur city we found that because of water scarcity and curse of Cheeria Nathji, old kings had consistently kind enough to have vision to built and developed water impounding structures. As a result of which since its foundation, old Jodhpur city is endowed with a large number of water impounding structures and with the time largest number in the world. These water impounding structures were considered as life line for the growth of the city. For tracing the journey of Jodhpur city water impounding structures can be taken as scientific evidences of growth rate and development steps of the Jodhpur city which were constructed and developed on the basis of their excellent geological, hydrogeological, geomorphological, geographical, civil, and architectural engineering knowledge. Despite of large number of water impounding structures in the Jodhpur city, it faced severe crisis of water till 1996 under such hardship water impounding structures played useful role in the supply of surface and ground water to steady growth of the city. However after year 1996, Jodhpur city receive plenty of water from Indira Gandhi Canal resulted in to fast rate of growth and development with its adverse effects in form of water logging problems. The paper embodies inventory, classification and common characteristics of water impounding structures of the Jodhpur city. Efforts have been also made to utilize history of construction of water impounding structures and water supply system to trace the pride journey of the Jodhpur city.

# **10.** Synthesis, *In-silico* and *in-vitro* activity of arylsulphonamides as non- nucleoside reverse transcriptase inhibitors against HIV-1

Anuradha Singh<sup>a</sup>, Madhu Yadav<sup>a</sup>, Ritika Srivastava<sup>a</sup> Rajinder Kaur<sup>b</sup>, Satish K. Gupta<sup>b</sup> and Ramendra K. Singh<sup>a</sup>,

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<sup>b</sup>National Institute of Immunology, Aruna Asaf Ali Marg, New Delhi-110067.

In silico studies, synthesis and *in vitro* activity of a series of arylsulphonamide derivatives as possible NNRTIs against HIV-1 have been discussed. Compounds designed on the basis of Lipinski's rule of five and extensive computational studies and having H-bond donor and acceptor sites were finally synthesized following green protocols and screened *in vitro* to assess their HIV-1 RT inhibitory activity using TZM-bl cells. *In silico* studies showed that these molecules formed H-bonds and exhibited  $\pi$ - $\pi$ ,  $\pi$ -+ interactions, with amino acids in the non- nucleoside inhibitor binding pocket, and formed more stable complexes (total interaction energy in the range of (-) 47.85 – (-) 77.01 kcal/mol) with HIV-1 RT in comparison to nevirapine and etravirine, (-) 45.79 and (-) 61.43 Kcal/mol, respectively, and, thus, lower EC50 values were predicted. The molecules,4-(4-chlorobenzenesulphonylamino)-N-(1H-indazole-5-yl)- benzamide showed significant inhibition of HIV-1 growth under *in vitro* conditions with EC50 value in the range of 4.89x10<sup>-5</sup> nM, however, its SI value was 2.45 only, which was much lower than nevirapine and etravirine. The reverse transcriptase analysis, based on luciferase reporter assay, of this compound proved its nature as a non-nucleoside reverse transcriptase inhibitor. The other compounds did not show significant anti-HIV activity under *in vitro* conditions.

### 11. Homogeneous Cosmological Model in General Relativity

#### R.K Tiwari and Rameshwar Singh

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We have investigated Robertson-Walker cosmological model with decaying vacuum density. We considered a special variation law in which the vacuum density  $\Lambda$  is proportional to the  $n^{th}$  power of Hubble parameter H i.e,  $\Lambda \propto H^n$  (where n is a constant). Physical, Kinematical and Statefinder parameters are evaluated and their behaviours are discussed. It can be seen that the values of Statefinders resemble  $\Lambda$ CDM model and so the model is in agreement with recent observations.

# **12.** Role of mineral acids in the acid rain phenomenon: A comparison due to weight percentage of acids

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### <sup>\*</sup>Dr. Kran Singh College, Rahlai, Agra, Uttar Pradesh.

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Lower atmosphere is filled with trace gas as air pollution.  $H_2SO_4$  is the main component. Heteromolecular homogenous nucleation of  $H_2SO_4$  has been considered for different mass functions. The critical composition of mineral acids (sulfuric, nitric, and hydrochloric) viz critical radius and Gibb's free energy of these acids have been calculated using different mass fractions as the functions of number of water molecules ( $n_A$ ) and number of acid molecules in an embryo. The critical radii have been found to decrease with increase in weight percentage of acid. Also, the calculated values of pH is positive for weight percentage <10, while it is negative of weight percentage>10.

### 13. Electrochemical Determination of Metal ions in Milk: A Fodder Resource Pollutant Assessment

Imran Khan, Umar Jan Pandit and S. N. Limaye

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Milk product is one of the important natural nutrients. A general analysis of standard milk records, each 100gm milk contains 88 % water, 5.26 % carbohydrate, 3.25 % fat, 3.2 % protein, 2 % vitamin and trace elements i.e. Ca (II) 113mg, Mg (II) 10mg, Na (I) 43mg, Fe (II)/ (III) 0.1mg, Zn(II) 0.4mg, Cu(II) 0.03mg, Pb(II) 0.03mg, Cd(II) 0.07mg, As(III) 0.07mg, Hg(II) 0.01mg and other trace elements Viz. K, S, Se and P have different concentration. The source of water for cattle's is the water resources available in the catchment area for cattle. Such water and grass / fodders used to feed buffalo and cow. Therefore, the probability of transfer of contamination is present in water and fodder to milk is increases. Hence the product necessary to health becomes hazardous and cause significant health problems.

Therefore we propose to determine the content of six metal ions in different milk samples (directly from teats) and water from cattle catchment area using polarographic and voltametric analytical methods. Analyses were performed after the chemical mineralization of the samples with nitric acid. As per our hypothesis, water is mostly contaminated by automobile, goldsmith and blacksmith workshop which are transferred to vegetation and to buffalo milk by different biological processes. This contamination is also spreading by adulterate of water in milk by milk man; either he used Catchment Area's water or any other source. Our result shows that concentration of metal ion in milk is more than 40% of sophistication of water.

# 14. <sup>57</sup>Fe Mössbauer Spectroscopic Study of organic rich sediments (source rocks) from test well CT-1 located in Chinnewala structure of Jaisalmer Basin, India

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Recently Oil and Natural Gas Corporation Ltd. (ONGCL), India drilled number of wells in Chinnewala Structure of Jaisalmer Basin. Earlier studies showed prospects of economically viable reservoirs of gaseous hydrocarbon in this structure. Presence of gas condensate in the structure for the first time in Jaisalmer basin was encountered by drilling but no indication of the presence of oil has been found. <sup>57</sup>Fe Mössbauer Spectroscopic study was carried out on the samples collected from different depth intervals of a representative well CT-1 located in Chinnewala Tibba Structure of Jaisalmer basin, (India). The results obtained are compared with the results already available in different structures of Jaisalmer Basin and other basins which are oil productive. The comparison shows that relative distribution of iron as a function of depth for the well CT-1 is significantly different from that reported from North Sea, EKG and Cambay basins, which are major oil fields. Our study shows that there exists a correlation between relative distribution of iron and oil prospects of the basin.

### 15. Finsler space subjected to a Kropina change with an *h*-vector

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In 1980, H. Izumi introduced the concept of *h*-vector. In this paper, we discuss the Finsler spaces  $(M^n, L)$  and  $(M^n, *L)$ , where \*L(x, y) is obtained from L(x, y) by Kropina change  $*L(x, y) = L^2(x,y)/bi(x,y) y^2$  and bi(x, y) is an *h*-vector in  $(M^n, L)$ . We also find the necessary and sufficient condition when the Cartan connection coefficients for both spaces  $(M^n, L)$  and  $(M^n, *L)$  are same.

### 16. Generalization of Semiperfect Ring

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Any right R-module M is called a CS-module if every submodule of M is essential in a direct summand of M. A ring is said to be CS-ring if R as right R-module is CS. In this paper we study semiperfect ring in which each simple right R-module is essential in a direct summand of R. We call such ring as a extending for simple R-module. Here we find that for such rings, every simple R-module is weakly-injective if and only R is weakly –injective if and only if R is self-injective if and only if R is weakly-semisimple. Examples are constructed for which simple R-module is essential in a direct summand.

### 17. Salt Gradient Solar Pond: An approach for Energy alternative

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Solar pond is a large body of saline water, exposed to ambient at top. Solar radiation penetrates through the saline water and heats it. Water has a property to lose the heat mainly by convection. Hence in principal, any exposed body of water will be warmed while exposed to sun and will be cooled immediately after the sunset. But in case of solar ponds, the convections are prohibited.

Hence it stores heat for very long time. Present trend of research is towards alternative sources of energy. Fossil fuel, the principal resource of energy, is getting depleted rapidly. The alternative sources of energy which is well known to everybody, but what we need is the technology to harness them in a cost effective manner. Salt gradient solar pond is an economical and viable source of energy.

# 18. Utilization of agro-waste material as potential adsorbent for waste water treatment

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Most of the effluents discharged by different industries are contaminated with metals which impose environmental and public health problems. Thus the need of improved management of these waste are important. Most contaminated waste water treatment techniques viz. coagulation, ionexchanging, advanced oxidation process etc. require high capital and operating cost and may produce large volume of wastes. Therefore, water treatment by biosorption is a promising technique for the removal of metals from aqueous environment due to lignocelluloses material. Tea industries produces large amount of tea wastes which is readily available almost everywhere. The use of absorption technology for the removal of contaminants of waste streams is favourable when biological treatments are not applicable. Utilization of agricultural waste for absorption is one of the alternative technologies for cleaning of industrial wastewaters. This part of the utilization of industrial wastes for wastewater treatment project aims to investigate the use of tea wastes as a potential absorbent, verify the chemical and thermal activation of the absorbent and investigate the absorption of Cd, Cr, Pb and Zn from synthetically prepared waste water. Toxic metal contamination of soil and water is a significant environmental and human hazard, and therefore its removal from the environment in a safe and efficient manner is of utmost importance. Hence, there is need for research and development of low cost and readily available absorbents which can remove toxic metals economically.

#### 19. A systematic study of potential development of solar power in India desert

#### Naveen Kumar, Kamlesh Kumar and Paati Purohit

#### Rajmata Krishna Kumari Girls' Public School, Jodhpur, Rajasthan.

Rajasthan, with its 300 days a year of sunshine and relatively cheap desert land, has set a goal even more ambitious than India's. In this year's state budget, the newly formed state government announced it hoped to install 25,000 megawatts of solar energy in the state within the next five years, and infrastructure to transmit that power to the national grid. Since the 1990s, the state has been home to a range of wind energy projects, with about 2,800 megawatts of wind capacity now installed, out of an estimated potential capacity of 5,000 megawatts. Altogether wind power in Rajasthan accounts for about 13 percent of India's wind energy production. But Rajasthan's Great Indian Thar Desert in district Jaisalmer, where the solar energy plants have installated that could help change the character of India's energy development.

Today the country has 2.28 million megawatts of power generating capacity, and about 12.4 percent of that comes from renewable energy. Of the 2,632 megawatts of solar power now installed in India, Rajasthan so far has only 730 megawatts, putting it in second place behind the state of Gujarat, with 916 megawatts, according to India's Ministry of New and Renewable Energy. But Rajasthan, India's largest state and 60 percent covered by sunny desert, is now attracting the world's interest as a solar hotspot.

"Around 1 lakh (100,000) square kilometers of barren land is available in the northwest arid belt of the state at cheaper rates that could be utilized for large scale solar projects. The government is formulating the policy to harness the enormous solar potential of the region to meet the country's growing energy requirements. Besides large solar installations, the government is studying the possibility of grid-connected rooftop solar photovoltaic units for households. The Solar Energy

Corporation of India estimates that 130 million homes could potentially be equipped with the units, creating 25,000 megawatts of generating capacity.

#### 20. On Bianchi type cosmological models in Lyra's geometry

#### R.K. Dubey

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Bianchi type cosmological models have been studied on the basis of Lyra's geometry. Exact solution has been obtained by considering a time dependent displacement field for constant deceleration parameter and varying cosmological term of the universe. The physical behaviour of the different models has been examined for different cases.

# 21. Development of a cost-effective technique to remove the arsenic from groundwater by oxidation-coagulation

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The potential of enhancing As(III) removal was investigated in a pilot study for the process of oxidation, coagulation and direct sand filtration at optimized pH. The process included pre-oxidation of As(III) to As(V) with potassium permanganate and co-precipitation of arsenic by adding ferric salt at optimized pH by addition of sodium bicarbonate as buffering agent and subsequent filtration of the water through a bucket sand filter. The arsenic level goes from initial 500-100 to 5-1  $\mu$ g/L when the water does not contain iron initially. The final pH of the water remains at about 7.3, which is within acceptable range for drinking. The pH of 8.3 provided by sodium bicarbonate has been brought to 7.3 by FeCl<sub>3</sub>, which is a Lewis acid and produces OH<sup>-</sup> ions by hydrolysis.

# 22. Study of Chemical State of Iron in Sediments of Test well DND-1 Located in Dandewala Structure of Jaisalmer Petroliferous Basin, Rajasthan, India

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Jaisalmer basin represents mainly the westerly dipping eastern flank of the Indus shelf and occupies an area of about  $3x10^4$  Sq. Kms. The palynological and geochemical studies have predicted good availability of hydrocarbons in this basin. The Cretaceous and Jurassic sediments are believed to contain source rocks in Jaisalmer basin. Number of studies carried out by several workers on source rock sediments collected from Jaisalmer basin has shown the presence of various iron-bearing minerals like pyrite, siderite, Fe<sup>3+</sup> in clay and Fe<sup>2+</sup> in clay minerals.

In present study, large number of sedimentary samples collected from test well namely DND-1 located in Dandewala structure has been studied using Mössbauer spectroscopy. Mössbauer logs were prepared by plotting relative distribution of iron bearing minerals with depth in a well. By careful analysis, we find that in Jaisalmer Formation (Middle Jurassic sedimentary sequence of Jaisalmer basin) there exists a similar trend of distribution of iron bearing minerals as in the Bilara Formation of Bikaner-Nagaur basin. It is seen that the Jaisalmer Formation comprises of two zones; zone A in which iron bearing minerals are present in significant amount and zone B in which iron bearing minerals are absent and simultaneous CaCO<sub>3</sub> laminated with phytoplankton is present. Our results are significant in context to the presence of biogenous component in Jaisalmer basin as it is known that marine sediments are more favourable for the formation of oil/gas in a basin.

# 23. Rao Jodha Desert Rock Park, Mehrangarh Fort, Jodhpur, India: Implications of its excellent geological, hydrogeological, lithophytic and historical heritage for possible potential site for Geopark.

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## <sup>1</sup>Department of Geology, J.N.Vyas University, Jodhpur, Rajasthan.

### <sup>2</sup>Rao Jodha Desert Rock Park, Mehrangarh, Jodhpur, Rajasthan.

The foundation of the world-famous Mehrangarh Fort of Jodhpur was laid on 12th May, 1459 by Rao Jodhaji on a hundred and twenty meters high rocky hill, six miles south of Mandore (the old capital of Jodhpur) known as Bhakurcheeria, the mountain of birds, or Cheeriatunk, the bird's beak. Geologically, this ridge is composed of rhyolitic rocks of the Malani Igneous Suite of 680-745 My at its base and sandstone of Jodhpur Group of Ediacara age of the Marwar Supergroup at top, which also marks the Unconformity. At the foothill of the Fort, on the way to Chandpole at Singorio Ki Bari, a Desert Rock Park is developing which is endowed with excellent geological, hydrogeological, historical and lithophytic site, named as Rao Jodha Desert Rock Park.

The Park was created by Mehrangarh Museum Trust in 2006 as a project to restore the natural ecology of a large rocky wasteland next to the Fort, 70 hectares in extent. The Park officially opened to the public in February, 2011. Today, Rao Jodha Park has become a well-known tourist place in Jodhpur. The aim of developing the park is also to give unique historical, geological, floral and hydrogeological knowledge of this place to students and tourists from India and abroad.

As you enter the gates of the Visitors Centre of Rao Jodha Park, the pathway is laid with blocks of Jodhpur sandstone (*chittar ka patthar*) displaying a variety of ripple marks, being sedimentary structures of the marine paleoenvironment displaying specific hydrodynamic conditions of deposition of this sandstone of the Ediacara period. Behind the main structure of the Visitors Centre – the Singorio Pol – many species of lithotypes (some of which are on the verge of extinction) brought from different parts of the Thar Desert are displayed with the aim of conserving them.

Only a short distance away from this exhibit lays a passageway or aqueduct leading to two ancient water-impounding structures built at the foot of Mehrangarh Fort, known as Ranisar and Padamsar. This passage is known as 'Hathi Nahar'. It was actually built by digging the sandstone (near Soorsagar) and rhyolite rocks (within the Park) so that the water could flow into the two lakes by gravity. During its course, Hathi Nahar exposed many peculiar geological features showing the nature

of volcanic activity in that precinct. It is actually an ancient canal which brought water from the catchment area from around Soorsagar, a place famous for Jodhpur sandstone quarries, to Ranisar. For a long time due to development activities and quarrying in the catchment area there was no water flow in Hathi Nahar which was filled by fallen boulders, pebbles and garbage, overgrown with thick vegetation. To redevelop a passageway down to Ranisar, the canal was cleaned and restored. Now it forms an excellent walking trail or gully to reach to the Ranisar water-impounding structure (one of the oldest hydro-geotourism sites in Jodhpur. This walking trail has excellent geological features in welded tuff and rhyolite rocks which represent a variety of volcanic activities and events around Jodhpur at about 680 My ago.

