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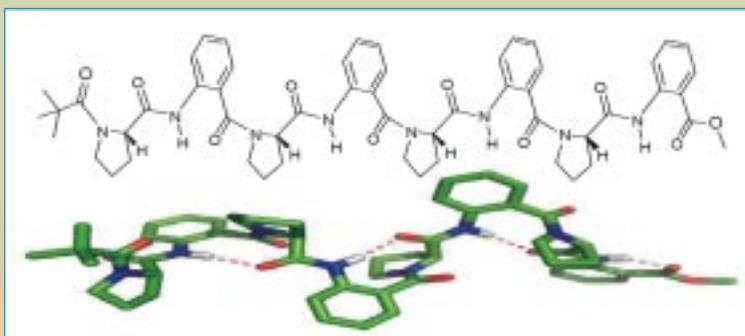


## Synthetic Protein Structures

Proteins — the long chains of amino acids, connected through peptide (amide) bonds — are critical components of every living cell. These vital biomolecules, have endless cellular functions that include catalyzing biochemical reactions, activating genes, enabling motion, etc.

Proteins exert their function by folding into intricate globular structures — a phenomenon that continues to grab the attention of scientists. Protein folding is integral to the functional activity of proteins. In addition to the structural/conformational preferences of the individual amino acids of a protein, the major contributory/dictating forces in protein folding are non-covalent interactions such as hydrogen bonding, Van der Waals forces and ionic interactions. It is widely anticipated that the ability to specify and design artificial/synthetic proteins (proteins containing unnatural amino acid building blocks) would eventually pave the way for developing artificial protein enzymes for use as medicines or as industrial catalysts. However, efforts in engineering new protein structures endowed with novel properties require considerable understanding of the intricate factors involved in protein secondary structure (conformation) modulation.

Scientists from National Chemical Laboratory (NCL), Pune, ([www.ncl-india.org](http://www.ncl-india.org)) have demonstrated that synthetic oligomers derived from conformationally constrained aromatic-aliphatic amino acid repeat motifs, show high degree of conformational ordering. Such oligomers form helical conformation reminiscent of protein helices. These findings were published in the recent issue of the Journal of American Chemical Society.



Conformationally ordered right-handed helical architecture derived from Ant-Pro hybrid building blocks



According to Dr Gangadhar J. Sanjayan from Organic Chemistry Division of NCL, the ability to specify a desired folded protein conformation with the use of hybrid building blocks would offer powerful scientific and practical benefits. First, such a 'hybrid' strategy would considerably expand the structural repertoire of synthetic protein structures. Secondly, one can design synthetic structures for intervening protein-protein interactions, an idea which is under active pursuit in the laboratory. For more information, please contact Dr G. J. Sanjayan

For further reading:

Sequence-Specific Unusual (1→2)-Type Helical Turns in  $\alpha/\beta$ -Hybrid Peptides, Panchami Prabhakaran, Sangram S. Kale, Vedavati G. Puranik, P. R. Rajamohanan, Olga Chetina, Judith A. K. Howard, Hans-Jorg Hofmann and Gangadhar J. Sanjayan, *Journal of the American Chemical Society* 2008, **130** (52), 17743-17754.

Sheet-Forming Abiotic Hetero Foldamers, P. K. Baruah, N. K. Sreedevi, B. Majumdar, R. Pasricha, P. Poddar, R. Gonnade, Ravindranathan and G. J. Sanjayan, *Chemical Communications* 2008, 712-714.

## Evidence for Early Uplift of Himalayas within the Central Indian Ocean

The discovery by Indian and British scientists that the Earth's strong outer shell — the 'lithosphere' — within the Central Indian Ocean began to deform and fracture 15.4-13.9 million years ago, much earlier than previously thought, impacts our understanding of the birth of the Himalayas and the strengthening of the Indian-Asian monsoon.

India collided with Asia around 50 million years ago as a result of plate tectonics — the large-scale movements of the lithosphere — which continues to this day. The new study, published in the March issue of the *Geological Society of America Journal of Geology*, focuses on the tectonics-related deformation of the lithosphere below the Central Indian Ocean.

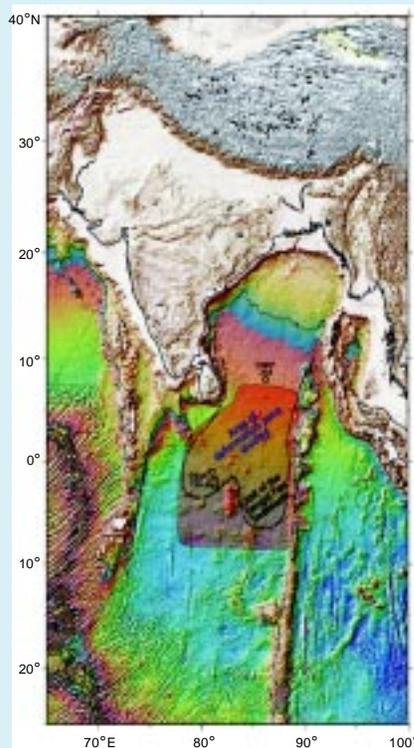
According to Dr K.S. Krishna and his team working at the National Institute of Oceanography (NIO), Goa, "Compression of the lithosphere has caused large-scale buckling and cracking." "The ocean floor has been systematically transformed into folds, 100-300 kilometres long and 2,000-3,000 metres high, and there are also regularly spaced faults or cracks that are evident from seismic surveys and ocean drilling," say the experts.

The onset of this deformation marks the start of major geological uplift of the Himalayas and the Tibetan Plateau, some 4,000 km further to the north, owing to stresses within the wider India-Asia area. Some studies indicate that it began around 8.0-7.5 million years ago, while others have indicated that it started before 8.0 million years ago, and perhaps much

earlier.

This controversy has now been dealt by Dr Krishna and his British colleagues Prof. Jon Bull of the University of Southampton, and Prof. Roger Scrutton of Edinburgh University. They have analyzed seismic profiles of 293 faults (vertical cracks in the ocean floor) in the accumulated sediments of the Bengal Fan. This is the world's largest submarine fan, a delta-shaped accumulation of land-derived sediments covering the floor of the Bay of Bengal.

