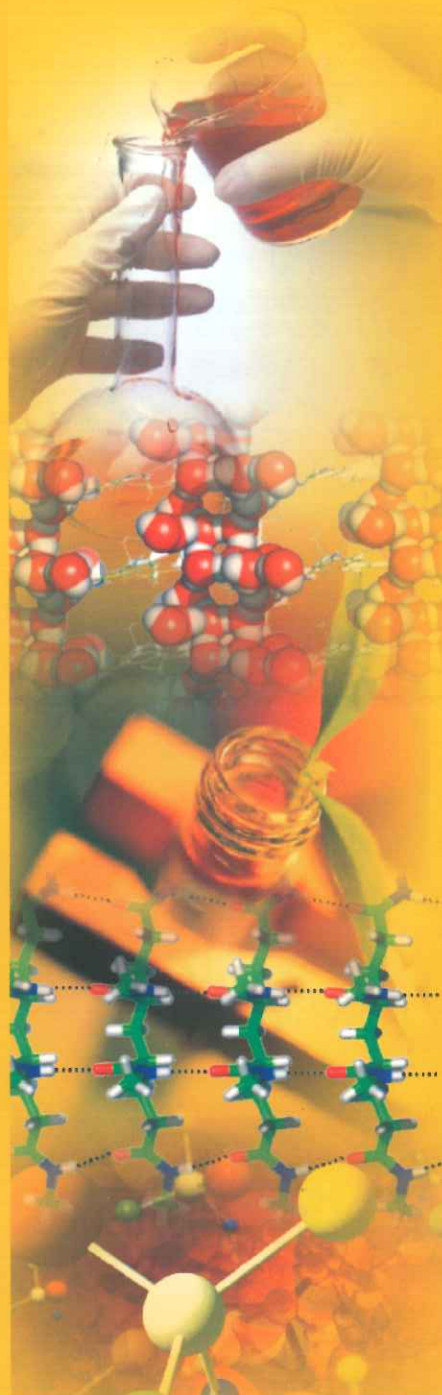
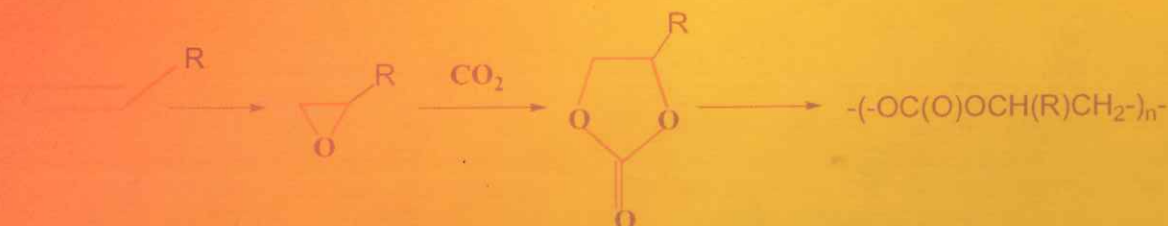


# Annual Report 2006-07



## राष्ट्रीय रासायनिक प्रयोगशाला



National Chemical Laboratory

**NCL** Annual Report 2006-07  
**NATIONAL CHEMICAL LABORATORY**

With best compliments from

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राष्ट्रीय रासायनिक प्रयोगशाला

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## निदेशक की कलम से



मुझे राष्ट्रीय रासायनिक प्रयोगशाला (एनसीएल), पुणे की वर्ष 2006-07 की वार्षिक रिपोर्ट प्रस्तुत करते हुए अत्यधिक हर्ष का अनुभव हो रहा है।

एनसीएल ने सभी क्षेत्रों में प्रगति का क्रम जारी रखा है। इसने रसायन विज्ञान तथा उससे सम्बन्धित विधाओं पर उनके सर्वाधिक मौलिक स्तर से अनुसंधान करके उन्हें उद्योगों और समाज के लिए उपयोगी बनाया है। हम विज्ञान एवं प्रौद्योगिकी को एक नए रूप में परिवर्तित करके उन्हें बाज़ार में प्रवेश दिलाने की दिशा में भी प्रयासरत हैं। एनसीएल में अनुसंधान एवं प्रवर्तन सर्वत्र व्याप्त है। यह केवल विज्ञान की खोज के लिए ही नहीं, अपितु विज्ञान को मुख्य रूप से समाज तक पहुँचाने के लिए है।

एनसीएल में बड़ी संख्या में कार्यरत शोध छात्रों तथा प्रतिष्ठित पत्र-पत्रिकाओं में इसके महत्वपूर्ण प्रकाशनों से विज्ञान के क्षेत्र में एनसीएल के योगदान का पता चलता है। हमने समीक्षाधीन वर्ष के दौरान प्रतिष्ठित पत्रिकाओं में 444 शोधपत्र प्रकाशित किए जिनका औसत इम्पैक्ट फैक्टर 2.39 प्रति शोधपत्र था। वर्ष के दौरान एनसीएल के 65 शोधछात्रों को पीएच.डी. डिग्री प्रदान की गई। वर्तमान में एनसीएल में चार सौ से अधिक शोधछात्र पीएच.डी. डिग्री के लिए कार्यरत हैं। सीएसआईआर की नेट परीक्षा उत्तीर्ण कर चुके अनेक छात्र पीएच.डी. हेतु अनुसंधान कार्य करने के लिए एनसीएल में प्रवेश लेना चाहते हैं। वर्तमान में प्रयोगशाला में उपलब्ध स्थान, सीमित संसाधनों तथा आवास-व्यवस्था को ध्यान में रख कर हम नेट परीक्षा उत्तीर्ण दो या तीन छात्रों में से केवल एक को ही प्रवेश दे पाते हैं। हम कुछ अतिरिक्त संसाधनों (आवास, प्रयोगशालाओं की जगह) को जुटाने का प्रयास कर रहे हैं ताकि हम वर्ष 2009 तक और एक सौ छात्रों को प्रवेश दे सकें।

हमने प्रौद्योगिकी के क्षेत्र में भी आगे बढ़ने के अपने अभियान को बनाए रखा है। वर्ष 2006-07 के दौरान एनसीएल के वैज्ञानिकों को 67 भारतीय पेटेंट तथा 31 विदेशी पेटेंट प्रदान किए गए हैं। रॉयल्टी से प्राप्त हमारी आय रु. एक करोड़ के आसपास हो गई है

हम समझते हैं कि एनसीएल के आकार को ध्यान में रखते हुए यह आँकड़ा फिर भी कम है। हमने सफलतापूर्वक दो पेटेंटों का लाइसेंस एक भारतीय कम्पनी को तथा पाँच पेटेंटों का लाइसेंस एक विदेशी कम्पनी को दिया है। सहभागिता के रूप में एनसीएल द्वारा विकसित बौद्धिक सम्पदा पर और आगे कार्य करने के लिए हमने एक नई कम्पनी को भी सहायता प्रदान की है।