The Rao Jodha Desert Rock Park is developing into an excellent educational centre and tourist attraction with unprecedented opportunities to learn about and enjoy the geological features of both rhyolite and sandstone along with hydrogeological features of Ranisar-Padamsar. The Park also showcases most of the floral lithophytes of the Thar Desert, growing in simulated natural conditions inside the Park. The present paper embodies all the historical, cultural and scientific aspects which will help to recognize it as world heritage site and a good Geopark site for society and for both Indian and international tourists.

### 24. Geoscientific Investigations to Search of Economic Mineralization in Phulad Ophiolite Suite, near village Phulad, District Pali, Northwestern India.

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The greatly needed as essential component for the modern technology, the Rare Earth Elements are being produced by china almost 97% of the global production. All of a sudden China has stopped all export of REE to India on strategic grounds, putting India handicap in many respect. Hence REE and Atomic minerals are now at the top of the priority list for the minerals to explore on India.

Ophiolite consists of herzolite or harzburgite commonly altered to serpentinite, gabbro, 'sheeted' basic dykes, sometimes with trondhjemite dykes or inter-dyke screens, pillow-bearing basic volcanic rocks, chert, pelagic limestone and argillite. Ophiolite thus describes sections of oceanic crust and upper mantle, along with sedimentary rocks deposited on the sea floor, emplaced as thrust slices onto continental lithosphere. The composition of these out-of-place fragments of ocean lithosphere, constrain their petrogenesis to back-arc or supra-subduction zone settings both of which are narrow in oceanic terms (6500 km wide) and are dynamically fragile, i.e. they are prone to perturbation by changes in plate boundary conditions .

Mineral deposits in ophiolite sequences are a common feature. A number of platinum-group element (PGE) oxides and hydroxides have been discovered in a PGE mineralization in the ophiolite complex. Some example of ophiolitic PGE deposits are: Primary platinum mineralization in Urals, Russia, PGE mineralization in Bushveld Complex South Africa, PGE mineralization in Manitoba, Canada. Chromite is an important accessory phase in ultramafic-mafic rocks and constitutes a part of orthomagmatic deposits where crystal-liquid equilibria processes dominate their formation Massive sulphides bodies are situated within the pillow lava section of many ophiolites.

A thick complex of mafic and ultramafic rocks closely associated with the Barotiya-Sendra sediments occur all through the length of SDFB and have been collectively referred to as **Phulad Ophiolite Suite**. The rocks of the Phulad Ophiolite Suite (POS) are exposed discontinuously in a ~300 km-long and 20 to 50 km-wide linear belt running from Ajmer in the north to Palanpur in the south.

Objective of the proposed study is to establish geological characteristic of Phulad ophiolite suite of rocks including geological setup, petrology, petrochemistry and Petrogenesis and to suggest the possibility of hosting economic mineralization in Phulad area of the Phulad ophiolite belt. Methodology proposed to be adoped will include Reconnaissance, topographical and small scale geological mapping, detailed Petrological studies using thin sections, detailed Geochemical studies including XRF and ICPMS studies of major, minor, trace and Rare earth elements, establishing a tectanopetrogenetic model and evaluation of economic potential. The proposed study will investigate possibility of economic mineral deposits in phulad ophiolite specially REE deposits in phulad ophiolite complex Which have a great scope for the search and need of the hour in National interest. Also PGE, Cu-Ni-Fe, Chromites and Base metal sulphides deposits are now very important deposits in the context of the India as a nation and needed to be explored in Phulad Ophiolite.

# 25. Higher-order sub-poissonian photon statistics in superposition of even and odd coherent states of light

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States of light, whose properties cannot be explained on the basis of classical theory, are called non-classical states. The non-classical nature of a quantum state can be manifested in different ways like squeezing, ordinary sub-poissonian photon statistics, higher order sub-poissonian photon statistics and various kinds of squeezing. Earlier study of non-classical states was largely in academic interest, but now their applications in quantum information theory have been well realized.

A coherent state  $|\alpha\rangle$  ( $\alpha$  is a complex number) defined as the eigenstate of the annihilation operator is the most classical state of light, but superposition of two or more coherent states may exhibit various non-classical effects. It has been realized that the even coherent state defined by  $|\alpha, +\rangle = K'[|\alpha\rangle + |-\alpha\rangle]$ , exhibit ordinary squeezing as well as Hong-Mandel's higher-order squeezing but not the ordinary sub--poissonian statistics while the odd coherent state defined by  $|\alpha, -\rangle = K''[|\alpha\rangle - |-\alpha\rangle]$  exhibits ordinary sub--poissonian statistics but not squeezing. In the present paper we study higher-order sub--poissonian photon statistics in the superimposed states,  $|\psi\rangle = \cos \chi |\alpha, +\rangle + \sin \chi$  $e^{i\phi} |\alpha, -\rangle of$  even and odd coherent states. We conclude that large percentage of higher order sub-poissonian photon statistics in the superimposed states  $|\psi\rangle$  can be obtained for low intensity of light. The variation of higher-order sub--poissonian photon statistics for different orders near absolute maxima with parameters  $|\alpha|, \chi$  and  $\phi$  have also been discussed.

### 26. Estimates of certain integral inequalities on time scales in two variables

#### Deepak B. Pachpatte

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The main objective of the paper is to establish explicit estimates on some integral inequalities in two variables which can be used in the study of certain qualitative properties of dynamical equations on time scales.

#### 27. Mathematical modelling for circular motion of satellites

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In this research paper I have calculated the time period of the motion of satellites. As we know that the satellites move under the attraction of the Earth in the same way as the planets move under the attraction of the Sun. The orbit of each planet is an ellipse with the sun at one focus. However the ellipticities of the orbit are very small, so that as a first approximation, we can take these orbits as circles with Sun at the centre. Also we know that the planets move under gravitational attraction of the Sun and that for motion in a circle with uniform speed  $\theta$ , a central attraction  $\theta^2/r$  is required with the help of these expressions the periodic time T of the satellite is calculated.

# 28. Environmental and health perspectives of hazardous and persistent organic pollutants

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#### <sup>2</sup>VKS University, Ara, Bihar.

As a consequence of rapid development a significant amount of organic chemicals have been dispersed into the environment, but the long term biological effects of most are unknown. On group of such chemicals are referred to as persistent organic pollutants (POPs) has been shown to exhibit potentially harmful effects in man and the environment. POPs are defined as organic substances, which posses toxic bio-accumulative characteristics, are persistent and prove to long range trans boundary atmospheric transport and depositions. In addition to being persistent, POPs are typically lipophillic, semivolatile and toxic. Some POPs are deliberately produced by the industry for a wide variety of applications while others are accidentally formed or released while others are accidently formed or released as by-product from various activities, such as chemical or industrial combustion processes. These are emitted into the environment as complex mixtures such as poly chlorinated biphenyls and PBDES. These are most hazardous and persistent chemicals. In order to highlight the effects of such hazardous and persistent POPs on environment and on the system of organs of man the studied and researches yet been done is not sufficient. The use of persistent organic pollutants should be controlled and minimized on need based.

# 29. A kinetic study of catalysed Solvolysis of nicotinate ester in water-DMF solvent systems

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Solvent effect of DMF after its gradual addition was studied on the thermodynamic parameters of the alkali catalysed solvolysis of Methly Nicotinate in water-DMF reaction media of varying composition ranging from 30% to 80% of DMF at five different temperatures ranging from 20°C to 40°C. With the addition of DMF to reaction media, enthalpy of activation ( $\Delta$ H\*) entropy of activation ( $\Delta$ S\*) and free energy of activation ( $\Delta$ G\*) all were found enhancing. On the basis of observation, it has been inferred that the entropy of activation enhances to lesser extent than enthalpy of activation and initial state of the reaction is solvated more than the transition state. The iso-composition activation energy values of the reaction of DMF in the reaction media. From this enhancement, it has been confirmed that the initial state of the reaction is solvated more than terms to reaction media.

# **30.** Synthesis and biological evaluation of novel triazole derivatives as antifungal agent

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Several substituted arylated N-(2-(2-benzylidine hydrazinyl)-4H-1,2,4-triazol-4-amine and 1-(2-(4H-1,2,4-triazol-4-yl)amino)-3-chloro-4-phenyl azetidin-2-one have been synthesized by the appropriate methods. Triazole on reaction with bromochloro propane gives N-(2-chloro ethyl)-4H-1,2,4-triazol-4-amine 1. The compound 1 on treatment with hydrazine hydrate yielded N-(2hydrazinyl ethyl)-4H-1,2,4-triazole-4-amine, **3** (a-j). These hydrazinyl derivatives on condensation with different aldehydes afforded N-(2-(2-benzylidenehydrazinyl)-4H-1,2,4-triazol-4-amine ,**3** (a-j) . These arylidines on reaction with chloroacetyl chloride in the presence of triethylamine yielded 2azetidinones, 4(a-j). All the synthesized compounds were evaluated for their antifungal activity against *Aspergillus niger*, *Aspergillus flavus*, *Fasuriam oxisporium* and *Trichoderma viride*. In the primary screening some of the products display acceptable biological activity. The structures of the synthesized compounds have been established on the basis of their spectral and microanalytical data.

# 31. Ligand-based QSAR Studies on the aromatic sulfonamides Inhibitors of the human trans membrane carbonic anhydrase isozymes XIV by CoMFA

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The ubiquitous metalloenzymes carbonic anhydrase (CAs, EC4.2.1.1) catalyze the interconversion between carbon dioxide and the bicarbonate ion at the physiological pH. The carbonic anhydrase XIV of extracellular isozyme is highly abundant in neurons and axons in the murine and human brain, where it seems to play an important role in modulating excitatory synaptic transmission. Ligand-based quantitative structure-activity relationship (QSAR) studies were performed on aromatic sulfonamides derivatives as a potential inhibitor of the human trans membrane carbonic anhydrase isozyme hCA XIV by comparative molecular field analysis (CoMFA) implemented in the SYBYL packages. The predictive ability of the model was assessed using a test set of five compounds. The best model has demonstrated a good fit having predictive r2 value of 0.796 and cross validated coefficient q2 value as 0.59 in tripos CoMFA region. Our results indicate that the steric and electrostatic factors play a significant role in CA XIV inhibition for the investigated compounds.

### 32. New perovskite-related oxides having high dielectric constant: 0.75Ba(Fe<sub>0.5</sub>Nb<sub>0.5</sub>)O<sub>3</sub> 0.25BaTiO<sub>3</sub>

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With the growing interest in the suitability of materials for device applications, a large number of ceramics have been developed in a wide variety of compositions and stable structure. Complex perovskite-related oxides have been of great importance since a number of materials exhibiting a wide range of unusual properties can be synthesized based on the perovskite structure. Complex perovskite oxides are widely used in various solid-state devices e.g., optical devices, multilayer capacitors, transducers, actuators, sensors etc. The conventional high temperature solid-state reaction root has been used to prepare polycrystalline samples of the compounds. Preliminary structural study using X-ray diffraction technique at room temperature suggests that  $0.75Ba(Fe_{0.5}Nb_{0.5})O_3$ - $0.25BaTiO_3$ , [BT-BFN] exhibit monoclinic phase. Scanning electron micrographs (SEM) show uniform grain distribution throughout the surface of the samples. Detailed studies of dielectric and electrical properties of the materials in a wide range of frequency (100Hz-1MHz) and temperatures (30-480°C) showed that these properties are strongly temperature and frequency dependent. Dielectric anomalies were observed for the solid solution of BFN with BaTiO<sub>3</sub> ceramics in the temperature dependence of dielectric constant ( $\varepsilon$ ) at 1.04, 10.80 and 51.50 kHz respectively, which may be attributed to ferroelectric to paraelectric transition.

#### 33. Hydrogen sulfide scrubbing by hollandites and metal intercalated hollandites

#### Manikandan Prabu and Kuppukkannu Ramalingam

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Hollandite was prepared and characterized by PXRD, IR, BET, SEM, EDX, HRTEM, XPS and TG-DTA techniques. XPS scans showed the presence of Mn  $2p_{1/2}$  signal at 654.2 eV and Mn  $2p_{3/2}$  at 642.6eV which can be attributed to the presence of Mn  $^{4+}$  and Mn<sup>3+</sup>. HRTEM of the hollandite showed the particles to be nanorods (< 20 nm). ICP-OES analysis showed the intercalation in the range of 1.09 to 2.99%. Order of increasing concentration of divalent metal ions is: Co < Zn < Ni < Cu < Cd < Pb. The observed order is an indication of the exchanging ability of the divalent ion with Ba<sup>2+</sup> ion of the hollandite in aqueous medium. Maximum scrubbing of H<sub>2</sub>S (27%) was observed for copper intercalated hollandite and a minimum (22%) for zinc intercalated hollandite. Overall H<sub>2</sub>S scrubbing ability followed the order: birnessite (18%) < hollandite (20%) < metal ion intercalated hollandite (27%) and the scrubbing efficiency is remarkable for a dry scrubber under laboratory conditions. BET measurements on select hollandites showed ~80% pore size. Hydrogen sulphide scrubbed hollandite showed relatively poor recyclability compared to intercalated material. Intercalated metal ion increases structural integrity, stabilizes the active metal against reduction and increases the scrubbing ability. The scrubber is recyclable by a simple heating process. The scrubber is benign to nature.

# 34. Interaction studies in $H_2O$ + $CH_3OH$ system at varying temperatures and pressures using ultrasonic velocity and density data

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The interaction study in  $H_2O + CH_3OH$  mixture has been carried out at elevated pressures and varying temperatures using ultrasonic velocity and density data. For this purpose Nomoto and Van Dael-Vangeel relations have been employed. In order to understand the thermodynamic properties of  $H_2O + CH_3OH$  mixture which provide accurate data for designs of solar thermal systems, the accurate measurements of excess volume (V<sup>E</sup>) isothermal compressibility ( $\beta_T$ ) and thermal expansivity ( $\alpha$ ) have been carried out by Safavou at 298.15 to 523.15K and upto pressure of 60MPa. Using some thermodynamic consideration their data were employed to compute ultrasonic velocity (u) and to study the interaction in  $H_2O + CH_3OH$  system under the varying physical conditions.

# 35. Polymorphic Transformations of CACO3 Scale: Synergistic Effect EDTA and NTA at various temperatures

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The influence of Nitrilotriacetic acid (NTA) and Ethylenediaminetetraacetic acid (EDTA) on the crystallization and morphology of CaCO<sub>3</sub> scale were studied at different temperatures from 60-230 °C. Scale samples were prepared from CaCl<sub>2</sub> solution using Na<sub>2</sub>CO<sub>3</sub> in a programmable autoclave and were characterized by XRD, Raman, FTIR and SEM techniques. The studies revealed that in the presence of a blended system of EDTA and NTA, aragonite is more stable and predominant polymorph. Occurrence of aragonite was observed in most of the samples at 60 - 230 °C. It was also observed that formation of aragonite and calcite ceased at 200°C resulting into samples with better vaterite composition. At 200 and 230 °C 65% of vaterite was formed which clearly indicate that NTA is more influential at this temperature.

#### 36. Physico-Chemical Quality Analysis of Ground Water

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The comparison of Physico-Chemical quality study of slum areas, developed areas and industrial areas in the underground water in patancheru mandal of Madak distrect Telangana state has been taken to evaluate of its suitability for domestic purpose. Altogether 15 water samples were collected from these areas. The quality analysis has been made through the estimation of PH, TDS, Calcium, Magnesium, Chloride, Nitrates, Phosphates, Conductivity, Total hardness, Turbidity. The study indicates the groundwater in the studied area is heavily loaded with inorganic ions and may pose serious health hazards if used longer periods. The studies are carried out between different analyzed quality parameters of the study area.

### **37.** Kinetic Studies of Os(VIII) Promoted Oxidation of Maleic Acid By Chloramine-T in Alkaline Medium

### Chandra Kumar Sinha

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Kinetics of oxidation of maleic acid (MA) by Chloramine-T (RNNaCl) in the presence of alkaline solution of osmium tetroxide as homogeneous catalyst have been studied in the temperature range 30 to  $45^{\circ}$ C. The results indicate first-order kinetics with respect to both chloramine-T and Os(VIII). First order kinetics in low concentration range of MA tends to zero-order at higher [MA]. Positive effect of variation of  $OH^-$  was observed on the rate of the reaction. Variation of ionic strength of the medium showed positive effect while negative effect of addition of p-toluene-sulphonamide (PTS), a reduct product of chloramine-T was observed on the rate of reaction. A suitable reaction mechanism was suggested and a rate law consistent with kinetic results was elucidated.

# 38. Modeling of Inhibitory Activity of Benzopyran Derivatives as COX-2 Inhibitors by QSAR Analysis

### Amrita Dwivedi and A. K. Srivastava QSAR Laboratory, Department of Chemistry, University of Allahabad, Allahabad–211002.

QSAR models were proposed for modeling of inhibitory activity of benzopyran derivatives as COX-2 inhibitors. Quantum chemical parameters based on Density Functional Theory (DFT-based), topological and physicochemical parameters were used for the present analysis. The QSAR models

show that DFT based descriptor affect the activity most and presence of H and  $-C(CH_3)_3$  at R<sub>1</sub> and R<sub>2</sub> position respectively enhances the activity. The predictive ability of QSAR models were cross validated by evaluating of the residual activity, appreciable cross validated R<sup>2</sup> values (R<sup>2</sup><sub>cv</sub>) by leave one out (LOO) technique. Based on the most dependable model obtained in present QSAR analysis, pIC<sub>50</sub> value is calculated for new nine COX-2 inhibitors designed in this work.