These scientists demonstrated that deformation of the lithosphere within the Central Indian Ocean started around 15.4-13.9 million years ago, much earlier than most previous estimates. This implies considerable



Himalayan uplift before 8.0 million years ago, which is when many geologists believe that the strong seasonal winds of the India-Asia monsoon first started.

“However,” says Dr Krishna, “the realization that the onset of lithospheric deformation within the Central Indian Ocean occurred much earlier fits in well with more recent evidence that the strengthening of the monsoon was linked to the early geological uplift of the Himalayas and Tibetan plateau up to 15-20 million years ago.”

Scientists believe that intensive deep-sea drilling within the Bengal Fan would provide better age estimates for the onset of deformation of the lithosphere in the Central Indian Ocean and concretize the recent findings. There are more weighty geological questions related to the geodynamics of the Indian Plate yet to be understood. Principal among these being the issue of how exactly did the ocean floor buckle and crack in space and time, and what will be the future course of this compressional activity in the Central Indian Ocean. Further scientists would like to gather new evidences for understanding of 1) why and how the Central Indian Ocean region has now become a site where mountains are rising up from the ocean floor and cracks are propagating within the crust; and 2) whether the present process could be a precursor to the formation of a subduction zone in the Central Indian Ocean.

The above research was funded by CSIR, and the United Kingdom's Royal Society and Natural Environment Research Council (NERC).

**For more information refer:**

- Early (pre-8 Ma) fault activity and temporal strain accumulation in the Central Indian Ocean, K.S. Krishna, J.M. Bull, R.A. Scrutton, *Geology*, March 2009, **37**, 227-230, doi: 10.1130/G25265A.

or contact Dr K.S. Krishna, Scientist, National Institute of Oceanography, Dona Paula, Goa- 403004, India; Email: krishna@nio.org, Phone: 91(0)832-2450384.

## Study of 'on water' Mechanisms of Organic Transformations

**W**ater is life's matter and matrix, mother and medium. 'There is no life without water.' (Albert von Szent-Györgyi Nagrapolt (1893-1986), Hungarian Biochemist, Nobel Prize for Medicine, 1937).

In a series of kinetic experiments, Dr Anil Kumar and his student working at the National Chemical Laboratory (NCL), Pune, ([www.ncl-india.org](http://www.ncl-india.org)) have observed the effect of salt additives for organic reactions taking place in heterogeneous aqueous media. The results thus obtained take us closer to the possibility of harnessing the power of hydrophobicity at the interface by offering an interesting paradigm about how water behaves at the interface.

It is well known that water has been used as the solvent of choice for the past millions of years by the most experienced chemist — the Nature. Yet, modern chemists are known to be wary of using water for synthetic purposes. In the recent past, organic chemists took great pains to exclude water, even in traces, from their reaction systems and preferred organic solvents for performing reactions. The growing awareness about the environmental hazards of the commonly used volatile organic compounds has forced the chemists to turn back to water. Water is environmentally benign, in addition to being cheap and readily available. So the disposal of its solvent vapours or solvent residues is not a problem.

The insolubility of the organic reactants in water or aqueous solutions was thought to be the most important hurdle in the industrial scale use of water as a solvent. But experiments have shown that effect of water on the heterogeneous reactions is exactly opposite. In fact, depending on the nature of the reaction, water was observed to accelerate most of the reactions dramatically on its interface if the reactants did not dissolve. This 'on water' approach developed by Sharpless and coworkers was instrumental in changing the perception of the scientific community. Many slow chemical transformations can progress much faster 'on water' as compared to the organic solvents. Complex organic molecules possessing biological activities can now be synthesized in the aqueous medium.

Very little is known about what drives the reactions so



fast at the interface between water and the organic compounds, though it is believed that the 'dangling' hydroxyl groups do the trick. The scientists at NCL, are trying to understand the molecular forces that accelerate the interfacial organic reactions. Dr Anil Kumar and his research group have been intrigued by the manifestation of hydrophobic effects in heterogeneous aqueous reaction systems resulting in rate acceleration. Realizing the tremendous potential of 'on water' strategy, Dr Anil Kumar and his student, Shraeddha Tiwari attempted to investigate the mechanistic aspects of such reactions.

NCL scientists chose a typical C-C bond forming organic reaction – between an aldehyde and a phosphorus ylide – known as the Wittig reaction. The ylide was insoluble in water and thus, provided the water-organic interface for the reaction. The application of kinetic and

thermodynamic tools then helped in unraveling the origin of the hydrophobic effect and the magnitude of its contribution in reaction progress. The study of such interfacial processes is a daunting task because of the difficulties in accuracy of analytical measurements and separation of individual rate-determining factors and extension of the mechanism to include the complexities of a heterogeneous process.

The most interesting observation from the experiments was that the addition of salts like lithium chloride and sodium chloride slowed down the reaction taking place in the aqueous suspensions. This was contrary to the effects of these salts on the rates of homogeneous aqueous reactions, where these salts are known to amplify the hydrophobicity and accelerate the reactions. The effect of these salts was inverted when the temperature was raised from room temperature i.e. 25 °C to 65 °C. At the higher temperature, the reaction went