एनसीएल ने समीक्षाधीन वर्ष के दौरान बाहरी स्रोतों से रु.22.15 करोड़ की धनराशि अर्जित की जिसमें उद्योग जगत से प्राप्त रु.13.30 करोड़ की राशि भी शामिल है। यह वर्ष प्रति वर्ष 20 प्रतिशत की बढ़ोतरी है। हमें इसका गर्व है कि एनसीएल विश्व की शीर्ष पचास सबसे बड़ी रासायनिक कम्पनियों में से दस कम्पनियों के साथ व्यावसायिक गतिविधियों में संलग्न है (केमिकल एण्ड इंजीनियरिंग न्यूज, जुलाई 24, 2006)। इससे एनसीएल को पूरे विश्व में अनुसंधान और विकास के क्षेत्र में एक सम्माननीय एवं विश्वसनीय सहभागी होने का गौरव प्राप्त हुआ है। आदित्य बिरला ग्रुप को दी गई एपीक्लोरोहाइड्रिन प्रक्रिया का कार्यान्वयन प्रगति पर है। इस कम्पनी ने रयोंग, थाईलैण्ड में 3000 टन प्रति वर्ष की क्षमता के अनवरत प्रदर्शन संयंत्र के निर्माण हेतु धन प्राप्त कर लिया है। एनसीएल ने एक मूलभूत इंजीनियरी पैकेज के निर्माण का कार्य पूरा कर लिया है तथा एबीजी द्वारा नियुक्त इंजीनियरी ठेकेदार के साथ मिलकर कार्य किया है। उपकरण के निर्माण का कार्य प्रगति पर है जिसका शुभारंभ वर्ष 2007 की तीसरी तिमाही में होने की संभावना है। सीएसआईआर की भारतीय नई सहस्राब्दि प्रौद्योगिकी नेतृत्व पहल के तत्वावधान में एनसीएल में चल रही दो परियोजनाओं ने प्रौद्योगिकी प्रदर्शन में महत्त्वपूर्ण प्रगति अर्जित की है। प्रयोगशाला में प्राप्त आँकड़ों के आधार पर एनसीएल ने एक सौ किलोग्राम प्रति बैच जैवभार का प्रभाजन-पूर्व संयंत्र तैयार किया है। इस संयंत्र को वर्ष 2007 की तीसरी तिमाही तक एक औद्योगिक स्थान पर स्थापित किया जाएगा। गन्ने के रस के किण्वन से प्राप्त कैल्सियम लैक्टेट के शुद्ध L(+) - लैक्टिक अम्ल में रूपान्तरण हेतु एनसीएल में एक अनवरत प्रायोगिक संयंत्र (2 किलोग्राम प्रति घंटा की क्षमता का) स्थापित किया गया है। हमें आशा है कि वर्ष 2007 की तीसरी तिमाही तक किसी एक औद्योगिक रिक्टर में किण्वन प्रक्रिया की पुष्टि हो जाएगी और वर्ष 2008 की तीसरी तिमाही तक एक 300 टन प्रति वर्ष की क्षमता का अनवरत डाउनस्ट्रीम रिकवरी संयंत्र स्थापित हो जाएगा। हमने एक नवोदय कम्पनी को ट्राइग्लिसिराइड का वसीय अम्ल एस्टर जैव डीज़ल में विपक्ष-एस्टरिकरण हेतु अनेक पेटेंटों का लाइसेंस दिया है। ये पेटेंट एक ठोस उत्प्रेरक हेतु एनसीएल को स्वीकृत किए गए थे। यह कम्पनी इन पेटेंटों पर आधारित एक प्रदर्शन संयंत्र स्थापित करने के लिए धन की व्यवस्था कर रही है। आशा है, वर्ष 2007 के अन्त तक धन की व्यवस्था हो जाएगी।

एनसीएल के एक विश्वसनीय प्रौद्योगिकी सहभागी होने की दिशा में ये कुछ महत्त्वपूर्ण मील के पत्थर हैं। हमने प्रौद्योगिकी हस्तान्तरण और कार्यान्वयन हेतु तीन प्रतिरूपों का सफलतापूर्वक

हस्तान्तरण और कार्यान्वयन हेतु तीन प्रतिरूपों का सफलतापूर्वक प्रयोग किया है। एपीक्लोरोहाइड्रिन के मामले में एनसीएल ने प्रारंभिक अनुसंधान एवं विकास सम्बन्धी कार्य किया है। इसके बाद पेटेंट और तत्सम्बन्धी जानकारी का लाइसेंस एक कम्पनी को दिया गया। एनसीएल ने उस कम्पनी के साथ मिल कर एनसीएल में ही छोटे स्तर पर प्रयोगों के द्वारा प्रक्रिया की व्यापारिक व्यवहार्यता को पुष्ट किया। एनसीएल ने मूलभूत इंजीनियरी पैकेज को भी तैयार किया। भारतीय नई सहस्राब्दि प्रौद्योगिकी नेतृत्व पहल के अन्तर्गत दो परियोजनाओं के मामले में परियोजना के कार्यान्वयन के प्रारंभिक चरणों से ही उद्योग जगत के साहचर्य के साथ सरकारी-निजी भागीदारी के रूप में कार्यक्रम तय किया गया था। अन्तिम परियोजना-जैवडीज़ल के मामले में एनसीएल ने पेटेंटों का लाइसेंस दिया और एक नवोदय कम्पनी की स्थापना में सहायता प्रदान की जिसने बदले में एनसीएल द्वारा अर्जित सुदृढ़ बौद्धिक सम्पदा को आधार बना कर बाजार में धन का उपार्जन किया। इन उदाहरणों से यह स्पष्ट होता है कि एनसीएल विज्ञान एवं प्रौद्योगिकी के माध्यम से समाज को धनी एवं सम्पन्न बनाने में अग्रसर है।

एनसीएल अपनी अनुसंधान एवं भौतिक संरचनाओं के निर्माण का कार्य जारी रखे हुए है। वर्ष के दौरान अनेक नई विश्लेषणात्मक सुविधाओं को जुटाया गया है जिसमें बहुपार प्रवाहमापी, लेज़र प्रकाश प्रकीर्णन उपकरण तथा एक अति शक्तिशाली उत्तेज्यवी लेज़र का समावेश है। एक उच्च निष्पादनयुक्त 32 नोड वाले कम्प्यूटेशनल क्लस्टर की भी स्थापना की गई है। एनसीएल ने अस्सी हजार वर्ग फीट के क्षेत्रफल में बनने वाले एक नए बहुलक एवं प्रगत पदार्थ प्रयोगशाला भवन की आधारशिला रखी। यह एनसीएल के अन्दर बनने वाली पहली ऐसी प्रयोगशाला है जिसका निर्माण पच्चीस वर्षों के अन्तराल के बाद हो रहा है। आशा है, यह प्रयोगशाला वर्ष 2008 की अन्तिम तिमाही तक पूरी तरह से तैयार हो जाएगी।

एनसीएल प्रवर्तन पार्क का शुभारंभ दिसम्बर 2006 में हुआ था। यह हमारे कार्यकलापों के प्रथम चरण की शुरुआत का द्योतक है। प्रौद्योगिकी व्यवसाय इन्क्यूबेटर वर्ष 2008 की प्रथम तिमाही तक पूरी तरह से काम करने लगेगा। इन्क्यूबेटर सुविधा की व्यवस्था हेतु एनसीएल ने कम्पनी अधिनियम की धारा 25 के अन्तर्गत उद्योगिता विकास केन्द्र नामक एक गैरलाभकारी नई कम्पनी की स्थापना की है। यह कम्पनी जनवरी 2007 को अस्तित्व में आई। इन नए प्रयासों से एनसीएल के लिए तथा कुल मिला कर देश के लिए ज्ञान के माध्यम से धनार्जन करने के अतिरिक्त नए अवसरों का निर्माण होगा।

हमारे अनेक वैज्ञानिकों ने एनसीएल को गौरवान्वित करने का क्रम जारी रखा है। डॉ. आशीष लेले को अभियांत्रिकी विज्ञान के क्षेत्र में शान्तिस्वरूप भटनागर पुरस्कार प्रदान किया गया। डॉ. श्रीनिवास होता को सीएसआईआर तथा भारतीय राष्ट्रीय विज्ञान अकादमी-दोनों ने वर्ष का युवा वैज्ञानिक पुरस्कार प्रदान किया।



हमारे अनेक वैज्ञानिकों को विज्ञान एवं प्रौद्योगिकी विभाग, भारत सरकार द्वारा जगदीश चन्द्र बसु और रामन्ना शोधवृत्तियाँ प्रदान की गईं। यह हमारे लिए गौरव का विषय है कि डॉ. आर.ए. माशेलकर ने सीएसआईआर के महानिदेशक के पद से सेवानिवृत्त होने के बाद एनसीएल में सीएसआईआर भटनागर फेलो के रूप में कार्यभार सम्हाला।