### **39.** The Structural Properties of tetragonal perovskites

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In this paper, a simple model of structural property prediction based on ionic charge theory of solid is proposed. The structural property of tetragonal perovskites (lattice constant) exhibits a linear relationship against the average ionic radii  $r_{av}$  (A°), along with the ionic charge product of the perovskites solids. This enables us to achieve improved prediction performance of the lattice constant of structurally known perovskites. We have applied the proposed relation to tetragonal perovskites and found a better agreement with the experimental data as compared to the values evaluated by earlier researchers.

# 40. Bulk modulus and cohesive energy of CsCl, alkali halides and alkaline earth chalcogenides semiconductors

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In this paper we proposed the Plasmon oscillations theory of solids formalism to CsCl, alkali halides and alkaline earth chalcogenides, group IV and II-VI semiconductor compounds with conduction d electrons the calculation of bulk modulus and cohesive energy. The present method is not limited to binary or ternary compounds but can also be use for all the semi-conducting and insulating compounds. The calculated values are in excellent agreement with the observed and calculated values of different researchers.

# 41. Integrated micro-biochemical approach for phyto-bioremediation of cadmium and lead contaminated soils using *Gladiolus grandiflorus* L cut flower

Dinesh Mani, Chitranjan Kumar and Niraj Kumar Patel Sheila Dhar Institute of Soil Science, Department of Chemistry, University of Allahabad, Allahabad-211002.

The integrated potential of vermicompost, elemental sulphur, *Thiobacillus* sp. (sulphur oxidizing bacteria) and *Pseudomonas putida* by growing gladiolus (*Gladiolus grandiflorus*) for phytobioremediation of cadmium and lead contaminated soils was investigated under pot experiment. The integrated treatment (6 g kg<sup>-1</sup> vermicompost, 0.5 g kg<sup>-1</sup> elemental sulphur and co-inoculation with

*Thiobacillus* sp. and *Pseudomonas putida*) promoted the dry biomass of the plant. The treatment was feasible for the enhanced accumulation of Cd up to 5.82 and 4.36 mg kg<sup>-1</sup> and accumulation of Pb up to 18.24 and 15.46 mg kg<sup>-1</sup> in corm and shoot, respectively. The treatment caused maximum remediation efficiency and bioaccumulation factor for Cd and Pb, showing feasible uptake (in mg kg<sup>-1</sup> dry biomass) of Cd and Pb at the contaminated site. Therefore, integrated use of vermicompost, elemental sulphur and microbial co-inoculation might be suggested for the enhanced clean-up of Cd and Pb-contaminated soils.

# 42. Effect of Organic matter and Phosphorus on the Uptake of Lead in Amaranthus (*Amaranthus spp.*)

Dinesh Mani, Neeraj Pal, Vishv Kumar Mourya, Niraj Kumar Patel and Indra Sen Tiwari Sheila Dhar Institute of Soil Science, Department of Chemistry, University of Allahabad, Allahabad-211002.

A pot experiment was carried out to assess the effect of Organic matter and Phosphorus on the uptake of Pb by *Amaranthus spp*. Vermicompost was applied @ 0, 2, 2.5 and 3 t ha<sup>-1</sup>, Single Super Phosphate (SSP) was applied @ of 0, 100, 150 and 200 kg ha<sup>-1</sup>, lead (PbCO<sub>3</sub>) was applied @ of 0, 5, 10 and 15 mg kg<sup>-1</sup> and replicated three times in a completely randomized design. Addition of 200 kg ha<sup>-1</sup> SSP increased the maximum dry biomass yield of *Amaranthus* by 34.5% over the control. The application of 15 mg kg<sup>-1</sup> Pb reduced maximum dry biomass yield of *Amaranthus* by 23.7% over the control and registered the highest accumulation of Pb in shoot and root of *Amaranthus* by 2.6, 3 fold over the control, respectively. Therefore, 200 kg ha<sup>-1</sup> SSP application may be recommended to enhance biomass yield of *Amaranthus spp*. and to reduce accumulation of lead contaminated soil by Plant.

# 43. Evaluation of heavy metals distribution and its role in physical properties of soil in sewage irrigated sites of Allahabad, India

Vishv Kumar Mourya, Neeraj Pal and Shailendra Kumar

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In present investigation, the depth-wise distribution of four heavy metals viz. Cd, Cr, Pb and Zn was observed, continuous use of sewage irrigation on agricultural land increased the DTPA-extractable Cd, Cr, Pb and Zn from  $0.081\pm0.01-0.270\pm0.01$  mg kg<sup>-1</sup>,  $0.084\pm0.005-0.46\pm0.02$  mg kg<sup>-1</sup>,  $0.082\pm0.002-0.80\pm0.033$  mg kg<sup>-1</sup> and  $8.40\pm0.16-16.40\pm0.432$  mg kg<sup>-1</sup> in surface soil (0-15cm), respectively. A very low amount of heavy metals (Cd, Cr, Pb and Zn) was observed in (45-60 cm) depth in comparison to surface soil (0-15 cm) in all the soil examined. Similarly accumulation of total heavy metals (Cd, Cr, Pb and Zn) from  $1.30\pm0.10-4.60\pm0.20$  mg kg<sup>-1</sup> in surface soil (0-15cm) respectively. A low amount of total heavy metals (Cd, Cr, Pb and Zn) mg kg<sup>-1</sup> and  $57.93\pm1.72-95.30\pm5.03$  mg kg<sup>-1</sup> in surface soil (0-15cm) respectively. A low amount of total heavy metals (Cd, Cr, Pb and Zn) was observed in 45-60 cm depth in comparison to surface soil (0-15 cm) in all the soil examined indicating low mobility of these metals down the depth. The soil organic carbon content in soils were positively and significantly correlated with DTPA-extractable Cd (r=0.81<sup>\*\*</sup>), Cr (r=75<sup>\*</sup>), Pb (r=0.61<sup>\*</sup>) and Zn (r=0.96<sup>\*\*</sup>), while clay contents showed negative impact on the extractability of these metals. Similar correlations of

total heavy metals with physical properties were observed positively, while pH and clay content showed negative impact.

# 44. Comparative study of polymer electrolytes using different dyes for the application of DSSC

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Different dyes in the PEO based polymer electrolyte composite film was prepared by sol gel technique. The properties of the film were studied by morphological measurement like optical microscope and infrared spectroscopy technique. The electrical properties measured by impedance spectroscopy show the effect of dyes on pristine electrolyte prepared by sol cast method.

# 45. Effect of synthesis process on ionic conduction and mobility of flyash based polymer composite electrolyte

Kamlesh Pandey, Mrigank Mauli Dwivedi, Atishay Dixit<sup>1</sup> and Nidhi Asthana

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### <sup>1</sup>Department of Electronics and Communication, University of Allahabad, Allahabad-211002

A new composite system, using a very low-cost material (flyash) was synthesized by two different techniques. This system was characterized by various experimental techniques. Changes in surface morphology have been observed in optical microscopy and Scanning Electron Microscopic (SEM) images. Variation of dielectric constant, dielectric loss, tangent loss and modulus spectra with frequency and temperature were studied with the aid of impedance spectroscopy.

# 46. Study of ionic conduction in ionic liquid based polymeric electrolyte with layered filler

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# National Centre of Experimental Mineralogy and Petrology, University of Allahabad, Allahabad-211002.

Ionic liquids (IL) are salts with low melting point close to room temperature. It has interesting solvent properties. IL is able to dissolve some polar as well as very small polar molecules. Polyvinyl formal-IL nanocomposite electrolyte with layered filler was synthesized by solution cast technique. Changes in surface morphology have been observed in optical microscopy and Scanning Electron Microscopic (SEM) images. Variation of dielectric constant, dielectric loss, tangent loss and modulus spectra with frequency and temperature were studied with the aid of impedance spectroscopy.

### 47. A Kinetic Study of the Solvent Effect of Aquo Acetone media on the Solvolysis of Formates

### R.T.Singh

# Professor of Chemistry and the former dean of the faculty of science, V.K.S University, Ara, Bihar

Studies on the kinetics of acid catalysed solvolysis of Butyl formate was carried out in aquo-Acetone media of varying composition ranging from 30 to 80% of Acetone at different temperatures (from 20°C to 40°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. Enhancement in the numerical values of free energy of activation ( $\Delta G^*$ ) with simultaneous decrease in the values of enthalpy of activation ( $\Delta H^*$ ) and entropy of activation ( $\Delta S^*$ ) of the reaction, reveals that Acetone acts as entropy controller solvent. The iso-kinetic temperature of the reaction was evaluated to be 280.8≈281.0 which reveals that there is weak but appreciable solvent-solute interaction in aquo-Acetone media. Effects of the ionic strength and [H<sup>+</sup>] ion have also been studied and it is inferred that the acid catalysed hydrolysis is the ion-dipole type of reaction and it follows A  $_{AC}^{2}$  mechanistic path in water-Acetone media.

### 48. Simulation of Dynamic pricing policy with price sensitive demand

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In diminishing market, demand of a product decreases and due to this, product may disappear from the market. One can reduce the selling price and generate the excess demand to earn more and to establish the product in the market. In competitive environment, the strategy is also applicable in entering the competition with others. The objectives of present paper are to develop a dynamic pricing policy to solve such types of problems in a diminishing market. The problem is solved by coming to terms with 'Kuhn Tucker imperatives and modalities', in this regard. A simulation study is appended to measure the effect of various parameters on optimal policy. The analysis reveals that for every business setup, there will be an optimal number of price settings for dynamic pricing policy that outperforms the static pricing policy.

### 49. Influence of Cr Doping on dielectric properties of CoFe<sub>2</sub>O<sub>4</sub>

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<sup>2</sup>Materials Science Laboratory, Department of Physics, J.N.Vyas University, Jodhpur-342001. Polycrystalline samples of pure and Cr-doped cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub> and CoCrFeO<sub>4</sub>) were prepared by solid state reaction route method. X-ray diffraction pattern infers that both the samples are in single phase with *Fd3m* space group. Slight reduction in the lattice parameter of CoCrFeO<sub>4</sub> has been observed as compared to CoFe<sub>2</sub>O<sub>4</sub>. The dielectric dispersion has been explained on the basis of Fe<sup>2+</sup>  $\leftrightarrow$  Fe<sup>3+</sup> hopping mechanism. The polarizations at lower frequencies are mainly attributed to electronic exchange between Fe<sup>2+</sup> $\leftrightarrow$ Fe<sup>3+</sup> ions on the octahedral site in the ferrite lattice. In the present system a part from n-type charge carrier (Fe<sup>3+</sup>/Fe<sup>2+</sup>), the presence of (Co<sup>3+</sup>/Co<sup>2+</sup>) ions give rise to ptype charge carrier. Therefore in addition to n-type charge carrier, the local displacement of p-type charge carrier in direction of external electric field also contributes to net polarization. However, the dielectric constant and loss tangent of CoCrFeO<sub>4</sub> have less amount of ferrous ion available for polarization as compared to that of CoFe<sub>2</sub>O<sub>4</sub>. The impedance spectra reveal a grain interior contribution to the conduction process.

# 50. QSAR analysis of Pyridinone derivatives as Non-nucleoside Reverse Transcriptase Inhibitors

#### Neetu Sharma and A. K. Srivastava

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Quantitative structure–activity relationship (QSAR) studies have been performed on a series of novel pyridinone derivatives that are non-nucleoside reverse transcriptase inhibitors. Various descriptors were calculated empirically and by density functional theory (DFT). Density functional theory-based descriptors were calculated at GGA-PW91 level. Several QSAR equations were formulated through regression analysis and tested with external and internal validation tests and the best equations were selected. The QSAR results revealed that the reverse transcriptase inhibitors activity could be modeled using different DFT- based descriptors such as softness (S), hardness ( $\eta$ ), chemical potential ( $\mu$ ) and lowest unoccupied molecular orbital energy (LUMO), Hydrophobic Parameter such as Partition Coefficient (LogP) and also empirical descriptors such as molecular weight (MW), surface tension (ST), index of refraction (IOR) and equalized electro-negativity (Xeq). Model equations were cross validated by leave one out (LOO) technique.

# 51. Synthesis and characterization of Fe<sub>3</sub>O<sub>4</sub>-activated carbon nanocomposite for removal of Ni<sup>+2</sup> metal ion from aqueous solution: Kinetics and Thermodynamics studies

#### Puja Rai and M.C. Chattoapadhayaya

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In the present study,  $Fe_3O_4$ -activated carbon nanocomposites were synthesized using chemical co-precipitation method for removal of Ni<sup>+2</sup> metal ions from aqueous solution has been investigated. Adsorption experiments were carried out in batch mode by varying parameter such as initial concentration, contact time, pH, adsorbent dosage,  $pH_{zpc}$  and temperature. The structure and surface morphology of  $Fe_3O_4$ -activated carbon nanocomposite was characterized by Scanning Electron Microscope (SEM), X-ray Diffracteometer (XRD), and Fourier Transform Infrared Spectroscopy (FTIR). The optimum initial concentration and contact time was determined to be 10mg/L and 100

min respectively for removal of Ni<sup>+2</sup> metal ion. Maximum adsorption was found to be at 4 pH. Adsorption isotherms were studied by Langmuir, Freundlich and Dubinin radushkevich isotherms. Langmuir isotherms were better fit for adsorption. Maximum adsorption capacity of nanocomposite for removal of Ni<sup>+2</sup> metal ion was determined to be 30 mg/g. Adsorption kinetics were analyzed using pseudo-first order and pseudo second order model. Adsorption kinetics follows the pseudo-second order model. Removal percentage of Ni<sup>+2</sup> metal ion on nanocomposite increases with increasing temperature, so the adsorption process was found to be endothermic and spontaneous in nature.

### 52. Pressure Derivatives of the Second Order Elastic Constants of La 1.85 Sr 0.15 CuO<sub>4</sub>

#### Seema Gupta

#### Department of Physics, Agra College, Agra-282002

The pressure derivatives of the second-order elastic constants of La  $_{1.8}$ Sr  $_{0.2}$ CuO  $_4$  are calculated from the knowledge of its second- and third-order elastic constants. The effect of pressure on the elastic constants of high temperature superconductor La  $_{1.85}$ Sr  $_{0.155}$ CuO  $_4$  (LSCO) has been studied theoretically using finite strain elasticity theory. The strain energy density  $\phi$  is estimated by taking into account the interactions of nine nearest neighbours of each atom in the unit cell of La $_{1.85}$ Sr  $_{0.15}$ CuO  $_4$ . The expressions for the effective second-order elastic constants of LSCO system have been derived in its strained state in terms of the natural state second- and third-order elastic constants. These expressions are employed to obtain the pressure derivatives of the effective second-order elastic constants. The results that the larger pressure derivative (d C<sub>33</sub>/d p) along c-axis direction than that along ab-plane, i.e. (d C<sub>11</sub>/d p), corroborates the observation that the layers close-up substantially under hydrostatic pressure while change in interatomic distance in a layer is smaller in La  $_{1.85}$ Sr  $_{0.15}$ CuO4.

### 53. Electro-polymerization reaction and their applications towards technology

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Controlled potential electro-polymerization of some aromatic compounds as Aniline, substituted aniline and phenol were carried out at the platinum electrode. Acetonitrile was used as organic solvent in the presence of lithium perchlorate as supporting electrolyte. The synthesized polymer shows excellent conductivity and electroattractive properties. Electro-polymerization has been studied by cyclic voltmeter and products were characterized by UV-Vis, FT-IR, <sup>1</sup>HNMR, <sup>13</sup>CNMR spectroscopy.

# 54. Synthesis and structural characterization of 3d coordination complexes with a new 2,4-dichloro-6-{(E)-[(5-chloro-2-sulfanylphenyl)imino]methyl}phenol Schiff base ligand

Brajendra S. Kusmariya and A.P. Mishra Synthetic Bioinorganic Chemistry Laboratory, Department of Chemistry, Dr. H.S. Gour Central University, Sagar – 470003. A new series of Co(II), Ni(II) and Cu(II) complexes of Schiff-bases derived from the condensation of 2-amino 4-chloro benzenethiol and 3,5-dichloro salicylaldehyde have been synthesized and characterized by various spectral techniques. The coordination behaviour of the Schiff-base towards metal ions has been proposed in the light of elemental analysis, spectral (FTIR, electronic, <sup>1</sup>H-NMR) and thermal studies. IR spectra show that ligand is coordinated to the metal ions in a tridentate manner. TG of the synthesized complexes illustrates the general decomposition patterns of the complexes. The SEM images show the crystalline nature of complexes. The ligand and its complexes exhibited interesting fluorescence properties.

# 55. Acoustic and viscometric studies of liquid mixture of atropine drug with Cu(II) metal ion in aqueous medium: Interaction studies

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Densities, viscosities and ultrasonic velocities have been carried out for ternary mixtures of Atropine sulphate drug (0.01 to 0.1M) in aqueous Cu(II)-ion solutions at three different concentration (0.1, 0.05 and 0.025 M) at 303.15 K and at atmospheric pressures. The acoustical parameters such as isentropic compressibility, intermolecular free length, specific acoustic impedance, relative association, free volume, internal pressure, viscous relaxation time, Gibb's free energy, attenuation coefficient, Rao's constant, and Wada's constant have been calculated from the experimental data. On the basis of the Jones-Dole equation viscosity data have been analyzed and the values of Falkenhagen coefficient A and Jones-Dole *B*-coefficient have been evaluated. The data have been interpreted in terms of molecular interactions and the variations in these parameters with concentration of solute give the information about intermolecular interactions.