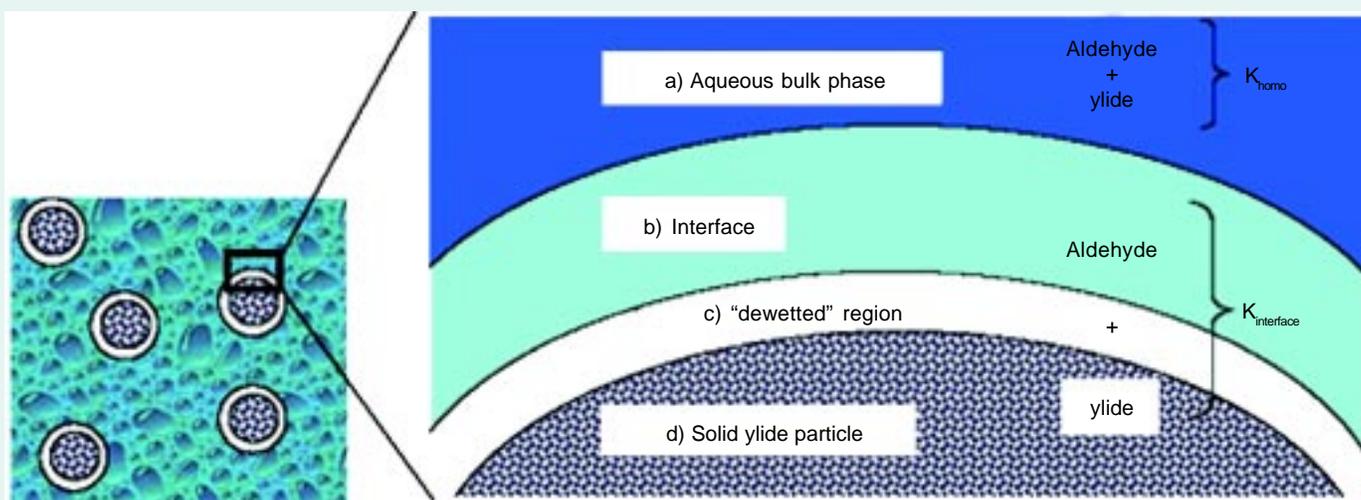
faster in the presence of the same salts. Such intriguing variation of salting effects with temperature had not been anticipated earlier. This unusual variation with temperature indicates that hydrophobic acceleration of reactions comprising 'on water' reactants is fundamentally different from that for homogeneous reactions.

The observations have led to interesting insights on the phenomenon of hydrophobicity. Further research in this area is being actively pursued, at the experimental as well as theoretical front. The study of 'on water' mechanisms of organic transformations will result in crucial advances in the extensive use of water as a reaction medium in large-scale industrial processes.

### For further reading:

S. Tiwari, A. Kumar, *Chem. Commun.* 2008, 4445.

For more information, please contact Dr Anil Kumar.



The Wittig reaction at the water- ylide interface



## Field Emission Scanning Electron Microscopy (FESEM) Facility at NAL

**S**urface Engineering Division of the National Aerospace Laboratories (NAL), Bangalore, is extensively engaged in the R&D activities related to nanostructured coatings, nanomaterials and surface properties of various new materials. Characterization of nanomaterials using electron microscope is vital for their microstructural properties. Conventionally, transmission electron microscope (TEM) is used to characterize the nanomaterials. Sample preparation for TEM is quite tedious and time consuming. Recent developments in the field of electron microscopy of the nanomaterials have led to the introduction of field-emission scanning electron microscope (FESEM). FESEM can be used to image all materials (conducting and non-conducting) with very high-resolution (approximately 1.0 nm). A state-of-the-art Carl Zeiss, Germany FESEM has been commissioned in NAL for imaging nanomaterials and nano-devices. Dr A. R. Upadhyaya, Director, NAL formally inaugurated the facility on 12 March 2009.

The FESEM system is also equipped with Oxford Instruments, UK, to make energy dispersive X-ray analysis (EDAX) of the material to be examined. Elements with atomic number greater than 5 can be detected by the high-resolution EDAX detector. Additional feature of the FESEM is that it is equipped with an electron back scatter diffraction (EBSD) set-up (also from Oxford Instruments, UK), which provides crystallographic information of the sample examined under FESEM.

This FESEM facility is open for all R&D activities of the laboratory and other R&D institutions/universities in India

## International Conference on Recent Trends in Environmental Impact Assessment (RTEIA- 2008) at NEERI



Dr T. S. Vijayaraghavan, delivering the Keynote Address.  
Seated on the dais (from left): Dr T. Chakrabarti, Shri J. M. Mauskar, Prof. Mark Hardy and Dr S. R. Wate

**A** three-day International Conference on Recent Trends in Environmental Impact Assessment (RTEIA-2008) was organized at the National Environmental Engineering Research Institute (NEERI), Nagpur, during 23-25 November 2008. This conference was organized to commemorate Late Dr Rajkamal Sarin, who made significant contributions to the field of environmental impact assessment during his tenure as Head, Environmental Impact and Risk Assessment Division at NEERI.

Inaugurating the conference Shri J. M. Mauskar (IAS), Chairman, Central Pollution Control Board (CPCB) who was the Chief Guest said that CPCB is thinking of implementation of zero emission discharge by industrial units, which is very important for protecting the environment. He urged the scientists to consider and review this issue during the conference and find out the solution. He said that industries will not favour any zero emission discharge technology, if its cost is very high, so economically viable technologies should be explored. Shri Mauskar emphasized on the regional approach for betterment of environment. Citing the examples of coal mining and other activities being carried out at various places, including Vidarbha region, he said that regional environmental assessment is important for improving the



environment. Shri Mauskar suggested scientists to ensure that the mistakes made by industries in developed countries should not be repeated in developing countries like India. Shri Mauskar stressed on the need to create a public domain and transparent database of all emissions and effluents from all industries in the country.

Delivering the Keynote Address, Guest of Honour Dr T. S. Vijayaraghavan, Chairman, Expert Appraisal Committee (Industry), Ministry of Environment and Forests, New Delhi, said that Environmental Impact Assessments (EIAs) are ensuring sustainable development in the country, which have been instrumental in providing better environment for everyone. He said that though people are living their lives in harmony, intellectual greens should be preserved and land given up for industrial purposes should be limited to the bare minimum.

Earlier, in his Welcome Address, Dr T. Chakrabarti, Acting Director, NEERI, briefed about the methods through which EIA has been brought to include aspects such as socio-economic effects of industries and corporate responsibilities, in an effort to make it practical and all-encompassing. He also added that the concept of EIA has been broadened to bring risk assessment under its purview.

The special invitee Prof. Mark Hardy, Dean, College of Science, Engineering and Technology, Jackson State University, Mississippi, USA, spoke about the origin and activities of his institution, and invited Indian organizations to

visit his academic institution, saying that it would be mutually beneficial.

Several dignitaries paid homage to Dr Rajkamal Sarin on this occasion and reminisced his valuable contributions in EIA studies made at the institute. Dr Chakrabarti, presented a plaque to Mrs. Shobha Sarin in the honour of Late Dr Rajkamal Sarin. Dr S. R. Wate, Director-Grade-Scientist and Head, EIRA Division, NEERI, proposed a vote of thanks.