हमने अपने दो सुप्रतिष्ठित वैज्ञानिकों को विदाई दी। डॉ. के.एन. गणेश भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान, पुणे के संस्थापक निदेशक बने और सजातीय उत्प्रेरण प्रभाग के प्रमुख, डॉ.आर.वी. चौधरी ने सेवानिवृत्ति के बाद अमरीका में कन्सास विश्वविद्यालय के रासायनिक एवं पेट्रोलियम इंजीनियरिंग विभाग में डीन ई. ऐकर्स प्रतिष्ठित प्रोफेसर के पद का कार्यभार ग्रहण किया। हम इन दोनों वैज्ञानिकों के नए सुखद भविष्य की कामना करते हैं। राष्ट्रीय रासायनिक प्रयोगशाला (एनसीएल) अपनी प्रगति-यात्रा के रोचक चौराहे पर खड़ी है। नेतृत्व एवं संकल्पनाओं- इन दोनों क्षेत्रों में बड़े-बड़े परिवर्तन होने जा रहे हैं। इसके समक्ष एक ओर भविष्य के लिए अनुसंधान के नए क्षेत्रों को तलाशने की बड़ी चुनौती है तो दूसरी ओर इसके साथ ही इसे अपनी क्षमता और पुरानी सुदृढ़ परम्पराओं को भी अक्षुण्ण बनाए रखना है। मुझे विश्वास है कि राष्ट्रीय रासायनिक प्रयोगशाला बखूबी इस चुनौती को पूरा करेगी।

मैं अपने सभी स्टाफ-सदस्यों, एन.सी.एल. की अनुसंधान परिषद और प्रबन्ध परिषद के सदस्यों, सी.एस.आई.आर., नई दिल्ली के महानिदेशक और सभी स्टाफ-सदस्यों तथा हमारे सम्मानित साझेदारों द्वारा दिए गए सहयोग और समर्थन के लिए उनके प्रति अपनी हार्दिक कृतज्ञता प्रकट करता हूँ। उनकी सलाह, सहयोग और विश्वास के बिना इन उपलब्धियों को प्राप्त करना असंभव होता

(एस. शिवराम)

(एस. शिवराम)



## FROM THE DIRECTOR'S DESK



It gives me great pleasure to present the Annual Report of National Chemical Laboratory, Pune for the period 2006-07.

NCL continues its march towards progress in all fronts from exploring chemical and related sciences at the most fundamental level to translating new and known science innovatively to applications in industry and society. We are also experimenting with new models for such translation, thus, providing an enabling environment for good science and technology to reach the market place. At NCL innovation is all pervasive, not only in the pursuit of science but also in defining the best manner in which science can reach society at large.

NCL's contribution to science is measured by the large number of research students it continues to attract and the quality of publications in peer reviewed journals. We have published four hundred and forty four papers in peer reviewed journals during the year in review with an average Impact Factor of 2.39 per paper. During the year sixty five students graduated with a Ph.D. degree from NCL. Currently we have more than four hundred students on roll pursuing a Ph.D. degree. There is a large demand from students qualifying in the CSIR NET examination to join NCL for their Ph.D research. Currently limitations of laboratory space and accommodation have restricted admissions to one in two or three NET qualified students. We are in the process of creating additional infrastructure (student accommodation, laboratory space) which will enable us to add on about hundred more students by mid 2009.

We have also continued to maintain our momentum on

the technology front. Sixty seven Indian patents and thirty one overseas patents were granted to inventors from NCL during 2006-07. Our earnings from Royalty inched towards the one crore (Rs 10 million) mark. We recognize that for the size of NCL this is still pitifully small. We successfully licensed two patents to an Indian company and five patents to an overseas company. We helped a start-up company of innovators- entrepreneurs to exploit an IP co-developed by NCL.

NCL closed the year with a total External Cash Flow of Rs.22.15 crores (Rs.221.5 million) with an industry contribution of Rs.13.30 crores (Rs.133 million). This is a 20 % growth, year on year. NCL also prides itself of being associated with ten of the top fifty largest chemical companies of the world (Chemical & Engineering News, July 24, 2006). Such associations bring substantial credibility to our laboratory as a respected and trusted partner for R&D across the world.

The process for a catalytic route for epichlorohydrin licensed to Aditya Birla Group continued its progress towards implementation. The company secured approvals for capital budget for constructing a continuous demonstration plant for 3000 tons per annum in Ryong, Thailand. NCL completed the preparation of the basic engineering package and worked closely with a detailed engineering contractor employed by ABG. Equipment fabrication is currently in progress with a start-up date for operation in third quarter of 2007. Two of the projects in execution at NCL under the auspices of New Millennium Initiative in Technology Leadership for India of CSIR (NMITLI) made significant progress towards technology demonstration. NCL designed and procured a 100 kg per batch biomass pre-fractionation plant based on the data generated in the laboratory. The plant will be installed in an industrial location and slated for commissioning by the third quarter of 2007. A continuous pilot plant (2 kg per hour) for converting calcium lactate (derived from fermentation of sugar cane juice) to pure L(+)-lactic acid was set up and commissioned at NCL. We expect to validate the fermentation process in an industrial reactor by the third quarter of 2007 and commission a 300 tons per annum continuous downstream recovery plant by the third quarter of 2008. We licensed a series of patents issued to NCL for a solid catalyst for trans-esterification of triglycerides to fatty acid esters (bio-diesel) to a start up



company. The company is raising capital to set up a demonstration plant based on these patents. Financial closure is expected to be achieved by end 2007.

These are important milestones in NCL's march towards being a reliable technology partner. We have successfully used three models for technology transfer and implementation. In the case of epichlorohydrin the early R&D was done by NCL. The patents and knowhow were then licensed to a company. NCL in collaboration with the company validated the commercial viability of the process through bench scale experimentation performed at NCL. The basic engineering package was also prepared by NCL. In case of the two NMITLI projects the programme was set up as a public private partnership with industry involvement right from early stages of project implementation. In case of the last project, namely, biodiesel, NCL licensed the patents and helped the birth of a start up enterprise, which in turn raised finances in the market, based on the robustness of the intellectual property generated by NCL. These examples clearly mark the coming of age of NCL with regard to translating science and technology into wealth in society.

NCL continues to build its research as well as physical infrastructure. Several new analytical facilities were added during the year, which included a multipass rheometer, laser light scattering equipment and a high power excimer laser. A high performance 32 nodes computational cluster was installed. NCL broke ground for a new 80,000 square feet Polymers and Advanced Materials Laboratory. This is the first new laboratory building in NCL, being built in over twenty five years. The laboratories should be ready for occupation by the last quarter of 2008.

NCL Innovation Park was formally launched in December 2006, marking the commencement of the first phase of the activity. The Technology Business Incubator will become fully operational by the first quarter of 2008. To manage the incubator facility NCL floated a new not for profit company under Section 25 of the Companies Act, christened, Entrepreneurship Development Center. The company came into existence in January 2007. These new initiatives will provide additional new channels of converting knowledge into wealth for NCL and the nation, at large.

Many of our scientists continue to make NCL proud. Dr

Ashish Lele was bestowed the SS Bhatnagar Prize in Engineering Sciences. Dr Srinivas Hotha had the unique distinction of winning both the CSIR and INSA Young Scientists award for the year. Several of our scientists were bestowed the J.C.Bose and Ramanna Fellowships by DST. We were also honored to welcome back Dr R.A.Mashelkar to NCL as a CSIR Bhatnagar Fellow after his superannuation as DG-CSIR. We also bid farewell to two of our distinguished colleagues. Dr K.N.Ganesh assumed charge as the Founding Director of the Indian Institute of Science Education and Research (IISER-Pune). Dr R.V.Chaudhari, Head of the Homogeneous Catalysis Division retired from NCL and went on to assume the position of Deane E. Ackers Distinguished Professor in the Department of Chemical and Petroleum Engineering, at the University of Kansas at Lawrence, Kansas, USA. We wish both of them very well in their new found careers.

NCL is at an exciting crossroad. A major transformation of both leadership and ideas is beginning to unfold. It faces the unique challenge of, on the one hand, heralding new frontiers of research for the future while at the same time preserving its strengths and strong traditions of the past. I am confident that NCL will meet this challenge admirably.

I wish to gratefully acknowledge the support and cooperation of all my staff, members of the Research and Management Council of NCL, DG-CSIR and staff of CSIR, New Delhi and our valued stakeholders. Without their counsel, cooperation and confidence, much of what was accomplished would have been impossible.