# 56. Synthesis, spectral, thermal and biological studies of Co(II), Ni(II) and Cu(II) metal complexes of bidentate Schiff base Ligand

### A.P. Mishra and Anjali Tiwari

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Schiff base metal complexes of Co(II), Ni(II) and Cu(II) derived from 2,3-Dimethoxy benzylidene-2-amino-6-chloro-4-nitro phenol (HL) have been synthesized and characterizations of the compounds have been done by elemental analysis, FT-IR, molar conductance, electronic spectra, <sup>1</sup>H-NMR, and thermal analysis. Analytical data reveal that all the complexes exhibit 1:2 (metal:ligand) ratio. IR data show that the coordination of ligand to metal is bidentate (donation from NO site). Thermal data shows the degradation pattern of the complexes which gives the idea about their stability. The Schiff base and their metal complexes show good activity against the *E.coli, S. xylosus* and *F. bacterium* bacterial strains. The antibacterial results also indicate that the metal complexes are better antibacterial agents as compared to the Schiff bases.

### 57. Computational studies on bisphenylbenzimidazoles (BPBIs) as non-nucleoside

#### inhibitors of HIV-1 Reverse Transcriptase

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Chemotherapy is the most effective weapon to meet out the challenges posed by drug resistant HIV mutants and also to hit the HIV reservoirs in humans. The low toxicity of NNRTIs in comparison to NRTIs inspired us to prepare better and safer second generation NNRTIs with an increased genetic barrier to the development of resistance. Molecular docking analyses have opened a versatile and fruitful pathway for developing effective anti- HIV agents. The protein ligand stabilization energies are highly useful tools in designing novel NNRTIs as effective inhibitors of HIV-1 RT. The designed ligands have shown high binding affinity with HIV-1 RT comparable to standard drug molecules - nevirapine and tetrahydroimidazo[4,5,1-jkj][1,4]benzodiazepin-2(1H)one and -thione (TIBO). Analysis of the docking results revealed that all molecules (bisphenylbenzimidazoles : BPBIs) formed hydrogen bonds with amino acids Lys101, Lys103, Tyr181, Tyr318 and exhibited  $\pi$ -stacking interactions with Tyr181, Tyr188, Phe227 and Trp229 present in the non nucleoside inhibitor binding pocket (NNIBP). The superimposition of contour maps on the active site of HIV-1 reverse transcriptase (HIV-1RT) revealed structural suitability of these inhibitors. The results provided insight into predictive and diagnostic aspects for better activity of this class of HIV-1 RT inhibitors.

# 58. *In-silico* designing of non nucleoside analogs of alkylated uracil as NNRTIs against HIV-1

Ritika Srivastava, Nidhi Singh, Anuradha Singh, Farha Naaz and Ramendra K. Singh

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Chemotherapy is one of the highly effective and more successful ways for the treatment of AIDS. A crucial step in the replication of HIV is the reverse transcription of viral ssRNA into proviral dsDNA by the virus-encoded reverse transcriptase enzyme. Inhibition of reverse transcriptase is considered one of the most possible approaches to prevent the spread of infection. There are two types of reverse transcriptase inhibitors; Nucleoside/Nucleotide Reverse Transcriptase Inhibitors (NRTIs/ NtRTIs) and Non Nucleoside reverse transcriptase inhibitors (NNRTIs). On the basis of low toxicity of NNRTIs in contrast to NRTIs, we have designed some molecules as NNRTIs. *In-silico* studies using DS 2.5 have shown that these molecules perform as NNRTIs while interacting at allosteric site on HIV-1 RT. The designed molecules have shown potential docking results when compare with nevirapine. Docking results revealed that all molecules formed hydrogen bonds with amino acids, Lys101, Lys103, Tyr181, Tyr318 and  $\pi$ - interactions with Tyr181, Tyr188, Phe227 and Trp229, present in the non nucleoside inhibitory binding pocket. The intended molecules have shown high binding affinity with HIV-1 RT analogous to standard drug molecule - nevirapine. The molecules reported herein showed complete adherence to Lipinski's rule of five.

# 59. Molecular modelling studies on tri-substituted triazine analogs as NNRTIs against HIV-1

### Farha Naaz, Ritika Srivastava, and Nidhi Singh

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Human immunodeficiency virus type 1 (HIV-1), the etiological agent of acquired immunodeficiency syndrome (AIDS), belongs to a family of retroviridae. HIV changes its ssRNA genetic material, through reverse transcription, into dsDNA – the provirus. This critical process of reverse transcription has, therefore, become the soft target for developing anti-HIV drugs. Presently, antiretroviral treatment that involves the use of a cocktail of drugs is referred to as HAART, is also unsuccessful due to mutational changes in the virus. Hence, to control the mutagenicity and thereby overcoming the problem of resistance, to attack viral reservoirs in the brain and circumventing pharmacokinetic problems, we have designed substituted tri-substituted triazine derivatives as probable NNRTIs against HIV-1.Computational studies using DS 2.5 have shown that these molecules adopted horse-shoe conformations while interacting at NNIBP of HIV-1 RT. All compounds exhibited well established hydrogen and  $\pi$ -bonds with amino acids present in non nucleoside binding pocket.

### 60. Fluorescent Prodrugs of Stavudine against HIV-1: A chemistry-based strategy

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The problems, like poor bioavailability and side effects have forced the scientific community to develop drug-conjugates with higher lipophilic character. In this direction, a rewarding chemistrybased strategy that has been successfully employed to solve drug formulation and delivery problems is fluorophore-tagged prodrug approach. Prodrugs can improve the solubility and bioavailability of known drugs and also improve drug targeting. So, we herein report the synthesis and biophysical properties of a series of fluorophore-tagged prodrugs of stavudine against HIV-1. The fluorophores have been designed with properties like high solubility in polar solvents, easy delivery into cells and imaging bio-macromolecules using chemical tagging. The fluorophores have been synthesized from the parent molecule 4-amino 1-8, naphthalic anhydride and amino caproic acid. These fluorophores are attached to stavudine via ester linkage. On the basis of fluorescence study, which is done in different solvents, like methanol, dioxane, methanol-water, it is confirmed that these molecules absorb in the UV-visible region and show good fluorescence property. The biological screening of these molecules is under process.

### 61. Ion transport Studies through Inorganic Precipitate Membranes

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To understand the mechanism of transport of ions through inorganic precipitate membranes the measurement of membrane potential was carried out by using different concentrations of univalent electrolyte solutions. The most effective parameter to understand the transport of ions through membranes, thermodynamically effective fixed charge density was evaluated by using a number of methods particularly those of T-M-S, based on thermodynamics of irreversible process. The values of some other parameters  $\alpha$ ,  $\beta$ ,  $\theta$ ,  $t_{app}$  and perm selectivity were also obtained for the same membrane by Kobatake procedure, equation was used under two limiting conditions namely  $\theta_c$  and  $\theta_d$ . It was found that  $\theta_c$  values were closer to those of T-M-S values and a close agreement was also found in between theoretical and observed values for the studied membrane. Therefore not only proved the existence of the membrane but also confirm the applicability of the theories of ion transport utilized to the membrane electrolyte system.

# 62. Micellar Effect upon Dephosphorylation of mono-2-MPPA ester by peroxy anions

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The micellar catalysed reactions between hydroxide or hydroperoxide anion and monophosphate ester of 2-methoxy phenyl phosphoramides has been examined in buffered medium (at pH 8.0-10.0) with borate ions. First order rate constant ( $K_{\psi}$ ) for the reaction of OH<sup>-</sup> with 2-MPPA go through maxima increasing with the concentration of cetyl trimethyl ammonium bromide (CTABr) micelles of CTABr are very effective catalysts to the reactions of phosphate mono ester. Rate enhancement depends upon the hydrophobicity of the nucleophile for the reactions of mono phosphate ester. Rate constants measured with HO<sub>2</sub><sup>-</sup> ions are approximately.

# 63. Effect of anionic micelles of Sodium lauryl sulphate on the reaction of hydroxide ion with mono-2-methoxy phenyl phosphoramides ester

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<sup>1</sup>Department of Chemistry, B.S.A. College, Mathura, Uttar Pradesh.

<sup>2</sup>Department of Chemistry, Janta College, Bakewar, Etawah, Uttar Pradesh.

The micellar catalysed reaction with hydroxide ion and mono phosphate ester of 2-methoxy phenyl phosphoramides (2-MPPA) has been examined in buffered solution medium (at pH 8.0-10.0) with borate ions. First order rate constant for the reaction of OH<sup>-</sup> ion with 2-MPPA through maxima inhibited the concentration of sodium lauryl sulphate (Nals); micelles of Nals are least reactive. Anionic micelles of [Nals] have little effect on the reaction rates probably because anionic micelles strongly inhibit the nucleophilic effect.

# 64. Mixed micelles of Sodium decyl Benzene Sulphonate and Sodium tetra decyl sulphate surfactants in aqueous media

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The mixed surfactant systems comprise of two anionic surfactants as sodium decyl benzene sulphonate and sodium tetra decy sulphate solution in presence of 1M Nacl concentration. The mole-fraction of the surfactant component in mixed micelle and the Rubingh's interaction parameter  $\beta$  to intercept the nature of interaction between surfactant mixture and factors governing them in aqueous media and control the product performance.

# 65. Effect of anionic micelles of Sodium lauryl Sulphate on the reaction of hydroxide ion with bis-4-chloro-3-methyl phenyl phosphate ester

Verma R.C.

### Department of Chemistry, Janta, college, Bakewar, Etawah, Uttar Pradesh

The micellar catalysed reaction with hydroxide ion and bis-phosphate ester of 4-chloro-3methyl phenyl (4-CMPP) has been examined in buffered solution medium (at pH 8.0-10.0) with borate ions. First order rate constant for the reaction of  $OH^-$  ion with 4-CMPP through maxima inhibited the concentration of sodium lauryl sulphate (Nals), micelles of Nals are least reactive. Anionic micelles of [Nals] have little effect on the reaction rates probably because anionic micelles strongly inhibit the nucleophilic effect.

# 66. Effects of electrolytes on the cloud point of mixed solutions of ionic and non-ionic surfactants

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The effect of electrolytes on the cloud point of ionic - nonionic surfactant solutions. When ionic surfactant is added to an electrolyte - free Triton X-100 solution, the cloud point increase as expected. However when small amount of electrolytes are added to the Triton X-100 solution in the presence of very low concentrations of sodium dodecyl sulphate the cloud point decrease in a ratio depending on the concentration of electrolyte and the nature of co -ion. This effect is due to the change of counter ion binding on the mixed ionic-nonionic micelles.

### 67. Comparing Directed and Random Routing Based on Lifetime Metric for Wireless Sensor Networks

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The main focus of this article is to achieve prolonged network lifetime with overall energy efficiency in wireless sensors networks through controlled utilization of limited energy. Major

percentage of energy in wireless sensor network is consumed during routing from source to destination, retransmission of data on packet loss. In this paper we first describe how on the increase of the networks size the lifetime is affected on implementing directed routing and random. Routing consumes the major part of energy usage in WSNs. Focus of the paper is on types of routing by which we can save energy. Simulation and results shows that this approach can save the overall energy consumption due to which the lifetime of wireless sensor network is prolonged.

### 68. Cross Layer Design for Network Lifetime Extension with Retry Limit for Retransmission by Sending the Traffic to multiple paths

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A cross layer architectural design has been the subject of research in wireless sensor networks. We achieve energy efficiency by balancing the traffic load created by each sensor nodes on multiple paths. Instead of shifting the traffic on a single route which would indeed increase the overhead, we shift the traffic on multiple paths. In this paper we propose, a cross layer strategy to improve the network lifetime by considering jointly the PHY, MAC and routing layers. We develop RLRTMP (Retry Limit for Retransmission by sending traffic to multiple paths). Initially at the network layer, we propose an efficient routing of reports to the sink node by balancing the energy throughout the network. Simulation report shows that 20 % of network lifetime is increased.

### 69. Spectroscopic Investigation of the Talcum Powder and its Potential Impact on Human Health

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This paper deals with the simultaneous analysis of various elements and compounds present in the talcum powder by D C Arc Optical Emission Spectroscopy (DC Arc-OES) and Attenuated Total Reflection Fourier Transform Spectroscopy (ATR-FTIR). Spectra of various samples of the talcum powder have been recorded in the spectral region 350-900 nm and 485-4000 cm<sup>-1</sup> respectively. The recorded spectra show spectral signatures of various elements and compounds with varying intensity. The scrutiny of the spectra reveals the presence of elements: sodium (Na), potassium (K), magnesium (Mg), calcium (Ca), iron (Fe), aluminium (Al), silicon (Si), manganese (Mn), chromium (Cr), cadmium (Cd), mercury (Hg), lead (Pb) and compounds Magnesium silicate, Magnesium silicate, Magnesium silicate and Calcium carbonate. The variation in concentration of the detected compounds in different sections has been observed through intensity variation. Out of these detected elements, the presence of element: Cd, Pb, Hg, Cr are dangerous to the human health. They can produce number of complications to the human body and can pose health hazards.

### 70. Novel and eco-friendly approach: synthesis of Isocoumarin derivatives in solvent –free conditions

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Efficient and environmentally benign heterocyclisation of O-halobenzoic acid and alkyne has been developed using [bmIm]OH as green catalyst. This methodology offers a metal and base free approach and is endowed with mild reaction conditions, high yields and better functional group tolerating ability. The recyclability and reuse of [bmIm]OH add the methodology a wide.

# 71. Kinetic influence of the new conformational polymorph of N-acetyl L-cysteine in Ru (III) catalyzed oxidation by methylene blue in acidic medium.

### Ranjana Sharma, Mahender Pal and K. K. Mishra Department of Chemistry, Rani Durgavati University, Jabalpur-482001

N-acetyl L-cysteine (NAC) has got diverse medicinal applications mainly due to its capability to support the body's antioxidant and nitric oxide systems during stress, infections, toxic and inflammatory conditions. It has potential for treating cancer, Alzheimer's disease, mutual toxicity and cardiovascular diseases. The oxidation of bioactive molecules, in general, involves metal ion catalysis facilitated by the participation of metal nanoparticles. Relatively, much attention has been paid to metals such as Pt, Pd, Ag, Au and Cu but less work has been carried out on the chemistry of Ru nanoparticles. In view of this Ru(III) catalyzed oxidation of NAC by a phenothiazine dye methylene blue (MB) has been investigated in acidic medium. Methylene blue has been widely used in the treatment of tumors and hepatitis C, in treatment of methemoglobinemia, plasmodium falciparum malaria etc. A minus half order (-1/2) kinetics has been observed in MB while the order in NAC in slightly larger than unity. Hydrogen ion retards the rate whereas the rate increases linearly with increasing [Ru(III)]. The addition of the reaction products does not affect the rate of reaction. The reaction is characterized by a large negative entropy of activation. Kinetics of the reaction suggest the participation of Ru(III) and Ru(IV) and a new conformational polymorph of NAC.

## 72. Synthesis, Spectral, Electrochemical and DFT Studies of Some *cis* –Dioxo molybdenum(VI) Complexes Involving Hydrazones Derived from 2-Hydroxyacetophenone

### R. C. Maurya, P. K. Vishwakarma, D. K. Rajak and J. M. Mir

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This paper reports the synthesis of four new dioxomolybdenum(VI) complexes of composition  $[MoO_2(L)_x(H_2O)]$  where, x = 2, LH = N-(2'-hydroxyacetophenonidene)- hydrazine (hahH, I); x = 1, LH = N-(2'-hydroxyacetophenonidene)benzoic acid hydrazide (habaH<sub>2</sub>, II), N-(2'-hydroxyacetophenonidene)isonicotinic acid hydrazide (hainaH<sub>2</sub>, III) or N-(2'-hydroxyacetophenonidene)salicylic acid hydrazide (hasaH<sub>3</sub>, IV). These complexes were obtained by the interaction

of bis(acetylacetonato)dioxomolybdenum(VI) with the said ligands in 1:2 metal-ligand ratio in case of ligand (I) and 1:1 metal-ligand ratio for the remaining three ligands in ethanol. All these complexes have been characterized by elemental analysis, molar conductance, magnetic measurement, <sup>1</sup>HNMR, IR, mass, electronic spectral and electrochemical studies. Molecular geometry optimizations, molecular surface electrostatic potentials (MSEP), vibrational frequencies calculations, bond lengths, bond angles and dihedral angles, natural atomic charges obtained by NBO and Mulliken population analysis and calculations of molecular energies, HOMO and LUMO were performed with the Gaussian 09 software package by using density functional theory (DFT) methods with Becke3–Lee–Yang–Parr (B3LYP) hybrid exchange-correlation functional and the standard LANL2DZ basis set for one of the representative complex, *cis*-[MoO<sub>2</sub>(haina)(H<sub>2</sub>O)](3). No imaginary frequency was found in the optimized model compounds and hence ensures that the molecule is in the lowest point of the potential energy surface, that is, a energy minimum. The results obtained from simulated Infrared spectra of the title compound show good agreement with observed spectral data. The experimental results, and the calculated molecular parameters, bond distances and angles, revealed octahedral geometry of the compounds.