The conference had four technical sessions on the following topics: EIA Practices — Regulations and Practices, New Trends in Environmental Monitoring, Modeling and Impact Prediction – Recent Trends and EIA and Climate Change. These technical sessions were chaired by Dr R. N. Singh, former Director, NEERI and Emeritus Scientist, National Geophysical Research Institute, Hyderabad; Dr M. Z. Hasan, Chairman, State Level Expert Appraisal Committee, UP; Dr Gurdeep Singh, Indian School of Mines, Dhanbad; and Dr S. Devotta, former Director, NEERI, respectively.

Next day, three technical sessions were organized on New

Trends in Environmental Management Practices, Public Participation and Corporate Social Responsibility and EIA, and Industry Perspective. These technical sessions were chaired by Prof. Maithili Sharan, Indian Institute of Technology, Delhi; Prof. I.V. Murali Krishna, Jawaharlal Nehru Technological University, Hyderabad and Mr Clement Chauvet, UNICEF, Delhi, respectively. The Poster Session which was inaugurated by Prof. Gurdeep Singh, Indian School of Mines, Dhanbad, had 50 posters. Cash awards were given to the best posters.

The conference concluded with a brain-storming session in which a panel of distinguished experts took part. Useful recommendations were made and an action plan was delineated for future implementation under different EIA studies. Over 200 delegates participated in the International Conference and the souvenir was also brought out on this occasion.

Earlier, a press conference was also organized at the Tilak Patrakar Bhawan, Nagpur, to address various issues related to environmental impact assessment in the country.



Souvenir being released by (from left):  
Dr T. Chakrabarti,  
Dr T.S.Vijayaraghavan,  
Shri J. M. Mauskar,  
Prof. Hardy and  
Dr S. R. Wate

## Indo-Korean Symposium in Organic Chemistry at NCL

The National Chemical Laboratory (NCL), Pune, organized a joint Indo-Korean symposium on organic chemistry entitled 'Contemporary organic chemistry and its future directions', during 12-13 January 2009. The joint scientific symposia in organic chemistry are being held since 1992 under the aegis of Indian National

Science Academy (INSA), New Delhi and Korean Science and Education Foundation (KOSEF). The present symposium was fourth in the series and the last one was held in Korea where eight eminent organic chemists from India had participated.

This symposium was the first in the series of NCL's Diamond Jubilee

year-long celebrations that aimed to bring together the practitioners of science from industry, academia and Government to NCL for scientific discussions and interactions

About 250 participants from different parts of the country attended the two-day symposium in which seven Korean and sixteen



Dr Sivaram delivering welcome remarks



Dr Ganesh Pandey giving background of the workshop



Prof. Kyu-Sung Jeong giving his remarks



Prof Goverdhan Mehta delivering special talk



Indian scientists presented a diverse spectrum of organic chemistry covered in eight scientific sessions spread over two days. 'Synthesis in Organic Chemistry' was the main aspect covered in this symposium. It dealt with diverse areas of contemporary organic synthesis.

In the symposium a special lecture was delivered by Prof. Goverdhan Mehta, IISc, Bangalore. Prof Mehta spoke on, 'A tryst with organic synthesis: Masters and molecules that changed our world'.

Dr S. Sivaram, Director, NCL, welcomed the delegates and hoped that these interactions will further strengthen the scientific collaborations between India and Korea. Dr Ganesh Pandey, Convener and Head, Organic Chemistry Division of NCL provided a brief background of the symposium. Each session dealt with different aspect of organic chemistry e.g. bioorganic chemistry, total synthesis, synthetic methodology and organic materials.

Prof. B.H. Kim from POSTECH, Pohang, in his inaugural presentation, dealt with the synthesis of modified nucleic acids and their use as chemical probes for sensing, polymer design, etc. He mentioned that modification by adding either steroid derivatives or cationic amine moieties to oligonucleotides has been found to enhance the cell permeability. He also discussed synthesis of modified oligonucleotides containing

fluorescent tags for use as molecular probes (molecular beacons) to detect single-nucleotide polymorphism (SNP) in nucleic acids, and to monitor secondary structures of various nucleic acids such as B-Z transition, G-quadruplex structures and DNA i-motif structures.

Prof. Sandeep Verma from IIT Kanpur, discussed designing of spherical hollow structures funded upon the ternary structures of the natural molecules and uses of these hollow structures as molecular containers for confinement and delivery applications.

The role of oligosaccharides at cellular level is a complex issue which has yet to be resolved. Similarly, the synthesis of complex oligosaccharides too needs special tactics and techniques. In his presentation, Dr A.K. Misra from Bose Institute, Kolkata, explained the recent successes of his group in the synthesis of biologically important oligosaccharides and also their mimics.

Total synthesis continues to be the final proof for the assigned structure of a natural product. In his presentation, Dr Lee from Sogang University, Seoul, presented the toughness of a total synthesis, especially when the structure of natural products is wrongly proposed, by demonstrating recent total synthesis of clavosolide A in his laboratory.

Dr S. Raghavan from IICT, Hyderabad, described the regio-

and stereoselective synthesis of 1,2- and 1,3-amino alcohols by oxidative functionalization of alkenes activated by an electrophile via participation of a sulfoxide/sulfilimine.

Prof. K.R. Prasad from IISc, Bangalore, in his talk provided a comprehensive compilation of recent synthesis of various natural products belonging to the polyol class by employing abundant chiral pool compounds.

Mimicking the secondary structure of proteins and peptides is a long standing research. In his presentation, Dr G.V.M. Sharma, Indian Institute of Chemical Technology (IICT), Hyderabad, explained some of the crucial design elements that his group employed to arrive at the helical peptides with a defined pitch and handedness.

Prof. S. Hazra from IIT-Kharagpur, gave a brief summary of his work in the area of developing asymmetric transformations and their application in the synthesis of some biologically significant molecules.

The versatility of titanocene(III) chloride as a radical generator was dealt in detail by Prof. S.C. Roy from Indian Association for the Cultivation of Science, Kolkata, by discussing experimentation with this reagent in the synthesis of various classes of natural products.

Prof. N. Jayaraman from IISc, Bangalore, has focused his research on multivalent transition metal

catalysts and its influence on the reaction rates. The design and synthesis of poly(ether imine) series of dendrimers and their trapping of the desired number of palladium atoms and use of these metal complexed dendrimers for some coupling reactions formed the basic content of his talk.