*S. Sivaram*

(S.Sivaram)



Vision

- To be a globally recognized and respected R&D organization in the area of chemical sciences and engineering.
- To become an organization that will contribute significantly towards assisting the Indian chemical and related industries in transforming themselves into globally competitive organizations.
- To become an organization that will generate opportunities for wealth creation for the nation and, thereby, enhance the quality of life for its people.

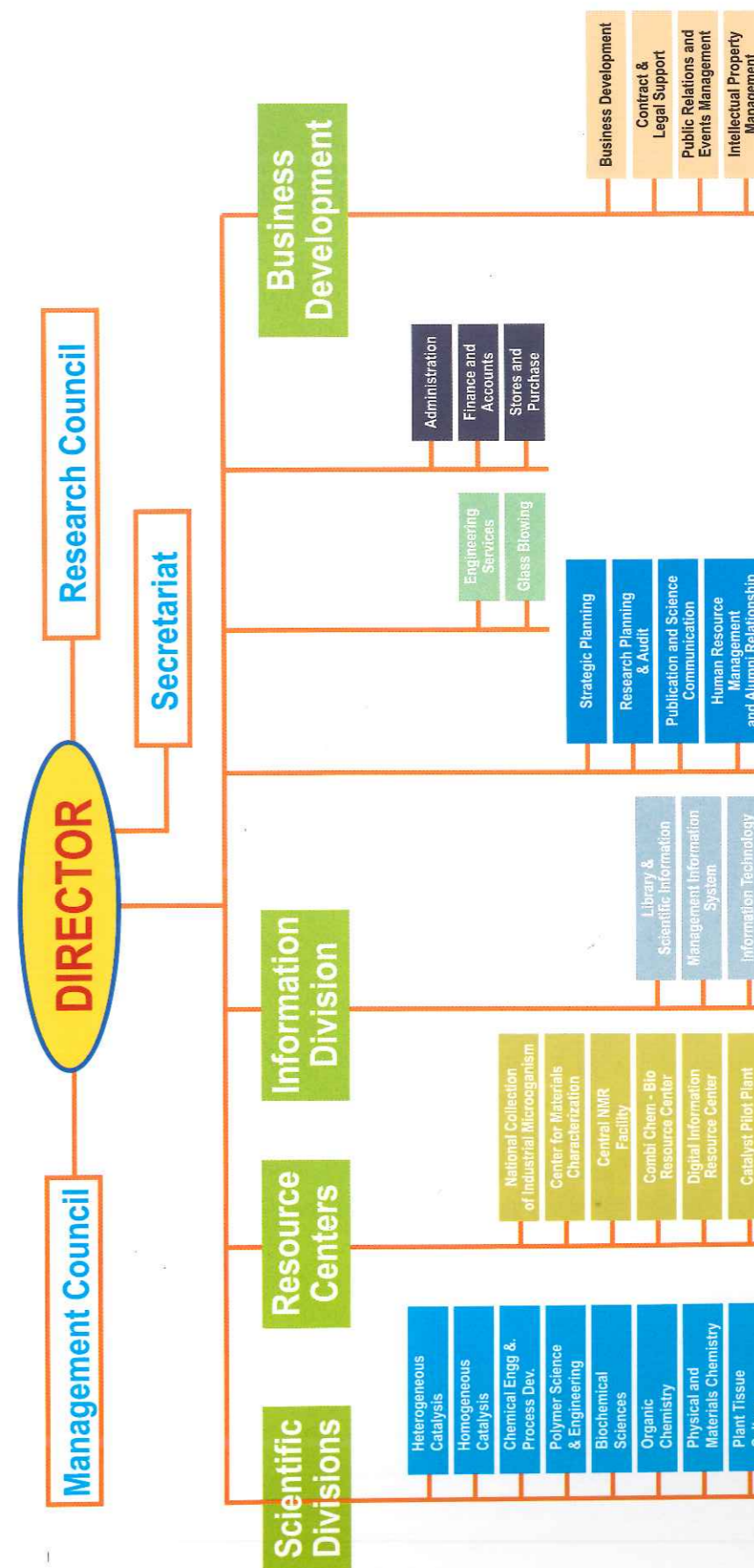
Mission

- To carry out R&D in chemical and related sciences with a view to eventually deliver a product, process intellectual property, tacit knowledge or service that can create wealth and provide other benefits to NCL's stakeholders.
- To build and maintain a balance portfolio of scientific activities as well as R&D programs to enable NCL to fulfill the demands of its stakeholders, present and future.
- To create and sustain specialized Knowledge Competencies and Resource Centers within NCL which can provide support to all stakeholders of NCL.

Guiding Principles & Values

- To be deeply committed to the success of our stakeholders.
- To create and sustain a self driven and self managed learning organization with a high degree of internal and external transparency.
- To encourage a culture of collective and principle-centred leadership.
- To value the dignity of the individual and deal with people with a sense of fairness and without bias, prejudice or favour.
- To nurture the highest standards of integrity and ethical conduct.

Organizational Chart





## Research Areas

## Catalysts

- Heterogeneous
- Homogeneous

## Biochemical Sciences

- Enzymology and microbiology
- Plant biochemistry and molecular biology
- Plant tissue culture

## Organic Chemistry

- Chiral synthesis
- New Synthetic methods
- Process chemistry for active pharmaceutical intermediates
- Multistep organic synthesis of complex organic molecules
- Chemical biology and Bio-organic chemistry
- Molecular diversity based chemical genetics

## Polymer Science and Engineering

- Polymer chemistry
- Polymer physics
- Complex fluids and polymer engineering
- Polymer and materials modeling

## Physical and Materials Chemistry

- Nanomaterials science and technology
- Materials chemistry
- Theory and computational science

## Chemical Engineering Science

- Reaction Engineering
- Process simulation and modeling
- Biochemical engineering
- Industrial flow modeling
- Process design and development of processes for fine chemicals and polymers

## Knowledge Competencies

- Chemical biology and Bio-organic chemistry
- Chemical Engineering Science
- Complex Fluids and Polymer Engineering
- Enzymology and Microbiology
- Heterogeneous Catalysis
- Homogeneous Catalysis
- Industrial Flow Modeling
- Materials Chemistry
- Nanomaterials : Science and Technology
- Organic Chemistry
- Plant Biochemistry and Molecular Biology
- Plant Tissue Culture
- Polymer and Materials Modeling
- Polymer Chemistry and Materials
- Process Design, Development and Engineering
- Theory and Computational Science

## Research Council (1 Jan. 2004 To 31 Dec. 2006)

## Chairman

**Prof. M.M. Sharma,**  
2/3, Jaswant Baug, Behind Akbarallys,  
VN Purav Marg, Chembur,  
Mumbai 400 071.

## Members

**Prof. S. Chandrasekaran,**  
Department of Organic Chemistry,  
Indian Institute of Science,  
Bangalore 560 012.

**Prof. Ajay Kumar Sood,**  
Chairman,  
Department of Physics,  
Indian Institute of Science,  
Bangalore 560 012.

**Prof. M.S. Ananth,**  
Director,  
Indian Institute of Technology,  
Chennai 600 036.

**Dr. K.V.S. Rao,**  
Head, Immunology Group,  
International Centre for Genetic  
Engg. & Biotechnology,  
ICGEB Campus, Aruna Asaf Ali Marg,  
New Delhi 110 067.

**Shri. Sujit Banerjee,**  
Senior Vice President, (Polymer)  
Planning Research and Business  
Development, RIL, Reliance Centre,  
19, Walchand Hirachand Marg,  
Ballard Estate, Mumbai 400 038.

**Dr. S. Sivaram,**  
Director,  
NCL, Pune 411 008.

## Dr. J.M. Khanna,

Executive Director and President,  
Jubilant Organo Systems Ltd.,  
1-A, Sector 16-A, Institutional Area,  
Noida 201 301.

## Dr. G. N. Qazi,

Director,  
Regional Research Laboratory,  
Canal Road, Jammu 181 001.

## DG's Nominee

## Dr. J.S. Yadav,

Director, Indian Institute of Chemical Technology,  
Uppal Road,  
Hyderabad 500 007.