# 73. Dioxovanadium(V) Complexes with Semicarbazone Ligands of Bioinorganic and Industrial Relevance: Synthesis, Characterization, DFT Calculations and Antimicrobial Activity

R. C. Maurya, D. K. Rajak, P. K. Vishwakarma J.M. Mir and B.A. Malik

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The interaction of bis(acetylacetonato)oxovanadium(IV), [VO(acac)<sub>2</sub>] with biomimetic semicarbazone ONO-donor ligands, LH in 1:1 mole ratio [where, LH = N-(4'-benzoylidene-3'-methyl-1'-phenyl-2'-pyrazolin-5'-one)-semicarbazone (bmphp-semH), N-(4'-butylidene-3'-methyl-1'-phenyl-2'-pyrazolin-5'-one)-semicarbazone (bumphp-semH), N-(4'-iso-butylidene-3'-methyl-1'-phenyl-2'pyrazolin-5'-one)-semicarbazone (iso-bumphp-semH) or N-(3'-methyl-1'-phenyl-4'-propionylidene-2'pyrazolin-5'-one)-semicarbazone (mphpp-semH)] in a mixed solvent (ethanol-methanol, 1:10) via aerial oxidation for 2-3 days yields dioxovanadium(V) complexes of composition  $[VO_2(L)(H_2O)]$ . The Synthesized complexes have been characterized by Elemental analysis, molar conductance, magnatic measurements, IR, electronic and mass spectral analysis, DFT studies have been carried out for one of the representative complex, cis-[VO<sub>2</sub>(bmphp-sem)(H<sub>2</sub>O)]. The molecular structure, vibrational wave numbers, infrared intensities, were obtained for molecule using the B3LYP density functional theory (DFT) with the standard B3LYP/6-31+G(d, p)/LANL2DZ basis set. Theoretical calculations invoking geometry optimization, charge distribution and molecular orbital descriptions- HOMO and LUMO were done using density functional theory. The absolute electronegativity ( $\chi_{abs}$ ) and absolute hardness  $(\eta)$  were obtained for molecule. The experimental results, and the calculated molecular parameters, bond distances and angles, revealed octahedral geometry of the compounds.

## 74. *Ab Initio*, Semi Empirical and DFT Quantum Chemical Aided Prediction of the Thermal Decomposition and Calorimetric Study of [RuHCl(CO)(TPP)(BYP)]

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In view of the conspicuous interests towards ruthenium carbonyl complexes, the present paper includes the synthesis and combined theoretical experimental studies of Ruthenium(II) carbonyl complex containing triphenylphosphine (TPP) and benzoyl pyridine (BYP) as co-ligands. The synthesized complex has been characterized by using FTIR, UV spectrophotometer and Cyclicvoltametric studies. All the experimental observations were compared with theoretical results. The geometric optimization with no imaginary frequency has been obtained using LANL2DZ/B3LYP combination for the complex and 631G/B3LYP for the ligands. More emphasis has been given towards the computational thermo analysis of the model compound. The quantum chemical calculations including *ab initio*, semi empirical and density functional methods were opted to act as a predictive tool for the possible decomposition reaction. Based on PM6/AM1, HF and DFT levels of theory the computed thermal data was studied comparatively and the output data has been found in full agreement with the expected results. Thermal free energy, thermal enthalpy and thermal entropy data procured from different levels of theory have been calculated for the model compound. Chloride and Carbonyl ligands have been predicted to be the first leaving groups based on computational thermal analysis. Based on the energetic calculations the reaction is feasible in the formation of stable product, the model compound of ruthenium.

### 75. Nuclear radiations affecting the freezing of liquid water

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Supercooled water freezes when nuclear radiations are passed through it, due to addition of electrostatic energy  $3(\text{Ze})^2/5r_i$  to the Gibb's free energy of formation of ice nucleus. The critical radius  $(r_i^*)$  of ice crystals is much less than that formed in absence of nuclear radiations  $(r_i, \text{homogenous})$ . Also, the supersaturation ratio is very small (0.01%) and nucleation rate  $(J_i^*)$  and equilibrium concentration [ $C(n_i^*)$ ] becomes very large. Thus, we see that  $S'_{v,i} < S_{v,i}$ ,  $G'_i < G_i$ ,  $r'_i < r_i$ ,  $n'_i > n_i$ ,  $J'_i > J_i$  and  $C(n'_i) > C(n_i)$ . Hence, we note that nuclear radiations enhance the formation of ice nuclei.

### 76. Formation of clouds by effective role of atmospheric ions

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In the lower atmosphere, the ions are produced as the result of ionization which occurs along the trajectory of high energy galactic cosmic rays due to radioactivity. These ions participate in ionmolecule reactions and ion induced nucleation. At a given supersaturation, the Gibb's free energy for the formation of critical nucleus, its radius and number of molecules in it are comparatively less than those in homogenous nucleation. As a result equilibrium concentration and rate of nucleation are found to increase. The ion induced nucleation is more effective at low supersaturation (even S<1). The phase changes of water vapour are more favored on negative ions than on positive ions. The rate and probability of nucleation is enhanced on ion induced nucleation of partially wettable, water insoluble planer as well as curved (convex and concave) substrates. There exists a threshold for angle of contact above which the effect of ions is dominant. Thus, there is effective role of ions and electric field in the formation of clouds. The electric field causes the lightning which in turn ionizes the air. Ultrafine aerosols are formed on ions.

# 77. Relaxation time and polarization of water vapour molecules affected by electric field induced nucleation

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The increase in polarizability of water vapour molecules in the nucleation of water vapour condensation and ice glaciations, result in increase of Gibb's free energy and hence the increase in nucleation rate, but at the same time decrease in relaxation time, the effective polarizability varies nearly inversely as the absolute temperature.

### 78. Hydrological assessment of water quality for drinking purpose in Agra city India

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This paper presents a geochemical evaluation of the various parameters of drinking water sources of Agra city. Groundwater quality shows wide variations which depends upon depth, hydrogeological conditions and human activities. Ten samples of bottled water were purchased from local markets. Four samples of different R.O. systems output waters being used; two samples of tap water from different locations were collected in clean sterile bottles while ground water samples were taken from bore wells from various locations in different parts of city.

Agra is situated on the banks of Yamuna River known for its brackish water, also the south-west side of city lies near fluoride rich area of Rajasthan. Therefore, the use of bottled water and domestic RO systems as source of drinking water is gaining momentum day by day. Therefore it is desirable to independently monitor the quality of these water sources. These facts make this study even more relevant. It is observed that the fluoride levels in bottled water are below recommended limits (0.07-0.35 mg/l) whereas in ground water fluoride levels are much higher. The groundwater samples also show higher values of hardness, TDS. The spatial distribution of fluoride, as estimated by geochemical assessment, agrees well with the incidence of dental and skeletal fluorisis. Apart from already affected people, a larger part of population is at risk. Similarly estimation of other parameters like hardness etc. agrees well with observed ill effects.

# 79. Novel facile and greener approach for the synthesis of 2,3,5,6-tetraryl-3,3*a*,5,6-tetrahydro-2*H*-pyrazolo[3,4-*d*]thiazole

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Three component, simple and direct cyclocondensation method has been developed for the synthesis of 2,3,5,6-tetraryl-3,3a,5,6-tetrahydro-2H-pyrazolo[3,4-d]thiazole **7** by combining aniline (1 mmole) **1**, benzaldehyde (2 mmole) **2**, mercaptoacetic acid (1 mmole) in presence of boric acid (20 mol%) as catalyst and surfactant CTAB (15 mol%) in aqueous medium with excellent yield, followed by cyclocondensation with arylhydrazene. Simple reaction conditions, short reaction time, ease of product isolation, use of cheap and readily available catalyst makes this manipulation very interesting from an economic and environmental perspective. The catalyst was easily recovered and reused without any considerable loss of activity.



# 80. Novel environmentally benign technique for the removal of fluoride, arsenic and coliform from Drinking water

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An environmentally benign homemade bio-sand filter is used for the removal of fluoride, arsenic and coliform from drinking water. This method is facile at rural area and has low cast. The physiochemical analysis of water samples had been done before and after the treatment time with filter using standard methods. Optimum operating time was determined for maximum removal of these impurities by running experiment for 2,4,6,8 and 10 hours respectively. The maximum reduction of fluoride, arsenic and coliform bacteria in percentage was 81.4, 91.1 and 100. These residual values are under the permissible limits prescribed by WHO and drinking water specification IS 10500. This method has advantages, such as simple work-up procedure, avoidance of organic solvent and highly sophisticated equipment, which will contribute in serving as a green process greatly.

### 81. [bmIm]OH Catalysed Four component one-pot Synthesis of Pyrazoloimidazole-2-thione-*N*-nucleosides

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A basic ionic liquid, 1-butyl-3-methyl imidazolium hydroxide [bmIm]OH has been used as an efficient catalyst for the novel synthesis of pyrazoloimidazole-2-thione-*N*-nucleosides by one-pot four component condensation reaction of aryl ribosylthiourea, chloroacetic acid, aromatic aldehyde and hydrazine hydrate at room temperature. This method includes marked improvements regarding to operational simplicity, reaction time, environmentally benign protocol, easily and reusable basic ionic liquid, avoiding hazardous organic solvents and toxic catalysts, which fulfil basic need of green chemistry.

### 82. Eosin Y catalyzed visible-light-promoted aerobic oxidative cyclization of 2aminobenzothiazole

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A mild and efficient one-pot visible light irradiated synthesis of 2-aminobenzothiazole from arylisothiocyanate and secondary amines have been reported in presence of eosin Y as an organophotoredox catalyst at room temperature under aerobic condition. This synthesis includes application of air and visible light as inexpensive, readily available, high atom economy, non-toxic and sustainable regents. This synthetic pathway is superior in comparison to all other alternative synthetic methods for 2-aminobenzothiazole.

# 83. Stability of mixed ligand complexes of Zn<sup>2+,</sup> Mn<sup>2+,</sup> Co<sup>2+</sup> and VO<sup>2+</sup> with meso 2,3 dimerceptosuccinic acid (DMSA) as a primary ligand and crotonic acid as a secondary ligand

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The formation of 1:1:1 ternary complexes of  $Zn^{2+}$ ,  $Mn^{2+}$ ,  $Co^{2+}$  and  $VO^{2+}$  with meso 2,3 dimerceptosuccinic acid (DMSA) as a primary ligand and crotonic acid as a secondary ligand have

been studied potentiometrically by employing the modified method of Irving and Rossoti at 30°C, 40°C and 50°C and keeping the ionic strength constant  $\mu$ =0.2M(KNO<sub>3</sub>). The stability constants determined follows the order: Mn<sup>2+</sup>  $\approx$  Zn<sup>2+</sup> > VO<sup>2+</sup> > Co<sup>2+</sup>. The thermodynamic parameters like free energy ( $\Delta G^0$ ), enthalpy ( $\Delta H^0$ ) and entropy ( $\Delta S^0$ ) have also been calculated using the standard equations.

### 84. Micellization of cadmium mono- and di- alkanoates in mixed organic solvent

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The molar conductance,  $\Lambda$  of cadmium alkanoates of mono- (hexanoic and decanoic) and di-(butanedioic and hexanedioic) carboxylic acid decreases with increasing alkanoate concentration, may be due to the combined effects of ionic atmosphere, solvation of ions, decrease of mobility and ionization and formation of micelles. In organic solvent, cadmium mono-alkanoates behave as moderate electrolyte, while cadmium di-alkanoates behave as weak electrolytes in dilute solutions. The critical micellar concentration (CMC), degree of ionization, and ionization constant of cadmium alkanoates of mono- and di-carboxylic acid in a mixture of benzene-methanol (50% v/v) have been determined by conductometric measurements. The scanning electron microscope studies of the solution of cadmium alkanoates beyond their critical micellar concentration confirm the formation of star shaped reversed micelles containing 8-10 monomers of alkanoate molecules. The size of micelles obtained in the range of micrometer.

# 85. Parametric analysis of offset-fed Microstrip patch antenna for enhancement in bandwidth

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A microstrip patch antenna for WiMAX and FWA applications is presented in this work. By properly feeding patch, various characteristic of microstrip antenna has been analysed. The overall dimension of this antenna is 28 X 30X 1.6mm<sup>3</sup>. An experimental result shows how antenna provides multi bands to enhance its role in communication. Good radiation pattern and applicable VSWR is obtained at the operating bands. The proposed antenna is thus suitable for wireless communication systems. Microstrip line with offset feed has been introduced, which improves the overall performance of antenna to fulfill requirements of multiband communication. Reduction in antenna size is done with slots cut in ground plane, which also provides impedance matching by diverting the ground current flow. Also parametric analysis has been done to analyze effect of length on return loss of antenna.

# 86. Synthesis, Characterization and Pharmacological Activity Evaluation of Curcumin Derivatives

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Curcumin 3,4-dihydropyrimidinones/thiones/imine have been synthesized using one-pot cyclocondensation of curcumin in solvent-free conditions, substituted aromatic aldehydes and urea/thiourea/guanidine in the presence of chitosamine hydrochloride as biodegradable and nontoxic catalyst under microwave irradiations. The synthesized product was purified by crystallization from ethanol and the process does not involve any hazardous solvent. All the synthesized curcumin derivatives **4a-o** was screened for antioxidant and anti-inflammatory activity. Biological activity data of the synthesized showed that most of the synthesized compounds exhibited greater antioxidant and anti-inflammatory activity than curcumin.

### 87. A Study on Supply Chain Management

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Today, holding and managing of an inventory is very important issue in our daily life as well as any business organization for efficient and smooth running. It is essential for all organizations like manufacturing industry, a five star hotel, a printing press or a hospital. In this paper we provide an overview of supply chain management, basic stages of a supply chain, supply chain decisions, modeling approaches to supply chain management and the common problems faced by supply chain management. The roles of supply chain management in sectors such as IT, ERP, health care, warehousing, and retail have been briefly illustrated. Finally we suggest directions for the future research.

### 88. An Inventory Model for Non-Instantaneous Deteriorating Items

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This paper presents an inventory model with non-instantaneous deteriorating items and stockdependent demand. Demand rate is taken to be stock dependent. Here shortage is not allowed. The necessary and sufficient conditions of the existence and uniqueness of the optimal solution have been shown. Finally we provided an inventory model with solution algorithm for minimum total relevant cost and optimal order quantity.

# 89. Oxidative kinetics of mannose by N-Chlorosuccinimide using Rh(III)-chloride as catalyst in alkaline medium

## Ashok Kumar Singh, Ritu Swamini Bala, Rashmi Srivastava, Jaya Srivastava and Shahla Rahmani

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The oxidation kinetics of mannose by N-Chlorosuccinimide (NCS) in alkaline medium has been reported at  $35^{\circ}$ C .The reaction follows first order kinetics with respect to [NCS]. First-order kinetics with respect to [OH<sup>-</sup>] was also observed throughout the oxidation for mannose. Inverse relationship between reaction rate and [Rh(III)] was observed. The rate is inversely proportional to [NHS] also. First-order kinetics observed at low concentrations of mannose changes to zero-order at its high concentrations. The results indicate negligible effects of [CI<sup>-</sup>], ionic strength and dielectric constant of the medium on the rate of reaction. Various activation parameters of the reactions were determined by studying the reaction at four different temperatures. Based on the kinetic results together with spectrophotometric information, a probable mechanism has been proposed for the oxidation of mannose by NCS and the rate law has been derived.

### 90. Investigation on practical existence of Dirac Monopole

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The aim of the paper is to highlight the necessity of thoroughly investigating the conditions of existence of magnetic charge and utilizing it in all fields of Communication Engineering. The idea of magnetic charge was first originated by P.A.M. Dirac in 1931 but it has not been observed anywhere in the outer atmosphere in spite of all efforts. This is why it has not been accepted in common literature. The paper describes the basic theory and some practical which show the existence of magnetic charge magnetic charge and electric charge is formed such that g x e = h where g = magnetic charge and electric charge is formed such that g x e = h where g = magnetic charge scan be separated by strong field giving perfect validity of Maxwell's Symmetrical Equations. It also shows the possibility of existence of magnetic charge in Ionospheric where electrons moving in circular orbit. This has to be investigated by organization like ISRO the consequences of arrangement on existence of magnetic charge will modify in communication engineering and science technology.

#### 91. Determination of Path loss using Hata model for GSM network

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This paper can be used in realistic planning of GSM networks, with the predicted path loss in area. For capacity enhancements of the network, GSM Engineers can use the path loss prediction models for intelligent placement of BTS's with certain antenna height and power. Path loss also facilitates Link budget analysis and Design in a telecommunication system. In a GSM like cellular network, Path loss is used for Frequency Re-use distance estimates so as to properly space the channels in Base stations (BS). Actual frequency assignment plans for the Base Stations are also

facilitated by the use of path loss. Better coverge predictions and interference reduction is what planning engineers get by using better path loss model.

The aim of this paper is to investigate the performance of various path loss models in different environments for determination of the signal strength with respect to various frequency ranges and distance for wireless network. A total of five path loss models, namely Free Space, Log-distance, Log-normal, Okumura/Hata, IEEE802.16d models have been reviewed with different receiver antenna heights in urban, suburban and rural environments. The estimated results produced by Free Space model were used as reference values. All estimated results of reviewed models were compared with the reference model values.

## 92. Mechanistic study of oxidation of xylose by protonated NCS using Rh(III)chloride as homogeneous catalyst

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The Kinetics and mechanism of oxidation of Xylose by N-chlorosuccinimide(NCS) in presence of Rh(III)-chloride as homogeneous catalyst in aqueous alkaline medium have been investigated at  $35^{\circ}$ C. The reaction is found to be first-order with respect to [N-chlorosuccinimide] and [NaOH] throughout their variation. Zero order kinetics with respect to xylose and inverse proportionality between pseudo-first order rate constants (k<sub>1</sub>) and [Rh(III)] were observed throughout their ten-fold variation. Rate of reaction is not influenced by the change in ionic strength ( $\mu$ ), dielectric constant (D) and [Cl<sup>-</sup>] of the medium. A reaction scheme, consistent with the kinetic data, spectroscopic information and activation parameters, was proposed.