Dr C.V. Ramana from NCL explained the importance of the design elements and strategy of a total synthesis especially when the focus is on the synthesis of libraries of small natural product molecules.

In the first lecture on the second day, Prof. D. Basavaiah from University of Hyderabad, who brought the Baylis-Hillman reaction into limelight, gave a brief account of this reaction and importantly the use of the derived adducts as novel synthons for nitrogen heterocycles.

Though, the reductive opening of benzylidene acetal is one of the widely employed protocol in carbohydrate chemistry, by employing innovative substrates and catalysts, Prof. S. Baskaran from IIT Chennai, in his talk dealt with the synthesis of a variety of natural products.

Dr K.V. Radhakrishnan, from National Institute for Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram, explained in detail a simple, yet elegant approach for the synthesis of disubstituted cyclopentanes synthons and their expeditious application for the preparation of glycosidase

inhibitors, antiviral and antitumor carbonucleosides.

Hybridization of organic molecules bearing characteristic properties, with nano-sized materials such as nanoparticles and carbon nanotubes is an attractive proposition in the contemporary research. It can improve the physiochemical properties of the nanosized materials, and create new materials possessing the unique properties, which are not present in the parent materials. Prof. Lee from Ewha Womans' University, Seoul, discussed her experience in the hybridization of ionic liquids, with nanomaterials, besides interesting physical properties of resulting nano-ionic hybrids.

Dr V.A.Kumar, dealt with the design, synthesis and execution of the structurally biased oligonucleotide analogues that bind strongly and sequence specifically to the target mRNA.

Prof. R.B. Sunoz from IIT-Mumbai presented recent research work from his lab that focuses on the application of computational studies to rationalize and predict mechanisms and also to reveal the factors responsible for stereoselectivity in a range of organocatalytic reactions.

Trimethylenemethane (TMM) has attracted much attention from physical organic chemist for its unique structural features. Prof. Lee from KAIST, Taejon, disclosed an alternative way to generate TMM

intermediates and elegant new ways to utilize this carbene intermediates in total synthesis of triquinane class of natural products.

Prof. F.A. Khan from IIT-Kanpur, gave the details about their in-house strategy that involves a novel ruthenium-catalyzed oxidation of 1,2-dihaloalkene moiety present in norbornyl derivatives to norbornyl  $\alpha$ -diketones and a cleavage reaction to furnish a short route to the highly substituted cyclopentenoid intermediates with high stereochemical control. The use of this intermediate in the synthesis of anti-retroviral drugs and glycosidase inhibitors was discussed.

Prof. K.H. Ahn from POSTECH, Pohang, gave a brief account of his recent contributions in the area of molecular sensors by taking their novel recognition motif *o*-CATFA that recognizes anions such as carboxylates and neutral amines through the formation of "reversible covalent adducts" by taking few selected examples of *o*-TFACA-based molecular systems that show unusual recognition and sensing behaviours towards these analytes.

Prof. Jeong from Yonsei University, Seoul, employed oligo-Indole-based approach for the development of new anion receptors and also novel foldamers that bind small hydrophilic halides in water by multiple hydrogen bonds with moderate affinities.



# Indo-Russian Workshop on Catalysis for Biomass-conversion and Environmental Engineering

The National Chemical Laboratory (NCL), Pune, organized a joint one-day Indo-Russian Workshop on Catalysis for Biomass-conversion and Environmental-engineering on 22 January 2009. The workshop was sponsored by Department of Science and Technology (DST), New Delhi, Government of India. The Russian team of six participants was lead by Prof. V. I. Bukhtiyarov, Deputy Director, Boreskov Institute of Catalysis (BIC), Novosibirsk, Russia, who was also the Convener of the workshop. A total of about 80 participants, from IIT-Madras, IIP, IICT, NEERI, Anna University Chennai, and NCL attended the workshop, besides one participant each from Australia and Denmark.

The workshop was held as a part of NCL's Diamond Jubilee Celebrations and it aimed to bring together various practitioners of science from industry, academia and Government to NCL for scientific discussions and interactions.

Dr S. Sivaram, Director, NCL, in his welcome remarks gave insights on why and how workshops of this kind are important to begin new avenues for collaborations and interactions within scientific community who share same views on the various issues related to chemistry. He encouraged the participants to have healthy interactions and understand the issues faced by world community.



Prof. V.I. Bukhtiyarov delivering his talk

He also emphasized on the significance of the topic chosen for the present workshop for both the countries. He elaborated on his vision on how chemists working in the field of catalysis can join hands and achieve the goals faced by world community in the conversion of biomass into chemicals and fuels.

Prof. Bukhtiyarov, apprised the participants regarding the facilities available and the research being carried out on biomass- conversion in various Russian institutes which come under the umbrella of Russian Academy of Science (RAS). He also informed that the next bilateral meeting will be held in Russia.

Dr Rajiv Kumar of DST informed that DST is working on joint programmes between Indian and Russian institutes with the help of RAS. He mentioned that the first MoU was signed between India and Russia way back in 1987 and again in 2007. DST and RAS have revived the ties and are looking forward to

have more interactions between the scientists from both the sides. He gave out details on how scientists from India and Russia can submit the joint proposals.

The workshop comprised two scientific sessions. Pre-lunch session was chaired by Dr P. L. Dhepe and the post-lunch session by Dr D. Srinivas, both from NCL.

The first session started with the talk by Prof. V. I. Bukhtiyarov on 'BIC infrastructure complex for development and commercialization of new catalysts and technologies: From fundamental to industrial level'. He briefed on various R&D facilities available at BIC. He also offered help in building new reactor systems for Indian scientists with the facilities available in his institute. He discussed the hydrodesulfurization project based on CoMo catalytic system. The next talk was by Dr Sadhana Rayalu from NEERI, who spoke on 'Catalysis for mitigation of global warming effects'. She introduced participants to sources of generation of green house gases and their adverse effects on the environment. She mentioned the work being pursued in her laboratory on the synthesis of microporous and mesoporous materials which can trap the green house gas, CO<sub>2</sub>, to form carbonates, decomposition of N<sub>2</sub>O and oxidation of methane. She also elaborated on synthesis and characterization of perovskites, photocatalytic water splitting and protein cage materials

for photocatalysis.