## Permanent Invitee, President of ICMA

## Mr. Deepak Mehta,

Managing Director,  
Deepak Nitrite,  
National Games Road,  
Shastri Nagar, Yerawada, Pune

## Permanent Invitee, CSIR

## Dr. O. P. Agarwal,

Head, R&D Planning Division,  
CSIR, Anusandhan Bhawan,  
2, Rafi Marg, New Delhi 110 001.

## Member Secretary

**Dr. G.S. Grover,**  
Head, Research Planning & Audit Unit,  
NCL, Pune 411008.



## RESEARCH COUNCIL

Research Council (1 Jan. 2007 To 31 Dec. 2009)

### Chairman

**Prof. D. Balasubramanian,**  
Research Director, L.V. Prasad Eye Institute,  
Road No. 2, Banjara Hills, Hyderabad 500 034.

### Members

**Prof. Dipankar Chatterji,**  
Molecular Biophysics Unit,  
Indian Institute of Science,  
Bangalore 560 012.

**Dr. Amit Biswas,**  
Senior Vice President (R&T)  
Reliance Industries Limited,  
Swastik Mill Compound,  
V.N. Purav Marg, Chembur,  
Mumbai 400 071.

**Prof. S. Chandrasekaran,**  
Department of Organic Chemistry  
Indian Institute of Science,  
Bangalore 560 012.

**Prof. S.K. Sopory,**  
Group Leader,  
Plant Molecular Biology,  
International Centre for Genetic  
Engineering & Biotechnology,  
Aruna Asaf Ali Marg,  
New Delhi 110 067.

**Prof. A.K. Shukla,**  
Director,  
Central Electrochemical Research Institute,  
Karaikudi 630 006.

**Dr. S. Sivaram,**  
Director,  
NCL, Pune 411 008.

### Member Secretary

**Dr. G.S. Grover,**  
Head, Research Planning & Audit Unit,  
NCL, Pune 411008.

**Dr. Pradip K. Bhatnagar,**  
Senior Vice President,  
New Drug Discovery Research  
Ranbaxy Laboratories Limited  
Plot No.20, Sector 18,  
Udyog Vihar Industrial Area  
Gurgaon 122 015

**Shri R. Saha,**  
Adviser & Head  
Science & Society Division  
Department of Science & Technology  
Technology Bhawan, New Mehrauli Road  
New Delhi 110 016.

**Dr. S. K. Bramhachari,**  
Director,  
Institute of Genomics and Integrative Biology,  
University Campus,  
Mall Road,  
Delhi 110 007.

**Dr. Naresh Kumar,**  
Head,  
R&D Planning Division  
Council of Scientific & Industrial Research  
Anusandhan Bhavan,  
Rafi Marg,  
New Delhi 110 001.



## MANAGEMENT COUNCIL

Management Council (1 July 2005 To 30 April 2007)