# **93.** Role of Rh(III) as an inhibitor in N-chlorosuccinimide oxidation of sorbose in alkaline medium: A kinetic and mechanistic study

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The Kinetics and mechanism of oxidation of Sorbose by N-chlorosuccinimide(NCS) in aqueous alkaline medium using Rh(III)-chloride as inhibitor have been investigated at  $35^{\circ}$ C. The order of reaction with respect to [NCS] and [OH]<sup>-</sup> was found to be unity. The rate of reaction remains almost the same throughout the variation of sorbose concentration. The significant feature of the reaction under investigation is that there is inverse proportionality between pseudo-first-order rate constant (k<sub>1</sub>) and [Rh(III)]. Inverse fractional order in [NHS] and nil effect in [Cl<sup>-</sup>] were observed. The reaction rates remain unaffected by the change in ionic strength ( $\mu$ ) and dielectric constant (D) of the medium. A reaction scheme has been proposed in the light of observed kinetic orders and spectroscopic information (Varian Cary 300 Bio UV-Vis spectrophotometer) collected in this regards.

# 94. Synthesis, characterization and antimicrobial activity of some new organophosphorus compounds

Kalpana Chaturvedi

#### Department of Chemistry, Agra College, Agra, 282002.

A series of biologically active organophosphorus compounds have been synthesized by the reactions of Phenylphosphonic dichloride/4-Chlorophenyl dichlorophosphate with 5substituted -2-mercapto-1,3,4-oxadiazole ligands. The compounds have been characterized on the basis of elemental analyses and spectral (IR, <sup>1</sup>H NMR <sup>31</sup>P NMR) data. All the compounds were screened for their antimicrobial activity. They were found to possess significant anti-microbial activity.

# 95. Analysis of frequency and temperature dependent behaviour of a fluorinated antiferroelectric liquid crystalline material for display application

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Temperature and frequency dependent dielectric and electro-optical response of a fluorinated antiferroelectric liquid crystalline material (S)-(+)-4-(1-methylheptyloxycarbonyl) phenyl4'-(6-perfluorooctanoyloxyhex-1 oxy)biphenyl-4 carboxylate (in short 7F6Bi) have been investigated. The dielectric studies have been carried out in the frequency range of 1Hz to35MHz under planar anchoring conditions of the molecules. Material exhibits paraelectric SmA\*, ferroelectric SmC\* and a wide temperature range (\*83 C)antiferroelectric SmC\*<sub>a</sub> phases. The soft mode relaxation due to the tilt fluctuation of molecules in the MHz region has appeared in the SmA\* phase, whose dielectric strength increases with decrease in temperature and follows Curie-Weiss law. The SmC\* phase shows Goldstone mode relaxation due to phase fluctuation of molecules with relaxation frequency - 10 kHz. The dielectric response of the SmC\*<sub>a</sub> phase exhibits unusually one relaxation mode due to antiferroelectric ordering of the molecules. Switching parameters viz. spontaneous polarization, switching time and rotational viscosity have also been determined with the help of polarization reversal technique. The maximum value of Ps is  $^{-}$  210nC/cm<sup>2</sup> and switching time is order of few milliseconds.

### 96. Synthesis, characterization and antifungal activity of some novel aryl N-(2-(1-(2-(4H-1,2,4-triazol-4-yl) amino)-3-chloro-4-phenyl azetidin-2-one derivatives

Mukesh Kumar Tyagi, S. K. Srivastava and S. D. Srivastava

Synthetic organic chemistry Laboratory, Department of Chemistry, Dr. HariSingh Gour Vishwavidyalaya (A Central University), Sagar Madhya Pradesh.

Several substituted arylated N-(2-(2-benzylidine hydrazinyl)-4H-1,2,4-triazol-4-amine and 1-(2-(4H-1,2,4-triazol-4-yl) amino)-3-chloro-4-phenyl azetidin-2-one have been synthesised by the appropriate methods and evaluated for their antifungal activity against *Aspergillus niger* (An), *Aspergillus flavus* (Af), *Fusarium oxisporium* (Fo) and *Trichoderma viride* (Tv). In the primary screening some of the products display acceptable fungal activity. The structure of the synthesised compound has been established on the basis of their spectral and microanalytical data.

# 97. Photoelectrocatalytic Oxidation of NADH by Visible Light Driven Plasmonic Nanocomposites.

#### Bijayalaxmi Jena

#### Department of Chemistry, Utkal University, Bhubaneswar-75100.

Here a new synthetic method has been demonstrated to develop raspberry shaped ZnO nanostructures (RB-ZnO). The RB-ZnO has been decorated with plasmonic gold nanoparticles (AuNPs) by adopting a facile wet chemical approach. The as-synthesized plasmonic nanocomposite (RB-ZnO-Au) has been thoroughly characterized by Transmission Electron Microscope (TEM), Scanning Electron Microscope (SEM) and XRD measurements. The photoelectrocatalytic performance of RB-ZnO-Au was checked towards the oxidation of reduced nicotinamide adenine dinucleotide (NADH). The RB-ZnO-Au shows excellent photoelectrocatalytic response driven in visible light. The over potential for the photoelectrocatalytic oxidation of NADH has been substantially decreased in case of RB-ZnO-Au modified electrode compared to RB-ZnO. The reduction in the recombination of photogenerated holes and electrons, expedite the electrocatalytic oxidation process, which substantially decreased the over potential and increased the oxidation current.

### 98. Synthesis, IR Spectral Studies and Biological Activities of some Rare Earth Metal Complexes with Biochemically relevant Ligand

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Biologically active La (III), Sm (III), Gd (III) and Dy (III) complexes were synthesized by using Furan-2-carboxylic acid (FCA) as ligand and were characterized by elemental analysis and spectral measurements. Coordination of the ligand atoms to the metal ion was deducted by IR spectral data. The in vitro antibacterial screening of the free acid and its metal complexes has been carried out against *Escherichia coli*, *Staphylococcus aureus*. Antifungal activities of all the synthesized compounds were screened for in vitro growth inhibitory activity against *Aspergillus fumigatus* and *Aspergillus niger*, *Aspergillus flavus* by using the cup plate method. Antimicrobial activities of the ligand increase on coordination with the metal ion and show more promising activity than the corresponding free acid, and the standard control antibiotics. Such increased activity of the metal chelates can be explained on the basis of Overtone's concept and chelation theory.

## 99. Determination of Heavy Metals in the Different Matrices of the Ganges River from Rishikesh to Allahabad through Differential Pulse Anodic Striping Voltametry

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River Ganges is considered to be the most pious river of India. That is why its increasing level of pollution becomes a major environmental concern. Due to industrial affluent, municipal sewage, household drainage etc, the increasing concentration of heavy metals as major pollutant is alarming. The present paper reported the concentration of heavy metals viz. cadmium, copper, lead and zinc ions in the different matrices of the river Ganges from Rishikesh to Allahabad. The concentration of these metals was determined through differential Pulse Anodic Striping Voltametry (DPASV) from the water and sediments of Ganges at different places from the above said locations. The results showed that the water at Narora barrage was maximum contaminated with Cd and Cu, while at Narora barrage and Jajmau, Kanpur, Pb and Zn were found at its maximum level than others. The Narora ghat river bank and Jajmau, Kanpur river bed sediments gave maximum amount of Cd, Cu and Pb while the maximum amount of Zn was found both in Narora bank as well as bed sediment and highest in the Jajmau river bank sediment.

# 100. <sup>57</sup>Fe Mössbauer Spectroscopy Reveals Presence of Toxic Iron Phases in Traditional Iron Rich Medicines

#### Bhavna Joshi and R.P.Tripathi

#### Department of Physics, Jai NarainVyas University, Jodhpur -342005.

Chemical phases of iron in large number of the Ayurvedic bhasma are investigated through Mössbauer Spectroscopy. Iron is found in oxide form as  $Fe_2O_3$  or  $Fe_3O_4$  or both in all the bhasma studied here irrespective of their nature their mode of preparation. The size distribution of iron particles is different for different bhasma. It is known that iron oxide is toxic to human body and it is also not easily absorbed in it. Mössbauer studies point to iron oxide being present in these bhasma and thus not safe for human consumption.

# 101. Synthesis and biocidal studies of oxalic acid dihydrazide and malonic acid dihydrazide and their metal chelates

#### Hariom Sharma and Beena Mishra

#### Govt. P.G. College, Dholpur, Rajasthan.

Oxalic Acid dihydrazide (O.A.D.H.) and malonic acid dihydrazide (M.A.D.H) were synthesized by the reaction of already synthesized hydrazides of phthalic acid, succinic acid, anthranilic acid and oxalic acid respectively with methyl salicylate and hydrazine hydrate respectively with salicylic acid hydrazine hydrate. The metal complexes of this hydrazide were prepared with Zn (II) Cd (II). All the compounds were characterized and screened for their biocidal studies against gram +ve (*S. aureus*) and gram –ve (*E. coli*) bacteria and two common fungi (*A.niger* and *C. albicans*) by serial dilution method in slant and both culture media. A comparative study of the activities of the synthesized compounds with their metal complexes has been given and explained.

#### 102. Photophysical Studies of 1-Formyl- 2-Pyrazolines

Pramod Singh, Geeta Joshinee Pant and M. S. M. Rawat

#### Department of Chemistry, HNB Garhwal University, Srinagar Garhwal, Uttarakhand.

2-Pyrazolines are versatile materials having various pharmaceutical activities. They are also used as brightening agents in the fields of textiles, paper, plastics and detergents. Nanoparticles of 1-

formyl 2-pyrazolines with different diameters ranging from ten to two hundred nanometers have been reported, obtained by different methods. These nonmaterials showed best fluorescence properties in solvents as compared to solute. Optical properties of the fluorescent compounds depend on the nature of solvents also. Solvent conditions such as solvent polarity and hydrogen-bonding affect the fluorescence properties. Energy transfer by organic nanoparticles of 2-pyrazolines changes the blue to red shift with dilution because solvatochromic effect due to the change in dipole moment of compounds. We have synthesized novel 1-formyl 2-pyrazoline derivatives and studied their fluorescence in chloroform at fixed concentration  $1 \times 10^{-5}$  M. Study of size dependent optical properties of the new compounds as polymer films is in progress.

# 103. Superspin glass to superparamagnetic state: an anomalous transition in collective spin dynamics of iron oxide nanoparticles

### K.Saikia and P.Deb

# Advanced Functional Material Laboratory (AFML), Department of Physics, Tezpur University (Central University), Tezpur, Assam.

Collective spin dynamics of magnetic nanoparticle assemblies can be modulated by controlling the interparticle interaction. Here, an anomalous transition of the superspin glass state to superparamagnetic state of iron oxide nanoparticles while transforming a uniform assembly system of iron oxide nanoparticles to a cluster system via an aggregation step is reported. The superspin glass state of the primitive assembly is confirmed from the observed zero-field cooled (ZFC) memory effect, while absence of both FC (field cooled) and ZFC memory for the cluster system stands for the superparamagnetic state. Henkel plots indicate the dipolar type of coupling among the particles in all three systems, while highest interaction strength is observed for the cluster system and the lowest for the primitive one. The ordered arrangement of the nanoparticles with intermediate interparticle spacing is realized to be responsible for the faster spin relaxation in the cluster system. The obtained cluster system with superparamagnetic characteristics can have potentials for biomedical applications.

### 104. Synthesis and Characterization of Pyrazole Containing Substituted [1,2,4] Triazole-3-thiol Derivatives.

### Suneel Sahu and S.P.Shrivastava

Heterocyclic Research Laboratory, Department of Chemistry, Dr. H. S. Gour Central University, Sagar, Madhya Pradesh.

The reaction of 4-Amino-5-subsituted-4H[1,2,4]triazole-3-thiol with 3-(4-substitutedphenyl)-1H-pyrazole-4-carbaldehyde in ethanolic medium. Produced the new substituted derivative of 4-{(3-Subsituted-phenyl)-1-phenyl-1H-pyrazol-4ylmethylene)-amino}-5-(substituted-phenyl) 4H-(1,2,4)triazole-3-thiol. The condensation of the newly synthesized Schiff and Mannich base compounds were elucidated by spectral methods IR, <sup>1</sup>H NMR, and elemental analysis.

### 105. Accelerating Universe Model with Time Varying G And $\Lambda$

### R.K Tiwari

Department of Mathematics, Govt. Model Science College Rewa - 486001.

We examined anisotropic and homogeneous Bianchi Type-I cosmological model containing a perfect fluid with time varying G and  $\Lambda$  by considering the anisotropy ( $\sigma/\theta$ ) per unit expansion scalar  $(\theta)$  as a function of scale factor (S), which yields a constant value of deceleration parameter (q). Solutions of field equations are obtained and various cosmological parameters are studied by taking different cases on EOS,  $p = \omega \rho$ . Physical consequences of the model are discussed. The model acquires isotropy at late times with accelerated expansion.

#### 106. Dielectric studies on silver nanoparticles dispersed in columnar discotic liquid crystalline material

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### <sup>2</sup> Raman Research Institute, Bangalore - 560080.

We report dielectric investigations on silver nanoparticles (size 6-7 nm and ~100 nm) dispersed discotic liquid crystalline material namely 2,3,6,7,10,11-hexabutyloxytriphenylene. The broad range (~  $65.0^{\circ}$ C) columnar hexagonal phase has been observed under differential scanning calorimeter for pure and dispersed material. The dielectric studies have been carried out in the frequency range of 10 Hz to 35 MHz under homeotropic anchoring conditions of the molecules. In the low frequency region, a relaxation mode has been observed in columnar hexagonal phase for pure as well as dispersed material. This relaxation mode generates near the isotropic to columnar phase transition with high value of dielectric strength ( $\delta \epsilon$ ) and it decreases towards the lower temperatures. It is observed that this relaxation mode becomes strong (with  $\delta \epsilon \sim 0.12 - 0.97$ ) due to inclusion of silver nanoparticles of size 100nm. In addition to this dielectric behaviour, the temperature dependent relative permittivity and ionic conductivity have been determined in temperature range of 40.0°C to 160.0°C. Dielectric permittivity for pure material increases from 3.05 to 3.19 due to silver nanoparticles of size 6-7 nm.

#### 107. Antimicrobial activity aspects of some newly synthesized hydroxamic acids and their complexes of transition metal ions of bioinorganic relevance

R.C. Sharma, Devendra Kumar and Virendra Pal Singh<sup>#</sup> Department of Chemistry, Institute of Basic Sciences, Dr.B.R.Ambedkar University, Khandari Campus, Agra-282002. <sup>#</sup>Department of Chemistry, Neelam College of Engg & Technology, Agra - 282007.

Six new metal complexes have been synthesized by the reaction of 3, 5-dinitro-N-caproyl benzohydroxamic acid (DNNCBHA)/ N-caproyl benzohydraxmic acid (NCBHA) with metal salts and characterized by repeated melting point determinations, running TLC for single spot, elemental analyses, IR, magnetic moment values and electronic spectral studies. The electronic spectral studies and magnetic moment values suggested octahedral geometry for Cu(II) and Ni(II) complexes and distorted octahedral geometry for Cu(II) complex. Both hydroxamic acids and their metal complexes were screened for their antimicrobial activity in vitro against gram +ve bacteria (Staphylococcus aureus) and gram -ve bacteria (Pseudomonas aeruginosa) and two fungi Aspergillus niger and Aspergillus flavus. Hydroxamic acids exhibited moderate activity which increased in the form of metal complexes. Among the metal complexes, Cu(II) complexes were found most active.

# **108.** Synthesis, spectral and antimicrobial studies of tetraazamacrocyclic complexes of bivalent transition metal ions of bioinorganic relevance

Devendra Kumar and Sandhya

# Department of Chemistry, Institute of Basic Sciences, Dr. B R. Ambedkar University, Khandari Campus, Agra-282002.

Eight new tetraazamacrocyclic complexes of the types  $[M(C_{32}H_{24}N_8O_4).2H_2O]$  (CH<sub>3</sub>COO<sup>-</sup>)<sub>2</sub> and  $[M(C_{14}H_{20}N_8O_4).2H_2O]$ (CH<sub>3</sub>COO<sup>-</sup>)<sub>2</sub>, where M= Co (II)/ Ni (II) / Cu (II) /Zn(II), have been synthesized by the reaction of oxaloyldihydrazide and benzyl/acetylacetone by adopting template method. All the synthesized compounds were characterized by running their TLC for single spot, elemental analyses, infrared spectral studies, <sup>1</sup>H-NMR spectral studies, magnetic susceptibilities measurements and electronic spectral studies. The elemental analyses and spectral analysis results revealed their Metal: Ligand (1:1) stoichiometry. Magnetic moment values and electronic spectral studies suggested octahedral geometry for Co (II), Ni (II) complexes while distorted octahedral geometry for Cu (II) complexes. Synthesized dihydrazide and all macrocyclic complexes were screened for antimicrobial activity against two bacteria *Staphylococcus aureus* and *Escherichia coli* and two fungi *Aspergillus niger* and *Aspergillus flavus*. ODH-AA Cu(II) complexes was found most active against both bacteria while ODH-AA Zn (II) complex was most active against both fungi.

# **109.** Synthesis and studies of complexes of Mn(II), Co(II), Ni(II) and Cu(II) with schiff base derived from p-methoxy phenyl glyoxal and O-phenylenediamine

### A.K. Sengar, P.K. Jadon and Rahul Yadav

#### Department of Chemistry, Narain College, Shikohabad-283135

The complexes having general formula  $[M(L)_2 Cl_2]$  where M = Mn(II), Co(II), Ni(II) and Cu(II), L = Ligand or Schiff base [N-N'-O-Phenylene-bis-(P-methoxy phenyl glyoxal imine)] have been prepared and characterized by elemental analysis, molar conductance, magnetic susceptibility, electronic and infra-red spectral studies.