The third talk was delivered by Prof. P. Selvam from IIT-Madras on 'Transition-metal-containing mesoporous molecular sieves: Highly efficient catalysts for selective oxidation reactions'. He gave a brief account of microporous and mesoporous materials and their advantages and disadvantages. He also discussed synthesis and characterization of metal incorporated mesoporous silicas and their applications in the oxidation reactions and photocatalytic activities. Next presentation was on 'Catalytic conversion of biomass for the biofuels production', delivered by Dr V. Yakovlev of BIC. He shared his views with the participants on the synthesis of bio-hydrogen from woody materials and also formation of bio-oils from wood.

A. K. Sinha from IIP, talked on the 'Co-processing of biomass-derived oils with petroleum fractions for the production of transportation fuels'. He spoke on the conversion of vegetable oil to biodiesel and green diesel. He said that green diesel is a step forward towards conserving the environment as it is free from oxygen. The next presentation was on 'Activity of mesoporous solid acid catalysts towards the synthesis of biodiesel over trans-esterification of triacetin' delivered by Prof. A. Pandurangan, Anna University, Chennai. He presented the work on the synthesis and characterization of several metal supported mesoporous silicas and their utilization in the trans-esterification reactions.

Dr D. Srinivas from NCL, spoke

on, 'Catalytic conversion of CO<sub>2</sub> to fuels and chemicals'. He mentioned that how conventionally CO<sub>2</sub> is used to synthesize methanol, carboxylic acids etc. He discussed various utilization pathways for CO<sub>2</sub>. He showed that CO<sub>2</sub> can also be fixed during reaction with amines to form carbamates. He presented his work on Ti and adenine containing mesoporous silicas. He also emphasized the fact that there still remain many other avenues for fixing up the CO<sub>2</sub>.

The first talk in the post-lunch session was by Dr I. L. Simakova, BIC, Novosibirsk on, 'Development of selective catalytic synthesis of multifunctional organic molecules from biorenewables using supported heterogeneous catalysts'. She discussed her work on hydrogenation of vegetable oils to produce partially or completely saturated vegetable oils. She further discussed catalytic deoxygenation of free fatty acids (FFA) and briefed on her future interests on which she would like to collaborate with Indian scientists. 'Utilization of biorenewable sources: Catalytic conversion of glycerol to commodity chemicals' was the next talk delivered by Dr N. Lingaiah from IICT. He showed how glycerol, a byproduct of biodiesel process can be used for synthesizing various chemicals and he specifically discussed his work on glycerol hydrogenolysis to form 1, 2 propane diol using various catalysts. The preparation and characterization of the catalysts was also discussed.

Dr T. B. Khlebnikova from BIC, spoke on 'Environmentally benign methods of fine chemicals synthesis using natural raw materials'. In her

presentation she discussed oxidation of organic substrates in the biphasic systems. She elaborated on oxidation of tall oils and castor oils using hydrogen peroxide. She showed her interest in developing new catalysts based on HPA for the synthesis of vitamins E and K and touched upon development of wood delignification catalyst.

Dr P.L. Dhepe of NCL delivered a talk on, 'Heterogeneous catalysts for the conversion of biomolecules'. He introduced participants to green chemistry principles and how those can be achieved by using biomass for the production of chemicals and using water as a solvent. He discussed his work on conversion of biomass using heterogeneous catalysts.

Ms. S. A. Khromova of BIC, delivered her talk on, 'Catalytic upgrading of bioliquids for biofuel production'. She discussed hydrodeoxygenation reactions, synthesis and characterization of various catalysts and their catalytic activities in hydrodeoxygenation of anisole. Dr E. A. Kozlova from BIC, delivered her talk on, 'Photocatalytic water splitting with hydrogen evolution in sacrificial organophosphorous donors and Ce<sup>3+</sup>/Ce<sup>4+</sup> shuttle charge transfer systems'. She commenced her talk with the introduction of soft chemical reduction (SCR) and photoreduction (PD) methods for deposition of metal on the surface of the support. She discussed the results for the Pt/TiO<sub>2</sub> catalyst prepared by both these methods in water splitting reaction and concluded that catalyst prepared by SCR is most active.



Last presentation was by Dr K. Sreekumar of NCL, on, 'Clean energy from biomass: Progress in developing fuel cell electrodes for effectively handling alcoholic fuels'. He detailed on utilization of alcohol, obtained from biomass, in fuel cells. He also discussed synthesis of electrodes and its importance for achieving highly efficient fuel cells. He discussed synthesis and characterization of carbon nanofibers and nanotubes and their use for the dispersion of platinum.

In the poster session twelve posters were on display, of which nine were by Indian participants and three from Russian side covering diversified fields ranging from biodiesel production, green diesel production, chemical's syntheses from biomass and further conversion of various products obtained from biomass such as glycerol to water gas shift reaction.

In the concluding remarks, Dr Sivaram thanked the audience for their enthusiastic and active participation during day long deliberations. He also hoped to see more fruitful collaborations between the researchers of the two countries by identifying the mutually interested fields. Prof. V. I. Bukhtiyarov also expected that more of such collaborations will be there in future.

## The deMon Developer's International Workshop at NCL

The deMon Developer's Ninth Annual Workshop was held at the National Chemical Laboratory (NCL), Pune, during 16-19 February 2009. The workshop, held normally every year, brings together the practitioners and developers of the software code deMon in order to assess and discuss new developments in the implementation and application of the code. About 50 participants, with half of them from abroad, attended the four-day international workshop. The workshop included 34 presentations spread over eleven scientific sessions.

The workshop was held as a part of NCL's Diamond Jubilee Celebrations that aimed to bring together practitioners of science from industry, academia and Government to NCL for scientific discussions and interactions.

Dr S. Sivaram, Director, NCL, welcomed the participants and Dr Sourav Pal, Convener of the workshop and Head, Physical and Materials Chemistry Division of NCL, gave background of the workshop. He remarked on his association with deMon 2K program and how this workshop would generate interactions of scientists from all over the world in development and use of deMon 2K code.

Prof. Dennis Salahub from University of Calgary, Canada, delivered the Plenary Lecture, reviewing the recent developments with respect to implementations and additions to the deMon2k code, and also laid out the agenda for the workshop. Other distinguished speakers included Prof. Andreas Koester (Instituto Politecnico Nacional, Mexico); Prof. Mark E.