### Chairman

**Dr. S. Sivaram**  
Director NCL, Pune 411 008.

### Members

**Dr. B.D. Kulkarni,**  
Deputy Director, NCL

**Dr. Rajiv Kumar,**  
Scientist, NCL

**Dr. Ganesh Pandey,**  
Scientist, NCL

**Mr. P. Venugopal,**  
Scientist, NCL

**Dr.(Mrs.) Veda Ramaswamy,**  
Scientist, NCL

**Mr. D.B. Pradhan,**  
Technical Officer, NCL

**Dr. Ashish K. Lele,**  
Scientist, NCL

**Mr. S. Chandrahas,**  
Senior F&AO, NCL

### Member-Secretary

**Mr. M.S. Vidyanathan,**  
Controller of Administration, NCL

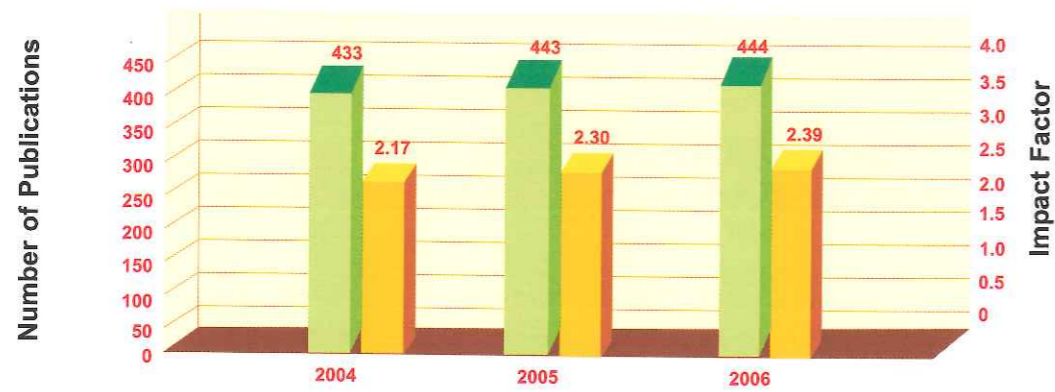




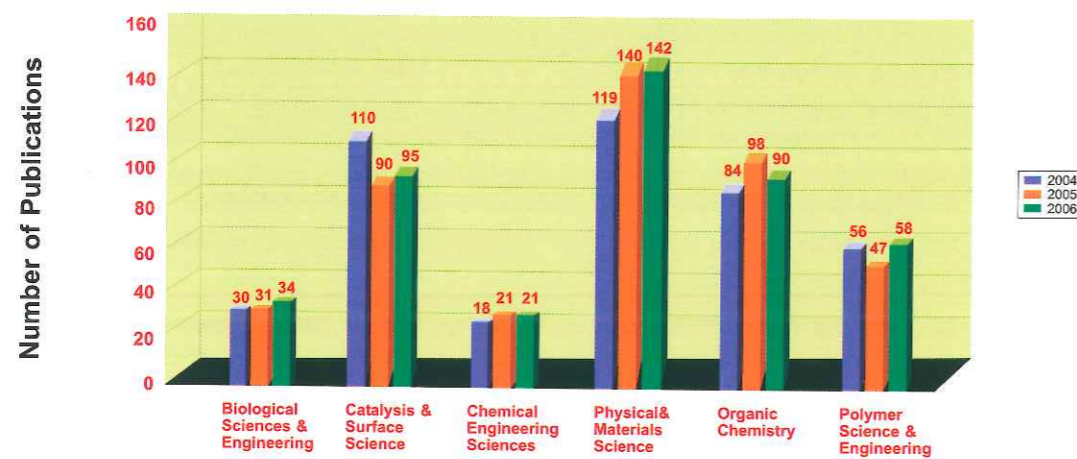
## PERFORMANCE INDICATORS

### SCIENCE PERFORMANCE INDICATORS

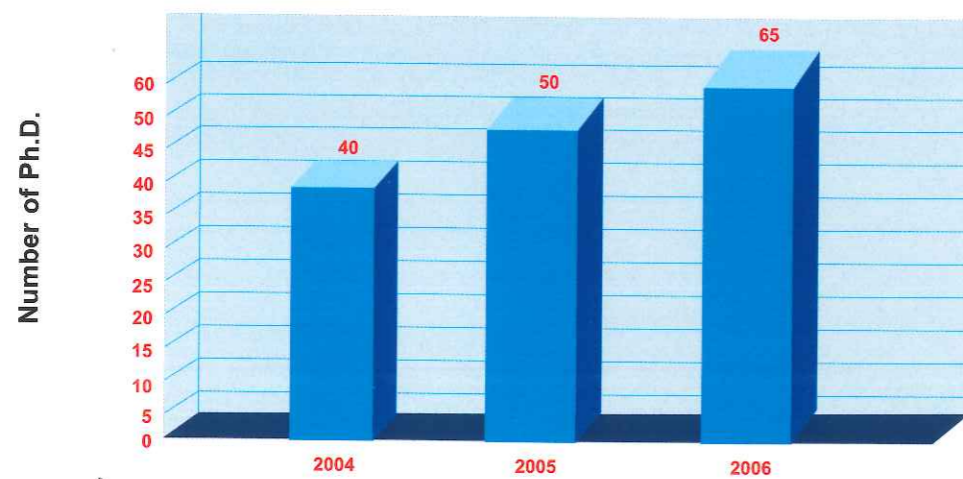
#### Publications



#### Area wise publications



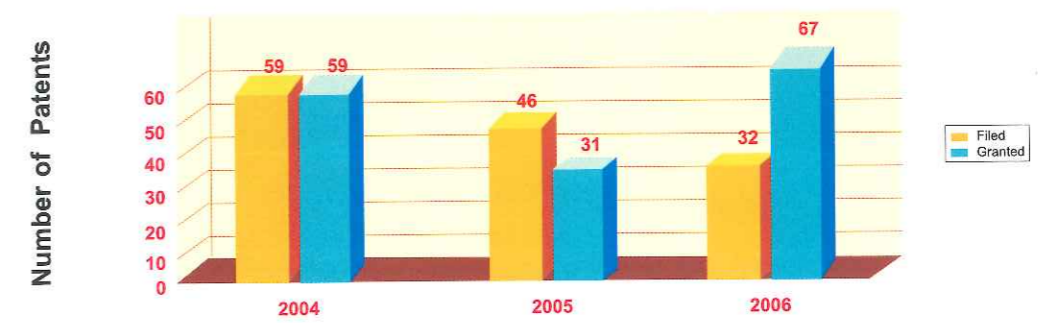
#### Ph.D. awarded



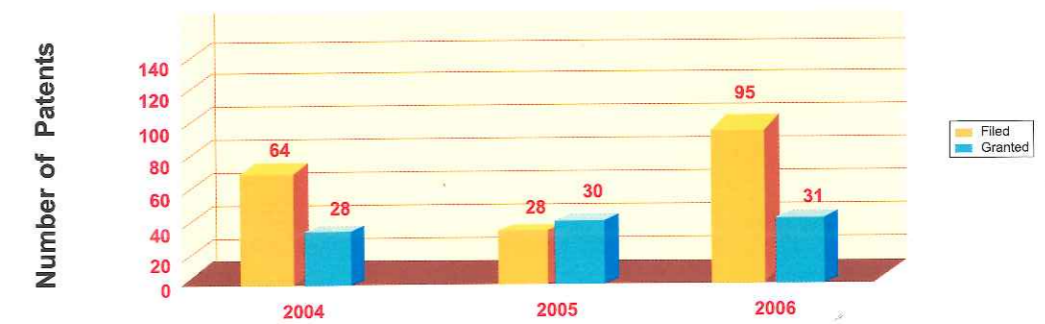
## PERFORMANCE INDICATORS

### TECHNOLOGY PERFORMANCE INDICATORS

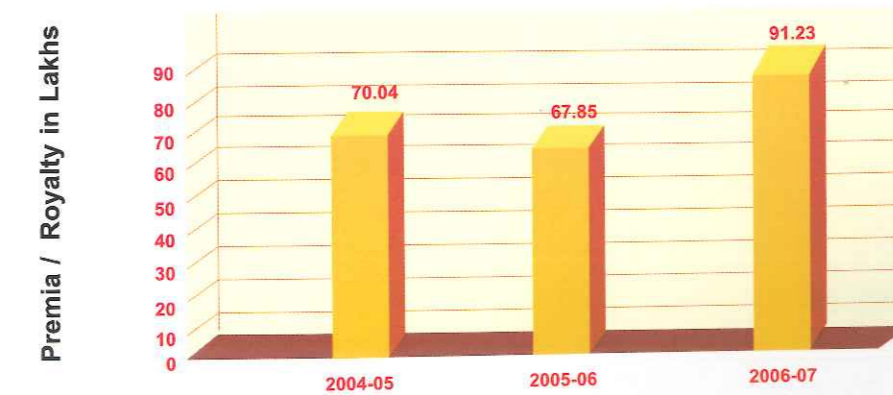
#### Indian Patents : Filed and Granted



#### Foreign Patents : Filed and Granted



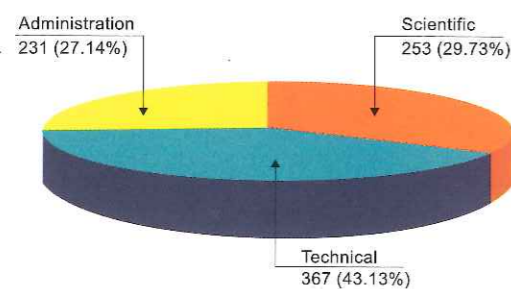
#### Premia / Royalty Earnings



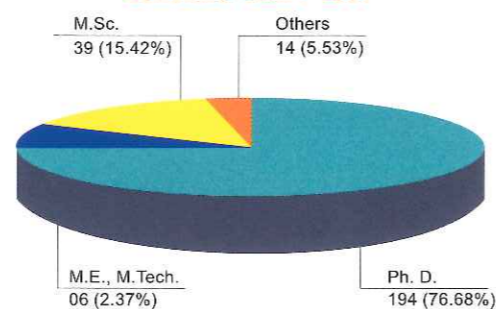


## HUMAN RESOURCE INDICATORS

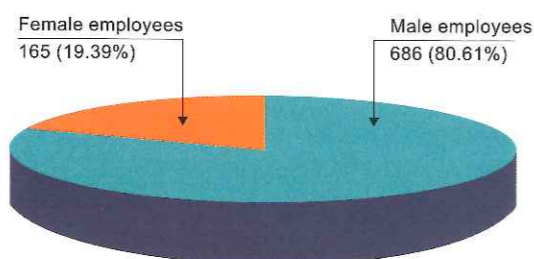
Total Staff : 851



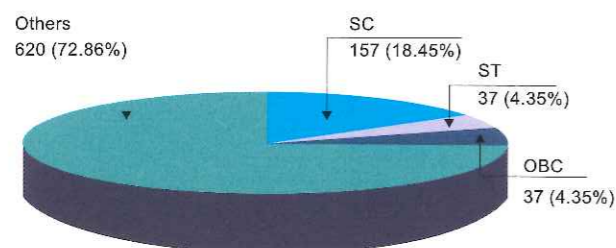
Scientific Staff : 253



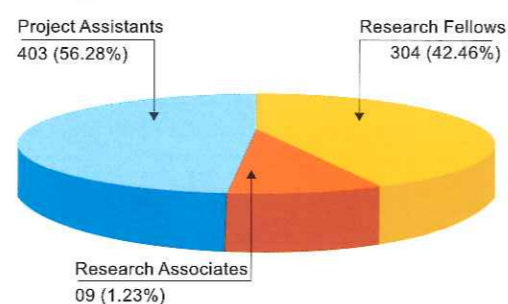
Male : Female ratio



SC, ST and OBC employees



Number of Students and Project Staff : 716



Scientist: agewise distribution

Grade	Number	Average age
Sci. B	27	36.01
Sci. C	29	39.99
Sci. E I	57	48.64
Sci. E II	93	52.49
Sci. F	39	55.63
Sci. G	07	55.69



## We welcome...

Name and date of joining	Subject	Qualifications
 Dr. R. Nandini Devi (3 May 2006)	Catalysis	Post Doctoral Fellow : Syracuse University, NY, USA; St. Andrews University, UK; Queen's University Belfast, UK.  Ph.D. (Chemistry) IIT Madras.  M.Sc. (Chemistry) IIT Madras.
 Mrs. Anuya Nisal (5 May 2006)	Polymer Science & Engineering	M.S. (Polymer Engineering) University of Delaware, USA.  B.E. (Polymer Science), Pune University
 Dr. Suresh Kumar Bhat (12 June 2006)	Polymer Science & Engineering	Post Doctoral Fellow (JSPS Fellow) : University of Tokyo, Japan; University of Fribourg, Switzerland.  Ph.D. (Physics), IIT Delhi.  M.Tech. (Applied Optics), IIT Delhi.
 Dr. Thulasiram H. V. (14 Aug. 2006)	Organic Chemistry	Post Doctoral Fellow : Dept. of Chemistry, University of Utah, USA; Dept. of Biochemistry, University of Iowa, USA.  Ph.D. (Organic Chemistry) Indian Institute of Science, Bangalore.