# **110.** Basic ionic liquid promoted reaction: An efficient and green protocol for one pot multicomponent synthesis of substituted furo[3,2c]pyridine derivatives

### I.R. Siddiqui, Hozeyfa Sagir and ShailendraTiwari

# Laboratory of Green Synthesis, Department of Chemistry, University of Allahabad, Allahabad- 211002.

An efficient, safe and facile route has been disclosed to synthesize a library of novel  $\{(2S,3S,7E)$ -7-Arylidine-2,3,4,5,6,7-hexahydro-5 methyl-3 arylfuro[3,2-c] pyridine-2 yl $\}$  (phenyl) methanone in high yield from the three-component reaction of N-methyl 4 piperidinone, aromatic aldehydes and 1-(2-oxo-2-arylethyl)pyridinium bromides in one- pot at room temperature by using basic ionic liquid. [Bmim]OH has been employed as a catalyst as well as reaction medium in this procedure that can be recovered and recycled for subsequent reactions without any appreciable loss of

efficiency. This novel protocol also avoids hazardous reagents/organic solvents and thus we herein report an eco-friendly alternative to the existing methods.

### 111. Monitoring of Fluoride Concentration in Ground Water of Jodhpur District in India: Correlation with Physico-chemical Parameters

#### Pallavi Mishra

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Western Rajasthan is most affected by water scarcity. Ground water is only source of dependence and sustenance of life. Advancement of human civilization has put serious questions to the safe use of ground water for drinking. Apart from its depletion due to excessive use, the quality has degraded due to transport of various organic and inorganic pollutants to ground water. Rajasthan is facing both the problems of quantity and quality of potable ground water. Water and health of living organisms are directly related. The occurrence of high fluoride concentration in ground water has now become one of the most important health related issues in many parts of western Rajasthan. In Rajasthan nearly 5 percent of country's human population has been recognized as a State endemic for Fluorosis. Due to excessive fluoride concentration in ground water cases of both dental and skeletal fluorosis are quite prevalent. Most severely affected areas are of Jodhpur, Nagaur, Barmer, Dungarpur, Tonk, Dausa, Sirohi, Udaipur, Sawai Madhopur and Karauli district. It seriously affects bones and causes problems like joint pain, muscular pains and non-skeletal manifestations.

In the present study fluoride concentrations in surface and ground water samples were determined in eight villages of Jodhpur district in India. Thirty-eight samples were collected and analyzed for fluoride content along with pH, electrical conductivity, total dissolved solids (TDS), total hardness, total alkalinity, chlorides (Cl<sup>-</sup>), sulfates (SO<sub>4</sub><sup>-</sup>) and nitrates (NO). Fluoride concentrations in surface and ground water samples of these villages varied between 1.5and8.0 mg/L. Groundwater samples contained high concentrations of fluorides compared to open well and pond water samples, which could be a major source of fluoride in water. Since the geological formation of this area consists of fluorite and fluoropatite. From the data, it is evident that the population in the study area is severely affected by fluorosis. Dental and skeletal fluorosis and deformation of bones in children as well as adults were observed in the study area indicating the consequences of excess fluoride

Therefore, for sustainable health and development, immense and immediate efforts are required to combat the problem. In the present communication the extent of problem, distribution of various physic-chemical parameters, their health effects, and remedial measures will be discussed comprehensively.

# 112. Thermodynamic and transport studies of some divalent transition metal sulphates and magnesium sulphate in water and binary aqueous mixtures of diethylene glycol

### R.C. Thakur and Ravi Sharma

# Department of Chemistry, School of Physical Sciences, Lovely Professional University, Phagwara, Punjab.

Viscosities of some divalent metal transition sulphate, viz. magnese sulphate, cobalt sulphate, nickel sulphate, copper sulphate, zinc sulphate and magnesium sulphate have been determined in

water and in binary aqueous mixtures of diethylene glycol (5, 10, 15, 20% by weight of DEG) at different temperatures (298.15, 303.15, 308.15, 313.15 and 318.15K). The measured viscosity data has been analysed by using Jones – Dole equation and B-coefficient are determined. The obtained parameters have also been interpreted in terms of ion –ion and ion – solvent interactions. The result is also analysed using transition state theory. In the present study, all these transition metal sulphates and magnesium sulphate act as structure makers in water and in DEG+water systems.

# **113.** Growth of kinetic Alfven wave in presence of beam velocities in an inhomogeneous magnetosphere with loss cone distribution function

# Sunil Kumar and A. K. Dwivedi

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Kinetic Alfven waves are examined in the presence of electron and ion beam and an inhomogeneous magnetic field with general loss-cone distribution functions. The theory of particle aspect analysis is used to evaluate the trajectories of the charged particles. The expressions for the field-aligned currents, perpendicular currents (with respect to  $B_0$ ), dispersion relation and growth/damping rate are derived. The effect of steepness of loss-cone distribution, electron and ion beam and in homogeneity of magnetic field is discussed. The plasma under consideration is assumed to be anisotropic and with low- $\beta$ . The results are interpreted for the space plasma parameter appropriate to the auroral acceleration region of the earth's magnetosphere. The theory is based on Dawson's theory of Landau damping for the analysis of electrostatic and electromagnetic waves. The advantage of this approach is its suitability for dealing with auroral electrodynamics and energy exchange by wave-particle resonant interaction.

In the present work we compute the effect of ion and electron beams and magnetic field in homogeneity on kinetic Alfven wave with general loss-cone distribution functions. The expressions for growth rate are derived. The results are interpreted for the auroral acceleration region of the earth's magnetoplasma. The variations of growth rate versus  $k_{\perp}\rho_i$  for different values of  $\varepsilon_{\rm B}$  taking the V<sub>De</sub>/ $\Omega_i$  and J constant. It is seen that higher magnetic gradient increases the growth rate. The destabilizing effect of magnetic field in homogeneity is clear as growth rate increases with  $k_{\perp}\rho_i$  and at higher values of  $k_{\perp}\rho_i$  becomes maximum. The variation of growth rate for different values of V<sub>De</sub>/ $\Omega_i$  taking the  $\varepsilon_{\rm B}$  and J constant, growth rate increases, V<sub>De</sub>/ $\Omega_i$  enhanced the growth rate of the wave. Whereas the growth rate for different values of J taking the V<sub>De</sub>/ $\Omega_i$  and  $\varepsilon_{\rm B}$  constant, again increases and becomes maximum at higher  $\varepsilon_{\rm B}$ .

# 114. Biogeochemical and Geobotanical Prospecting of Pd – Zn deposit of Zawar mines area dist Udaipur (Rajasthan)

### S.K. Trivedi

Department of Geology, Faculty of Science, J.N.Vyas University, Jodhpur, Rajasthan.

The metalliferous zawar area about (67 sq. km.) in situated between the 24' 18' 48'' and 24'22'48'' and long. 73'40. and 73'45'24''E, at a distance of about 43 km from Udaipur. The various hills of this area are known by local names and are rich in pd, zn and related minerals. Biogeochemical and Geobotanical studies on the Pd-Zn deposit of Zawar mines were carried out.

First, to use plant involving visual observation and second to analyze chemically, various part of the plants was prospected. The use of floral species have high capacity to uptake metal in their organs among others, so they can use as a guide or good indicator plant for particular mineral content of the plant cover in order to detect mineralization. The Pb-Zn concentration in plant and soil has been evaluated among the different species namely: *Capparis serpiaria, Euphorbia tirucalli, Hibiscus gibbsoni, Hyptis suaveolens, Pongamia, pinnata, Leucaena leucocephala, Sesamum indicum* and *Zinnia elegans*.

### 115. Geomorphology, Origin and Source of Salt in Saline Lakes of Rajasthan

### S.R. Jakhar

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Saline lakes/playas are present throughout northwestern Rajasthan (in the Indian Thar Desert) specifically in the region west of the Aravalli Mountains, i.e. the region in the rain shadow for the south-west monsoon. The area has a negative water balance with rainfall of 100–500 mm/a and the higher average annual temperature ranges between  $45^{\circ}$  and  $50^{\circ}$  C hence the potential evapotranspiration ranging between 1500-2000 mm/a. There are about 20 salt playas/lakes, out of these 8 to 9 are producing salt about 12 lakh tonnes (8% of total production of India) every year from their brine. These highly saline playas are characterized by alkaline brines, centripetal drainage and absence of any outflow. The basements of the lakes are mainly composed of rocks of Precambrian age and they are covered by silty clays, sands, gravels with intercalations of halite, gypsum, calcite etc. of Quaternary age. The isotopic studies on these playa brines, carried by some workers, disprove their marine connection and suggest that they are replenished by rainwater and surface runoff. They have confirmed meteoric origin and related the higher salinity to the dominance of evaporative conditions. Apart from tectonic origin, it is also suggested that during the late Pleistocene excessive siltation at the river and formation of sand dunes across the river channels led to the formation of these shallow (1–3m depth) closed basin playas.

### 116. Comparing the magnetic influence of Eu and Cu on SnO<sub>2</sub> nanoparticle host

### Pawan Chetri and Amarjyoti Choudhury

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Structural and magnetic property of Eu and Cu doped  $SnO_2$  nanoparticles are studied by XRD and magnetic measurement systems.  $SnO_2$  system in nano-regime found to show an appreciable amount of magnetism. The inclusion of these two different entities as 1% dopant enhances the magnetism in their respective systems. The magnetic moment achieved by Cu 1% doped  $SnO_2$ nanoparticles is far more than that achieved by a Eu 1% doped  $SnO_2$  nanoparticles. The reasons for the difference in magnetic influence by these two dopants are discussed thoroughly. We did some atomistic level theoretical calculation based on density functional theory to cross check the experimental findings.

### 117. Eco- Friendly approach for metropolitan pollution control

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Pollution is the darker side of technological development. The urban air pollution has increased all over the world in past few decades to an alarming state. Indian cities have also reported a very high level of air contamination in recent surveys done by air pollution monitoring authorities. The present paper gives an over view of air pollution all over the world with special emphasis to the dangerous levels of air pollution indices in Indian cities. It highlights the causes of this scenario. The statistical data of motor vehicle born air pollution is correlated with the changing life style and attitude of urban residents. It proposes the comprehensive greener and cleaner approach for air pollution control in urban residential localities integrating various aspects of pollution control together. The importance of town planning in air pollution control in urban localities, and significance of mass transport systems is described. Importance of bicycle revolution is also discussed. It suggests the use of advanced information technology based air pollution monitoring system also. Such a system can provide effective means for urban air pollution monitoring and shall enable pollution control authorities to adopt suitable means of air pollution control in real time.

# **118.** Supercapacitance behaviour of conducting polyaniline/expanded graphite nanocomposites prepared by in situ oxidative polymerization

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An electrode material based on polyaniline (PANI) with expanded graphite (EG) sheets was synthesized via *in situ* oxidative polymerization of aniline in the presence of various proportions (5% and 10%) of EG. The samples were characterized by FTIR, SEM, TGA, XRD and electrical conductivity measurements. FTIR and XRD revealed the interaction between EG and PANI. The dc electrical conductivity (11.5 S/cm) of the prepared composite was dramatically enhanced compared to pure PANI (1.32 S/cm). The high specific capacitance of PANI/EG composite was obtained 460.4 F/g in the potential range from 0 to 0.50 V at 2 mA compared to 245.2 F/g of pure PANI by Galvanostatic charge - discharge analysis. The incorporation of EG into PANI matrix have a pronounced effect on the conductivity and electrochemical capacitance performance of the PANI/EG nanocomposites.

#### 119. Future of nanotechnology in memory devices

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Till now, there have been chips made from silicon, with innumerable transistors on it. But according to Moore's law, the silicon chips are now falling small for placing transistors. Therefore, the chip manufacturing has now switched over to nanomaterials, and has got success in finding several nanoscale substitutes of silicon in making chips. Substitutes like Indium Gallium Arsenide, Vanadium Oxide Bronze, carbon nanotubes etc. have been predicted by scientists. It has been found that these nanoscale substitutes have more information carrying capacity at much low power consumption in comparison to silicon, which also proves that they are more economical to use, with much faster speed. The synthesis techniques of these nanoscale substitutes has also been developed, which have also been discussed. Thus, within the next two decades, computer chips made from these

predicted substitutes will completely replace currently used silicon chips. The future of nanocomputing is speeding up at an unexpected rate.

# **120.** Induction of plasmonic resonance and enhancement of the electrical conductivity in the columnar mesophase of discotic liquid crystalline material

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Experimental characterization of the composites of colloidal Gold Nano Particles (GNPs) in the columnar discotic liquid crystal namely Hexabutyloxytryphenylene (HAT4) has been carried out. Thermophysical properties have been investigated by differential scanning calorimetry (DSC), UV-Vis spectroscopy, polarizing optical microscopy (POM) and dielectric spectroscopy. GNPs have been dispersed in the concentrations of 0.2 wt% in pure HAT4. Phase sequences as obtained from DSC and POM for pure HAT4 and its composite with GNPs are as follows:

Pure HAT4: Cr-(86.3 °C)-Col<sub>hp-</sub>(145.3 °C)-Iso

HAT4+0.2% GNPs: Cr-(85.9 °C)-Col<sub>hp-</sub>(137.7 °C)-Iso

The above phase sequence suggests that the  $\text{Col}_{hp}$ -Iso transition temperature is depressed; however melting temperature remains almost same. In the columnar mesophase DLCs behave like onedimensional conductor. Our studies show that the colloidal GNPs increase the ionic conductivity of HAT4 by about two orders of magnitude in columnar phase. At 90 °C the ionic conductivity of pure HAT4 is  $7.8 \times 10^{-10}$  Sm<sup>-1</sup> and that of composite sample is  $2.9 \times 10^{-7}$  S-m<sup>-1</sup>. At 135 °C the ionic conductivity of pure HAT4 is  $3.7 \times 10^{-9}$  S-m<sup>-1</sup> and the composite  $9.7 \times 10^{-7}$  S-m<sup>-1</sup>. These results suggest that GNPs improved stacking of the disc-like molecules within the columns and possessing high charge mobility. Dielectric permittivity measured parallel to the column axis in the homeotropic aligned sample is increased. In case of pure and dispersed sample permittivity increases from 3.0 to 3.2 at a temperature 90 °C and frequency 100 kHz. Increase of conductivity may be exploited to enhance efficiency of photovoltaic cells.

# 121. Synergistic amalgamation of metal oxide nanoparticles and liquid crystal for display applications

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Changes in the electro-optical, thermodyanamical and dielectric properties of 4-pentyl-4'cyanobiphenyl (5CB) due to dispersion of metal oxide nanoparticles have been studied. Dielectric spectroscopy for planar and homeotropic aligned samples has been carried out in the frequency range 1Hz–40 MHz. Polarized light microscopy images confirm the proper alignment of molecules in the nematic phase. Threshold and switching voltages, dielectric anisotropy, relaxation frequency, dielectric strength and activation energy of an observed relaxation mode have been determined as a function of concentration of nanoparticles. The electro-optical experiments show that the steepness of the transmission–voltage curve improves while threshold voltage for Freederickz transition decreases due to dispersion. Dielectric studies show that the presence of alumina nanoparticles decreases the effective longitudinal component ( $\varepsilon'_{\parallel}$ ) of dielectric permittivity while has no effect on transverse component ( $\varepsilon'_{\perp}$ ) of dielectric permittivity. The dielectric relaxation study of the homeotropic aligned samples shows that the relaxation frequency corresponding to the flip-flop motion of the molecules about their short axes decreases due to dispersion of nanoparticles.

#### 122. Compact I-shaped slot loaded half disk patch antenna for dualband operation

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#### Department of Electronics and Communication, University of Allahabad, Allahabad-211002.

This paper presents a generalized approach to design compact microstrip patch antenna for dualband operation by introducing the two L-shaped slot in the half circular disk patch and found dual resonance frequency at 8.51 GHz and 13.81 GHz and the bandwidth of the proposed antenna for lower and upper resonance frequency is found to be 4.39 % and 7.31 % respectively. By introducing the two shorting pin resonance frequency is shifted to lower side and found to be 2.5 GHz and 5.05 GHz. It is easy to adjust the higher and lower band by changing the dimensions of notch and slot. The frequency ratio is found to be 1.622 while with shorting pin the frequency ratio is increases 2.02. The theoretical results are compared with IE3D simulation results which are in good agreement.

## 123. Ediacaran Microbial Mat-Induced Sedimentary Structures (MISS) from the Siliciclastic Girbhakar Sandstone of Marwar Supergroup, Bhopalgarh area, District -Jodhpur, Rajasthan, India.

V.S. Parihar, V. Gaur, S.L. Nama and S.C. Mathur

#### Department of Geology, Jai Narain Vyas University, Jodhpur -342005.

Girbhakar Sandstone is youngest sequence of the Jodhpur Group of Marwar Supergroup known as Girbhakar Sandstone Formation. It is well exposed in and around Bhopalgarh area and situated about 70kms North-East of Jodhpur. Under present investigation author's report well - preserved Microbial Mat -Induced Sedimentary Structures (MISS) from western block of Girbhakar Sandstone of Marwar Supergroup in Bhopalgarh area. These Microbial mat -induced sedimentary structures (MISS) are identified as Kinneyia mat structures, Arumberia banksi mat structures, Wrinkle mark structures, Mat deformed structures, Mat related mat growth and Mat sand surface structures. These Mat structures are, occur in patches on the top and sole of various colored light brown, brown, pinkish white, brownish and pinkish to purple fine and medium to fine grained sandstone bedding surfaces. The Wrinkle mark structures and Kinneyia ripple sedimentary structures were commonly found in Precambrian siliciclastic facies. These structures may response of microbial activity and suggested that the Mat-induced sedimentary structures were formed when the sand devoid of mud content was made cohesive by the presence of microbial mats. The presence of Microbial Mat - induced sedimentary structures were represents Ediacaran period on the basis of its worldwide occurrences and can be assigned Ediacaran age to the Girbhakar Sandstone of Bhopalgarh area.