Prof. Dennis Salahub delivering the Plenary Lecture

Casida (Institut de Chimie Moleculaire de Grenoble, France); Prof. Thomas Heine (Jacobs University, Germany); Prof. Annick Goursot (Institut Charles Gerhardt, France); Prof. Klaus Hermann (Abt. Theorie Fritz-Haber-Institut, Germany); Prof. Lars Petersson (Stockholm University, Sweden) and Dr Tzonka Mineva (Institut Charles Gerhardt, France).

In addition to the members of the deMon2k family, the ninth annual workshop also included several invited guest speakers such as Prof. Shiv N. Khanna (Virginia Commonwealth University, USA); Prof. Ravindra Pandey (Michigan Technical University, USA); Prof. K.D. Sen (University of Hyderabad); Prof. Rajiv Pathak (University of Pune); Prof. Sridhar R. Gadre (University of Pune); Dr Mrinalini Deshpande (Nasik); Dr V. Subramanian (Central Leather Research Institute, Chennai); Dr Swapan Ghosh (Bhabha Atomic Research Centre, Mumbai); Dr K. R. S. Chandrakumar (Bhabha Atomic Research Centre, Mumbai); Dr Kumar Vanka (NCL, Pune) and Dr Sailaja Krishnamurty (Central Electrochemical Research Institute, Karaikudi). In addition, several young researchers – post-doctoral fellows and Ph.D. students – in the field of computational chemistry were given opportunity to make oral presentations. In the discussion session the developers of deMon2k took stock of current state of implementations of the deMon2k code and chalked out future plans to incorporate further additions and changes to the code.

## Syed Hussain Zaheer Medal Lecture at CECRI



Prof. K.T. Jacob of IISc delivering the Syed Hussain Zaheer Medal Lecture at CECRI

The prestigious Syed Hussain Zaheer Medal of the Indian National Science Academy (INSA) for the year 2007 has been awarded to Prof. K.T. Jacob, INSA Distinguished Professor, Department of Materials Engineering, Indian Institute of Science, Bengaluru. The medal awarding function was organized by the INSA Madurai chapter at the Central Electrochemical Research Institute, Karaikudi, on 12 February 2009. Prof. Jacob was presented the Medal with citation by the Distinguished Prof. J.C. Ahluwalia, former Professor of Chemistry, IIT, Delhi and former INSA Council Member.

Accepting the Award, Prof. Jacob delivered the Medal Lecture on 'High temperature electrochemical route for the extraction of titanium from rutile'. Prof. Jacob commenced his lecture by highlighting the industrial importance of titanium metal, due to its high 'strength vs weight' ratio. Owing to its unique properties, especially its low weight, it has replaced much of steel in the aircraft industry. Other major areas of its use are in chemical industries and in marine environment due to its excellent corrosion resistant characteristics. Also, it can replace major steel in all transport sectors but for its cost acting as the constraint.

He mentioned that Hunter and Kroll's processes are the current methods of production of titanium metal in the form of sponge. These processes use sodium and magnesium metal to reduce titanium tetrachloride at 900 °C. The sponge metal has to be melted and subjected to downstream production. Oxygen is soluble in metallic titanium up to 32 atom %, above which it starts to form compounds. Hence, these operations, including the primary production has to be done in air-free environment. Otherwise, the metal will become brittle and useless. Among these two metallothermic reduction processes, Hunters process is rarely used due to the hazardous nature of sodium, although the quality of sponge produced by Hunter process is better than Kroll's process.

India possesses good quality ilmenite as well as some quantity of



rutile. However, India currently meets her requirements of titanium and its alloys through import. Hence, to meet the needs of titanium and to add value to ilmenite, DMRL, Hyderabad, has developed a modified Kroll's Process, whose energy requirement is high and is around 30 kWh/kg of the metal. Further intensive efforts are needed for minimizing the energy requirement.

Subsequently, Prof. Jacob pointed out that global research activities aiming electrochemical production of titanium metal are in progress. The recent studies on reduction of titanium chloride by two compartment method developed by Ginatta of Italy advocate for total energy consumption of around 18 kWh/kg of titanium particles. In early 1990s, a Japanese group (K. Ono *et al*) indicated the possibilities for the electrocleaning of titanium surface, i.e., removal of oxide layer and oxygen on titanium surface to about 50 ppm by treating the titanium sheet as cathode in molten calcium chloride electrolyte. In late 1990s, D.J. Fray, T.W. Farthing and G.Z. Chen (Cambridge University) reported a process for the removal of oxygen from a pellet of titanium dioxide and claimed the production of titanium particles with less than 200 ppm of dissolved oxygen. Another group in Japan (Ono/ Suzuki, Kyoto Univ.) also declared their success in deoxidation of titanium dioxide in molten calcium chloride melt. However, voltammetric studies have revealed that the titanium particles obtained on larger scale operations contained around 500 ppm of dissolved oxygen which could not be used for high-tech production. Nevertheless, these extensive investigations have paved way for obtaining very high pure titanium metal required for sputtering applications. However, the cost of high purity titanium is about 9 times higher than commercially pure titanium. Further, thin foils of titanium metal can be deoxygenated electrolytically in molten calcium chloride. Thus the area of electrochemical extraction of titanium poses still challenging research issues.

Earlier, Dr V. Yegnaraman, Scientist 'G' and Head, Electrodeposition and Electrocatalysis Division of CECRI welcomed the gathering. Dr G. Marimuthu, Head, Department of Animal Behaviour & Physiology, Madurai Kamaraj University, Madurai and Secretary of INSA Madurai Chapter, proposed a vote of thanks.

### Earth Day celebrated at NISCAIR

Day long events marked the Earth Day celebrations at NISCAIR on 22 April 2009. Funded by the Ministry of Earth Sciences, NISCAIR organized a painting competition for school children in the forenoon. Ninety nine children from 8 schools and wards of NISCAIR staff participated in the painting competition. Three prizes each in the junior, middle and senior categories and three special prizes were awarded to the winners of the painting competition.

A lecture on "Climate Change: Impact Assessment and Management" was delivered by Dr P.L. Uniyal of Delhi University who enlightened the gathering including the school children about the process of climate change, its impact and management measures. He also gave away the prizes to the winners of the painting competition.