## PERFORMANCE INDICATORS

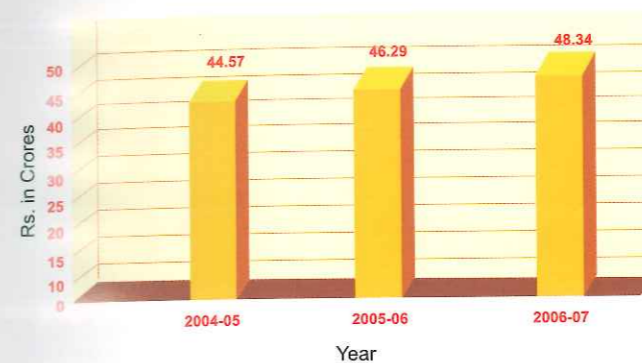
Name and date of joining	Subject	Qualifications
 Dr. Chetan J. Gadgil (6 Nov. 2006)	Computational Biology	Post Doctoral Fellow : Mathematics, University of Minnesota, USA.  Staff Scientist, GlaxoSmithKline R&D, USA.  Ph.D. (Chemical Engineering), University of Minnesota, USA.
 Dr. Mugdha Gadgil (13 Nov. 2006)	Mammalian Cell Engineering and Gene Expression	Post Doctoral Fellow : University of Minnesota, USA; Scientist, Invitrogen Corp, MD, USA.  Ph.D. (Chemical Engineering), University of Minnesota, USA.  B. Chem. Eng., UICT, Mumbai.
 Dr. Sayam Sen Gupta (16 Dec. 2006)	Catalysis and Materials Science	Post Doctoral Fellow : The Scripps Research Institute, La Jolla, CA, USA; Humboldt Fellow at Technical University, Munich, Germany.  Ph.D. (Chemistry), Carnegie Mellon University, Pittsburgh, USA.
 Arti Harle (8 Feb. 2007)	Electron Microscopy	Scientist B; IMT-Chandigarh; Research Assistant; SAIF, IIT- Mumbai; Scientific Assistant, RSIC, Nagpur University.  M.Sc. (Zoology) Nagpur University.



## PERFORMANCE INDICATORS

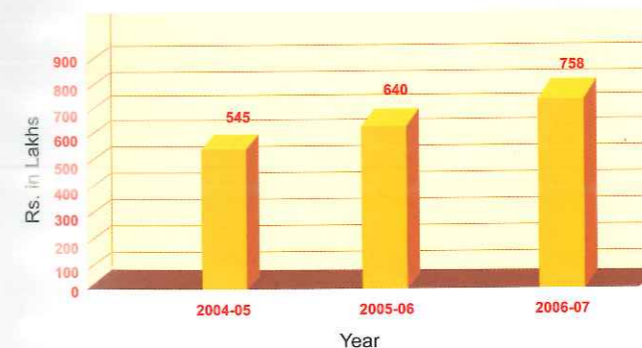
### FINANCIAL PERFORMANCE INDICATORS

#### CSIR budget

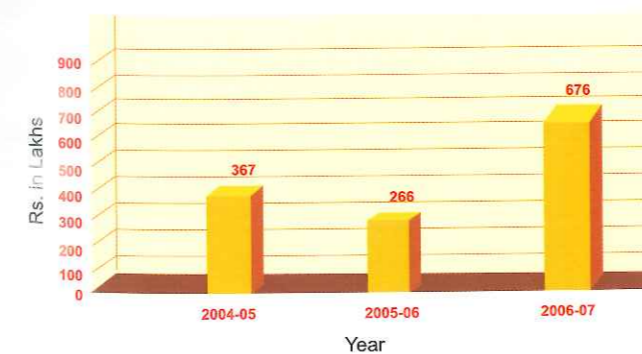


(CSIR Budget : 34.04 + Network Project : 10.53)  
(CSIR Budget : 39.96 + Network Project : 06.32)  
(CSIR Budget : 43.38 + Network Project : 04.18 + NMITLI Projects : 00.78)

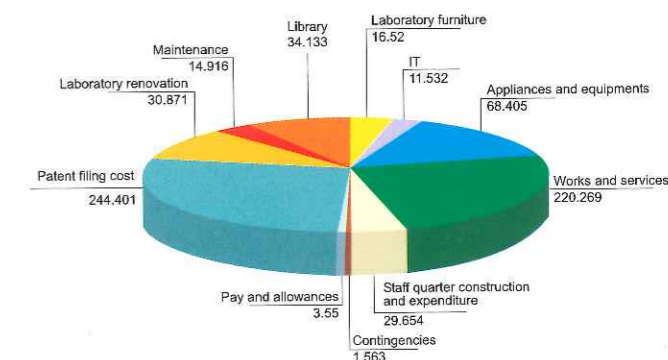
#### Laboratory reserve: Receipts



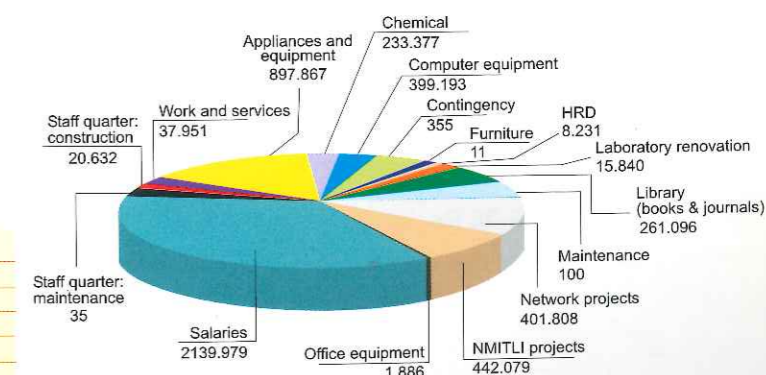
#### Laboratory reserve: Expenditure



#### Expenditure: Laboratory reserve 2006-2007 (Rs.675.872 Lakhs)



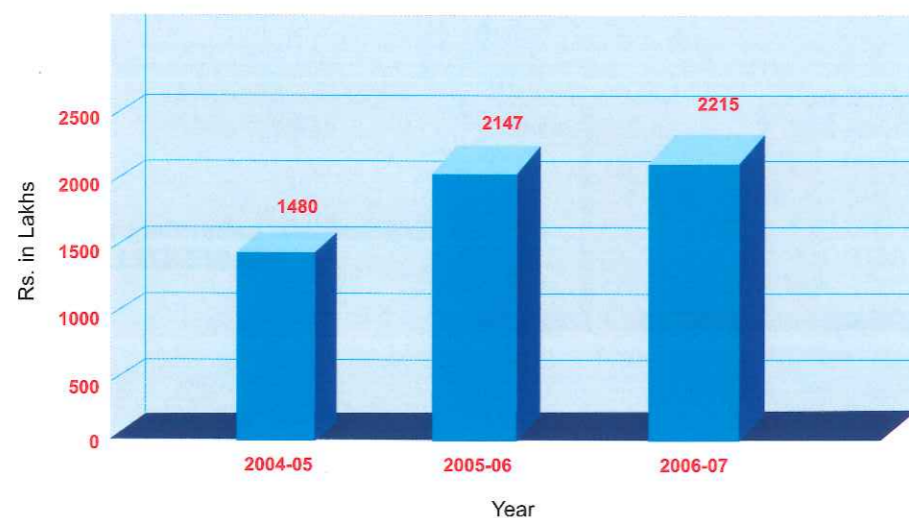
#### Expenditure: CSIR and Network Projects 2006-2007 (Rs.5360.939 Lakhs)