# 124. *Ophiomorpha* and *Margaritichnus* Trace Fossils from Bariyara section of Fatehgarh Formation of Barmer Basin, Western Rajasthan, India.

V.S. Parihar, S.L. Nama, C.P. Khichi, N.S. Shekhawat and Snehlata Mathur *Department of Geology, Jai Narain Vyas University, Jodhpur -342005.* 

The present paper is first reporting of *Ophiomorpha* and *Margaritichnus* trace fossils from the Bariyara section of the Fatehgarh Formation of Barmer Basin located about 6km south of Fatehgarh town which situated about 70kms north of Barmer on NH-65. The Ophiomorpha trace fossils are found in white colored fine grained calcareous sandstone from lower siliciclastic sequence where as Margaritichnus trace fossils occurs in dark brown colored medium to fine grained ferruginous sandstone of middle phosphorite -siliciclastic sequence of the Fatehgarh formation of Barmer Basin. The Ophiomorpha trace fossils were mainly produced by crustaceans and shrimps where as Margaritichnus trace fossils were interpreted as worm -like sediment eating animals such as Sipuncalid ?; Priapulid ? or possibly hydrozoa. The ichnological and sedimentological investigations suggests near coastal shallow water depositional environment for the Fatehgarh Formation of the Barmer Basin. The Margaritichnus trace fossils (Permian -Cretaceous) and Ophiomorpha trace fossils (Permian –Recent) have long ranging however, very difficult to assign a particular age but the associated facies contain Microvertebrate assemblages has earlier recorded from the same section (Mathur et. al., 2006) which assigned Cretaceous age to the Fatehgarh Formation of the Barmer Basin. The paper embodies various aspects including geological attributes, systematic ichnology and depositional environment of the Fatehgarh Formation.

# 125. Sarnu Formation of the Barmer Basin, western Rajasthan, India: Implication for Hydrocarbon prospects and Economic significance

### C.P.Khichi

### Department of Geology, J.N.V. University, Jodhpur, Rajasthan.

The Barmer Basin is a Mesozoic-Tertiary intra-cratonic rift basin located in the heart of the Thar Desert in the western part of India with around 6,000 m of sediment fill overlying Proterozoic basement. The sediments of the Barmer basin are categorize in to pre-rift, syn-rift and post-rift sediments as the basin is bounded by various faults (rift). These rifts were resulted due to the breakup of the Indian craton from the Gondwana Super continent in Early Cretaceous time and followed by a significant tectonic history to form source, reservoir and structural trap rocks for hosting the Hydrocarbon deposits. The syn-rift sediments are exposed at Sarnu, Barmer and Fatehgarh area. They are Sarnu Formation, Barmer hill Formation and Fatehgarh Formations. The Sarnu hill Formation comprising thinning and fining upward sand bodies with intervening siltstones. This formation is exposed at the south-western margin of the Barmer basin. Sisodia and Singh (2000) correlate this formation with Jodhpur Group of Late Proterozoic age. Earlier Dasgupta, (1973) mapped this formation which contains plant fossils and assigned Early Cretaceous age.

Cairn India Ltd. first came into Rajasthan in 1997 for hydrocarbon exploration and more than two dozen wells were discovered since 2004. These fields are Mangla, Aishwarya, Bhagyam, Vijya and Kameshwari and a further to date, 25 discoveries holding an estimated 7.3 billion barrels of oil (boe) and 175,000 barrel oil per day production from the Barmer Basin of which cairn India is operating 70% holding and 30% by ONGC. The siliciclastic sediments of Sarnu Formations mainly form the

reservoir rocks for the hydrocarbon occurrences of the Barmer Basin. The Sandstone of Sarnu Formation has significant implications pertaining to hydrocarbon occurrences. The paper embodies facies analysis, depositional environment and hydrocarbon prospect of the Sarnu Formation.

### 126. Barmer hill Formation of the Barmer Basin, western Rajasthan, India: Implication for Hydrocarbon prospects and Economic significance

### N.S.Shekhawat

#### Department of Geology, J.N.V. University, Jodhpur, Rajasthan.

The Barmer Basin is a Mesozoic-Tertiary intra-cratonic rift basin located in the heart of the Thar Desert in the western part of India with around 6,000 m of sediment fill overlying Proterozoic basement. The sediments of the Barmer basin are categorize in to pre-rift, syn-rift and post-rift sediments as the basin is bounded by various faults (rift). These rifts were resulted due to the breakup of the Indian craton from the Gondwana Super continent in Early Cretaceous time and followed by a significant tectonic history to form source, reservoir and structural trap rocks for hosting the Hydrocarbon deposits. The syn-rift sediments are exposed at Sarnu, Barmer and Fatehgarh area. They are Sarnu Formation, Barmer hill Formation and Fatehgarh Formations. The Barmer hill Formation exposed along the south - western boundaries of the basin. It rests unconformably on the basement of Malani Rhyolites. The Barmer hill Formation is comprised of fining upward sedimentary sequence of sandstone and clasts supported conglomerate.

Cairn India Ltd. first came in to Rajasthan in 1997 for hydrocarbon exploration and more than two dozen wells were discovered since 2004. These fields are Mangla, Aishwarya, Bhagyam, Vijya and Kameshwari and a further to date, 25 discoveries holding an estimated 7.3 billion barrels of oil (boe) and 175,000 barrel oil per day production from the Barmer Basin of which cairn India is operating 70% holding and 30% by ONGC. Sandstone of Barmer hill Formation considered equivalent to lower siliciclastic sequence of the Fatehgarh Formation of Cretaceous age also formed reservoir rocks in the southwestern margin of the Basin. Dasgupta and Compton assigned Cretaceous age for the Barmer hill Formation which contains angiosperm flora and pollen assemblages along with leaves and pieces of stems. Sandstone of the Barmer hill Formation have good permeability and porosity and are quartzose in nature therefore considered as good oil reservoirs. From the development drilling results and further evaluation of the Barmer Hill Formation which overlying the Mangala and Aishwariya Fatehgarh sandstone reservoirs, identified significantly increased potential in the basin. Fields in other parts of the Barmer Hill are being under development and have demonstrated recovery factors in the range of 7% to 20%. The estimated gross recoverable resources from the Barmer Hill (From Mangala and Aishwariya) and other fields have almost doubled to 140 mmbbls. Since the Barmer Hill oil reservoir is comparatively less permeable, the plan is to fracture horizontal wells in reservoir to optimize the well count and deliver high production rates. The present paper embodies geological attributes and hydrocarbon prospective of the Barmer Hill Formation of the Barmer Basin.

### 127. Spin Squeezing by the action of ladder operator on an atomic coherent state

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<sup>1</sup>Department of Physics, Udai Pratap College, Varanasi – 221002. <sup>2</sup> Department of Physics, Bhavan's Mehta Mahavidyalaya (V S Mehta College of Science), Bharwari, Kaushambi – 212201. Spin squeezing is an important non-classical effect in quantum optics with potential applications in metrology and quantum information processing. Such type of squeezing can be generated interaction of radiation with a collection of atoms using various atomic models. The Dicke model is an important atomic model which describes interaction of a quantized radiation field with N two-level atoms located within a distance much smaller than the wavelength of the radiation. In the present paper, we study the generation of spin squeezing using the action of lowering ladder operator on an atomic coherent state for a collection of N two-level atoms in ground states considering Dickle model. We investigate the conditions on the various interaction parameters for occurrence of spin squeezing. We also discuss the variations of spin squeezing factor with various relevant parameters.

# 128. Perovskite of $Ba_{0.2}Sr_{0.8}Ni_{0.8}Fe_{0.2}O_{3-\delta}$ as a Cathode material for intermediate temperature Solid oxide fuel cell and its Electrochemical and microstructural characteristics

Vandani Rawat and Mahesh Chandra Chattopadhayaya Department of Chemistry, University of Allahabad, Allahabad- 211002.

The Nickel containing cobalt free Perovskite oxides of  $Ba_{0.2}Sr_{0.8}Ni_{0.8}Fe_{0.2}O_{3-\delta}$  (BSNF) were synthesized as a new cathode material for intermediate temperature by Glycine nitrate process. Nitrates of Ba, Sr, Ni and Fe were used as precursor and Glycine as self-combustion reaction matter. X-Ray diffraction and Scanning electron microscopy measurement were carried out of BSNF cathode material. The Pellets were sintered at 900°C for 2hr and electrochemical impedance was measured at different temperatures. The conductivity measurement showed the highest value as 0.081 S cm<sup>-1</sup> at 650 °C. The minimum Area specific resistance value measured was 0.783  $\Omega$ cm<sup>2</sup> at 650 °C. The results shows that BSNF can work as a good alternative of cobalt free, low cost and intermediate temperature cathode material for Solid oxide fuel cell.

# **129.** Decoloration treatment of a hazardous dye, Methylene blue from aqueous solutions using functionalized nanoalumina

Sushmita Banerjee and M. C. Chattopadhyaya Department of Chemistry, University of Allahabad, Allahabad – 211002.

The performance of humic acid functionalized nanoalumina (HAFA) was investigated in adsorptive removal methylene blue dye from an aqueous solution by performing batch experiments. The adsorbent was characterized with Fourier transform infrared spectroscopy and scanning electron microscopy. The adsorption behavior and operational parameters were examined by monitoring various process variables namely the pH, initial dye concentration, contact time, temperature, adsorbent dosage and ionic strength. Maximum removal percent of 98% observed at a temperature of 313 K, pH 8.0 and initial dye concentration of 10 mg/L. The isotherm data was interpreted by fitting them into various adsorption isotherm models such as Langmuir, Freundlich and Redlich Peterson moreover data found to be highly consistent with the Redlich-Peterson model. The estimation of thermodynamics parameters suggest that dye adsorption process is spontaneous and endothermic in nature. The kinetics data was represented by Pseudo-first order model and Pseudo-second order model. The study of sorption dynamics conveyed that adsorption process is governed by film

diffusion mechanisms. The experimental results confirmed that HAFA is a promising adsorbent for the adsorptive removal of dye methylene blue from aqueous solutions.

# **130.** Studies of Adsorption performance of Bio-nanocomposite for the removal of methyl orange dye from aqueous solution

#### Amita Jaiswal

# Environmental Chemistry Research Laboratory, Department of Chemistry, University of Allahabad, Allahabad -211002.

Layered double hydroxides (LDHs), anionic clay was prepared by Co-precipitation method at constant pH and modified it with chitosan. The characteristics of chitosan intercalated layered double hydroxides (CTS/LDHs) was examined by X-ray diffractometer (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), Transmission Electron Microscopy (TEM), and Thermogravimetric Analysis (TGA). The adsorption performance of this material for hazardous dye, methyl orange (MO) was studied. Experiments were conducted at different initial concentration (50-300ppm), different adsorbent dose (0.1-1.0g), temperature (303-323K), pH (2-10) and different contact time (15-20 min). Adsorption kinetics were best described by the pseudo-second order model. The equilibrium data were better fitted by Langumir isotherm compared to Freundlich isotherm. The adsorption of methyl orange increased with operating temperature, indicating as endothermic process. Regeneration of the bio-nanocomposite was feasible. These results suggested that the CTS/LDHs can be used as an absorbent for the removal of MO from aqueous solution.

# 131. Humic acid (HA) coated Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles for removal of malachite green from aqueous solutions: Kinetics, equilibrium and spectroscopic analysis

Ravindra Kumar Gautam, Pavan Kumar Gautam and J.D. Pandey

# Environmental Chemistry Research Laboratory, Department of Chemistry, University of Allahabad, Allahabad -211002.

Humic acid (HA) coated Fe<sub>3</sub>O<sub>4</sub> nanoparticles (Fe<sub>3</sub>O<sub>4</sub>/HA) were synthesized by Coprecipitation method and characterized for TEM, SEM-EDS, XRD, FTIR, TGA/DTG, BET surface area, VSM, SQUID and through the determination of  $pH_{zpc}$ . The Fe<sub>3</sub>O<sub>4</sub>/HA nanoparticles was used for the removal of malachite green from aqueous solutions. The removal of malachite green is strongly dependent on pH of the medium. The process was very fast initially and the maximum adsorption was observed within 30 minutes of contact time. The kinetics of the removal, tested with pseudo-second – order and intra-particles diffusion model, showed better agreement with pseudo-second-order rate kinetics. This adsorption data was modeled with Langumir and Freundlich isotherms. Thermodynamic studies have also been performed. The results have established good potentiality for Fe<sub>3</sub>O<sub>4</sub>/HA nanoparticles to remove malachite green from aqueous solutions.

# **132.** Adsorption of Tartrazine onto biosorbent of *Pongamia pinnata* seed pod: Kinetic, equilibrium and mechanistic modeling

# Pavan Kumar Gautam, Ravindra K. Gautam, Sushmita Banerjee and J.D. Pandey *Department of Chemistry, University of Allahabad, Allahabad- 211002.*

Adsorption of a food dye Tartrazine onto biosorbent of *Pongamia pinnata* seed pod has been studied on aqueous solutions. The batch adsorption experiments were conducted using simulated aqueous solutions and the effects of initial dye concentration, pH of solution, contact time and temperature were investigated. The prepared biosorbent was characterized using FTIR, SEM, elemental analysis and through the determination of  $pH_{zpc}$ . The equilibrium data were modelled with Langmuir and Freundlich isotherms. The rates of adsorption were found to confirm to the pseudo-second-order kinetics with good correlations (R<sup>2</sup>>0.99). The thermodynamic studies showed that the Tartrazine-biosorbent system is spontaneous, exothermic and favourable in nature.

# **133.** Efficacy of integrated approach of ground water management in Rajasthan for sustainable socio-economic development

### D.D. Ozha

#### Chemical Laboratory, Ground water development, Jodhpur-342003.

Water is a precious natural resource and is essential for both life as well as livelihood. Unlike many other commodities it cannot be manufactured and the given resource has to be preserved and managed in a systematic, scientific and sustainable way. India is facing water stress in many of its states, particularly in Rajasthan. Providing access to clean and safe drinking water to more than 55 million population of the state spread over the entire length and breadth of this huge state is a serious challenge, more so, when ground water, which is source of dependence, is rapidly depleting every year. Periodic occurrences of droughts and famines have further aggravated the problem. Poor availability of perennial surface water sources, less recharge, depleting water table and deteriorating water quality make the drinking water supply still more difficult. Out of 32 districts in Rajasthan, water table is depleted in 29 districts. It is obvious that as a consequence of depletion in ground water table and other geo-chemical factors, increased concentration of nitrate, fluoride and salinity in ground water have adversely affected the lives of human beings, floras and faunas. This has ultimately adversely affected the socio-economic status of the inhabitants too. Therefore, for sustainable health and socio-economic development integrated approach of water resource management comprising mandatory Roof Top Rainwater Harvesting, Rejuvenation and proper maintenance of traditional water bodies, judicious use of water in agriculture and domestic purpose, construction of ground water recharge structures, Jal Chetna (water awareness) through education using audio-visual aids and enforcement of ground water legislation are some of the managerial methods to be adopted for the welfare of mankind. Participation of stakeholders and community as well as NGOs plays an important role in the management of this natural resource.

# **134.** Using dried biomass of Parthenium for the removal of malachite green dye from aqueous solution

#### Praveen Rai and Vriddhi Nigam

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The objective of our present investigation were to study the potential of dried biomass of Parthenium (DBP) as a low cost adsorbent to remove the malachite green dye from aqueous solution and also the study of equilibrium isotherms, kinetics of the process and the rate of adsorption. For this purpose a batch adsorption experiment was carried out to observe the effect of pH, contact time, initial metal concentration, adsorbent dose and temperature on the adsorption. Equilibrium data were fitted to Langmuir and Freundlich isotherm models. The adsorbent was characterized by Fourier Transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscopy (SEM) to study the functional groups and surface morphology of the adsorbent respectively. Results showed that DBP has high potential as an adsorbent for the removal of malachite green dye from aqueous solution.

# **135.** Preparation, characterization and batch adsorption study of activated carbon for the removal of heavy metals from aqueous solution

Vriddhi Nigam and Praveen Rai

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In the present investigation an activated carbon was prepared from low cost plant material and their application in waste water treatment. For this purpose the dried biomass of Thuja (*Platycladus orientalis*) commonly known as morpankhi has been used to prepare activated carbon using perchloric acid. The activated carbon prepared from the dried biomass of *Platycladus orientalis* (ACDBPO) was characterized by Fourier Transform Infrared Spectrophotometer (FT-IR) and scanning electron microscopy (SEM) to study the functional groups and surface morphology of the material respectively. To study the potential of activated carbon derived from dried biomass of Thuja for the removal of Ni from the aqueous solution, a batch adsorption experiment was carried out to observe the effect of pH, contact time, initial metal concentration, adsorbent dose and temperature on the adsorption. Equilibrium data were fitted to Langmuir and Freundlich isotherm models for equilibrium study. Data obtained from batch experiment has been also used for kinetics and thermodynamics study. Results showed that ACDBPO has been found to have high potential as an adsorbent for the removal of crystal violet dye from aqueous media.

### 136. Heteropolyacid catalyzed synthesis of 8-methyl-2-aryl/alkyl-3oxabicyclo[3.3.1]non-7-ene derivatives through (3,5)-oxonium-ene reaction

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A variety of aldehydes undergo a smooth coupling with (4-methylcyclohex-3-en-1-yl) methanol in the presence of 2 mol % of phosphomolybdic acid in dichloromethane to afford 3-oxabicyclo[3.3.1]non-7-ene in good yields through 3,5-oxonium-ene cyclization under mild conditions. The use of inexpensive, nontoxic, and readily available heteropoly acid catalyst makes this method simple, convenient and environmental friendly.