Earlier, Mr Ashok Chawla, Chairman of the Earth Day Celebrations Committee spoke about the importance of Earth Day and the need for conserving the natural resources. Dr Gangan Prathap, Director, NISCAIR, welcomed the gathering and presided over the function.



**Top:** Dr Gangan Prathap, Director, NISCAIR, welcoming the distinguished gathering during the Earth Day Celebrations at NISCAIR.  
**Above:** The painting competition being held at NISCAIR

### **Dr Shivendra Nath Rai gets National Mineral Award**

**D**r Shivendra Nath Rai, Scientist 'G' at National Geophysical Research Institute (NGRI), Hyderabad, has been conferred the National Mineral Award-2007 in recognition of his significant contributions to the field of Groundwater Exploration through predictive models and geophysical studies.



Dr Rai has developed new generation of analytical mathematical models to predict water table fluctuations in different aquifer systems. Models prepared by him have also found application in ground water resource management through the selection of appropriate recharging or pumping techniques. Models prepared by Dr Rai are capable of predicting the rise and decline of the water table depending on the increase and decrease in the recharge or pumping rate. He has also made sustained efforts in the field of groundwater exploration through geophysical surveys, notable amongst these is locating potential zones within and below the Deccan traps as well as in the rocks of Gondwana Supergroup in Maharashtra.

Dr Rai is recipient of National Hydrology Award of Indian Association of Hydrologist. He is Vice-President of International Association of Hydrogeologist (IAH), Fellow of Indian Geophysical Union (IGU), Indian Association of Hydrologist and Member of many scientific bodies. He has published more than 60 research papers in International and National journals, many chapters in books and edited two books on hydrological sciences.

### **Ms Tanpreet Kaur to meet Nobel Laureates in Germany**

**M**s Tanpreet Kaur, a research student working for her Ph.D. jointly with Prof. K.N. Ganesh, Director, IISER-Pune and Dr Asish Bhattacharya, Scientist, National Chemical Laboratory (NCL), Pune, has been selected for the prestigious DST Department of Science and Technology -DFG (German Research Foundation) Award for "Participation in the 59th meeting of Nobel Laureates and Students in Lindau, Germany" which is scheduled to be held during 28 June – 3 July 2009. About 20 Nobel Laureates and more than 600 young researchers from around the world will meet at Lindau. Each year since 1951, Nobel Prize winners in Chemistry, Physics and Physiology / Medicine have been meeting in Lindau, Germany, to discuss major issues of importance to their fields with students from around the world. The meetings include lectures by the Nobel Laureates, round-table discussions and informal small-group meetings with the Nobel Prize winners. The DST has been sending a group of students/young researchers to these meetings, since 2001. This year, DST is sending 44 students covering three categories namely: undergraduate students, masters students and doctoral students, and young post-doctoral scientists in the field of Chemistry. The 2009 Lindau Meeting will be dedicated to chemistry.



### **Honours and Awards won by CLRI Scientists**

**D**r P.T. Perumal, Scientist-G and Head, Organic Chemistry, Central Leather Research Institute (CLRI), Chennai, has been honoured with Elsevier Award for his pioneering and outstanding contribution to the area of organic chemistry.

**Dr J. Raghava Rao**, Scientist, Chemical Lab, CLRI has been awarded the Indira Gandhi Paryavaran Puraskar Award (IGPP) by the Ministry of Environment and Forests for his pioneering and outstanding contribution to the area of Environmental Protection.



## *Appointments/Announcements*

### **Dr K.C. Gupta takes over as Director, IITR**

**D**r K.C. Gupta, Acting Director, Institute of Genomics and Integrative Biology (IGIB), New Delhi, has taken over as Director, Indian Institute of Toxicology Research, (IITR), Lucknow, w.e.f. 27 March 2009. The areas of specialization of Dr Gupta are 'Bioorganic chemistry, nucleic acid synthesis & design'. His recent work relates to the development of nano-particle- aided transfection reagents for delivery of genes and their toxicity assessment and oligonucleotide based biochips as diagnostic tools for detection of genetic diseases. He has published over 80 publications in national and international peer reviewed journals. He also has to his credit 15 patents, both national and international, and has been instrumental in transferring two technologies in the area of nucleic acid chemistry.



Dr Gupta is a Fellow of the National Academy of Sciences (Allahabad). He has guided over 12 students for their Ph.D. programme and an equal number are pursuing their doctoral programme under his guidance.

### **Prof. Ram Rajasekharan takes over as Director, CIMAP**



**P**rof. Ram Rajasekharan, Professor of Biochemistry at the Indian Institute of Science, (IISc), Bangalore, has taken over as Director, Central Institute of Medicinal & Aromatic Plants (CIMAP), Lucknow, w.e.f. 4 April 2009. He took charge from Dr P. S. Ahuja, Director, Institute of Himalayan Bioresource Technology (IHBT), Palampur, who was holding additional charge of Director, CIMAP.

The major research interests of Prof. Rajasekharan include lipid metabolism, signal transduction in plants and bio-pesticide. After doing Ph.D. from IISc in 1987, he proceeded to University of Illinois, USA for his Post Doctoral Research. He has also worked in Biotechnology Division of prestigious Du Pont Company, USA.

### **Nominations invited**

### **Prof. G. N. Ramachandran Gold Medal for Excellence in Biological Sciences & Technology for 2008**

**T**he Council of Scientific & Industrial Research (CSIR) invites nominations for the Prof. G. N. Ramachandran Gold Medal for Excellence in Biological Sciences & Technology for the year 2008. The award is bestowed every year to an outstanding Indian scientist, who has made conspicuously important contributions, applied or fundamental, in the inter-disciplinary subject/field of Biological Sciences and Technology. The award would be given for the work done primarily in India during ten years preceding the year of the award. The Gold Medal is presented during the Indian Science Congress.

Nominations addressed to Dr Rajesh Luthra, Head, Human Resource Development Group, CSIR Complex, Library Avenue, Pusa, New Delhi 110 012 should be sent as per prescribed proforma (10 Copies) along with reprints of five most significant publications of the last 10-year's period by 29 May 2009. The details of the award and the prescribed proforma for nomination may be downloaded from the website <http://csirhrdg.res.in>

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