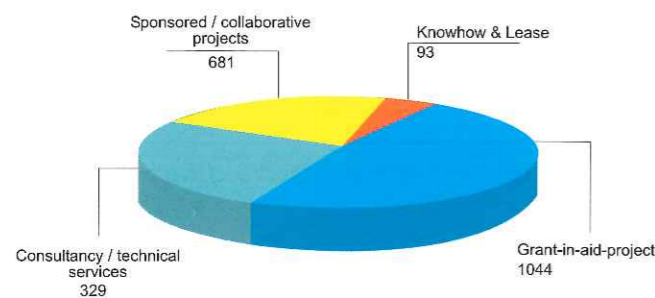


## PERFORMANCE INDICATORS

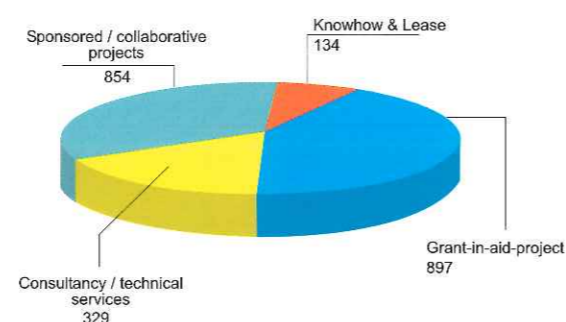
### External Income



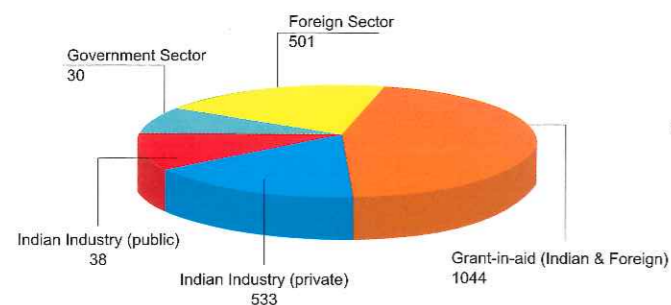
### ECF : Project wise break-up 2005-06 Rs. 2147 Lakhs



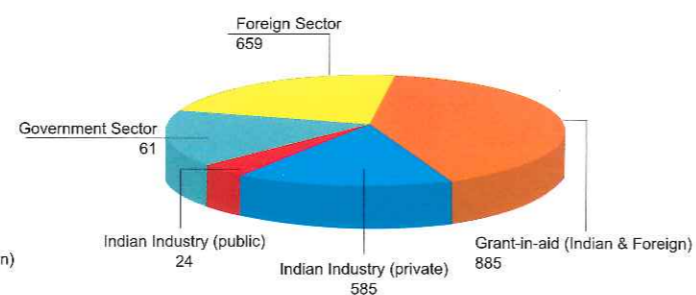
### ECF : Project wise break-up 2006-07 Rs. 2215 Lakhs



### ECF : by source 2005-06 Rs. 2147 Lakhs



### ECF : by source 2006-07 Rs. 2215 Lakhs



## PERFORMANCE INDICATORS

### FINANCIAL PERFORMANCE INDICATORS

#### Capital and recurring expenditure on R&D (2005-2007)

Rs. in Lakhs

Source	Capital		Recurring	
	2005-06	2006-07	2005-06	2006-07
CSIR	1146	1299	315	233
Lab Reserve	46	324	18	0
External Projects	720	355	1330	1444
Network Projects	415	196	301	206
NMITLI Projects	147	227	124	215
Total	2474	2401	2088	2098
%	54	53	46	47

NMITLI - New Millennium Indian Technology leadership Initiative

#### Ongoing publicly funded mission mode and internal projects (2006-07)

Sr. No.	Description	Rs. in Lakhs
1	CSIR NMITLI	77.94
2	Major publicly funded projects (DST, DBT, NPSM, SDC, McNIGHT etc.)	894.47
3	X Five year plan network projects	417.87
4	Internal projects *	95.85
	Grand Total	1489.13

\* - Funded from Lab Reserve of NCL

#### Scientific Budget (2006-07)

Funding Source

Rs. in Lakhs

	Recurring	Capital	Total
CSIR	200	200	400
LR	567.65	840.24	1407.89
Total	767.65	1040.24	1807.89

10 Lakhs=1 Million



## PERFORMANCE INDICATORS

### 1. OUTPUTS AND OUTCOMES

#### Select outputs and outcomes of NCL during 2004-2007

Category of benefit	Benefit	Indicators	2004-05	2005-06	2006-07
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in foreign peer-reviewed journals/ publications(Calendar year)	395	414	425
		Number of papers published in Indian journals(Calendar year)	24	17	19
		Average Impact Factor	2.17	2.30	2.39
		Number of patents filed in India (Calendar year)	59	46	32
		Number of patents commercialized / assigned	4	2	5
		Number of major national/ regional collections, compilations databases	3	3	3
	Highly trained man-power (Calendar year)	Number of PhDs produced	40	50	65
		Number of NET/GATE qualified students joined	35	30	28
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	8	4	NA
		Number of national and regional workshops, seminars organized	12	12	11
Pride and standing among nations; National image	Number of international awards won	1*	1**	1***	
	Memberships of major international academies and learned societies (Cumulative membership years)	7	7	7	
	Memberships of editorial boards of international peer-reviewed journals (Cumulative membership years)	26	30	31	
	Number of papers in foreign peer-reviewed journals	395	414	425	
	Number of IF research papers	387	379	426	
	Number of foreign patents granted (Calendar year)	28	30	31	
	Representation in global affairs	Official(s) in global/ trans-national organizations like the UN, WHO etc - IUPAC (Cumulative years of office held) (Data given in no. of years)	6	6	4

\*- IZA: Dr Paul Ratnasamy

\*\*- TWAS: Dr. K.N. Ganesh

\*\*\*- Khwarizmi International Award: Dr. R. P. Singh

1 Crore = 10 Million



## PERFORMANCE INDICATORS

### OUTPUTS AND OUTCOMES

Category of benefits	Benefit	Indicators	2004-05	2005-06	2006-07
Private goods	Research, consulting, teaching and analytical	Total earnings from projects done for Indian & Foreign businesses/ industry (Rs. in Crore) (Industrial ECF, excluding Grant-in-Aid)	9.28	11.02	13.17
	Continuing education	Total earnings from continuing education/ training programs (Rs. in Crore)	NA	0.17	NA
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (Rs. Crore)	0.70	0.68	0.91
Strategic goods and options	Contributions to projects involving valuable opportunities in the form of technology option	Money inflow from NMITLI projects and other similar strategic projects (Rs. in Crore)	5.68	4.70	0.78
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (Rs. in Crore)	5.33	10.44	8.97
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	Number of papers in foreign peer-reviewed journals	395	414	425
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	10	17	17
		Number of PhDs granted where lab scientists were research guides	40	50	65
		Number of staff who are members of National academies (Cumulative)	27	27	27
		Number of Bhatnagar awardees Cumulative)	13	13	14
		Number of Padma awardees (Cumulative)	4	5	5
	Lab's standing with industry	Total worth of projects with industry (only industry: both Indian & foreign) (excluding Grant-in-Aid) (Rs. in Crore)	9.28	11.02	13.17

\* - Individuals who are members of more than one academy have been counted only once.

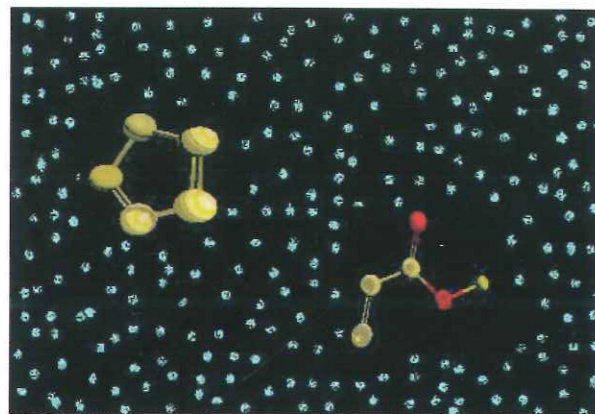


## TOP PAPERS (2006)

Pandey G., Banerjee P., Gadre S.R., Construction of enantiopure pyrrolidine ring system via asymmetric [3+2]-cycloaddition of azomethine ylides, *Chemical Reviews*, 106(11), 4484-4517

Tiwari S., Kumar A., Diels-Alder reactions are faster in water than in ionic liquids at room temperature, *Angewandte Chemie - International Edition*, 45(29), 4824-4825

**Abstract:** A comparative study indicates that water, rather than room-temperature ionic liquids (RTILs), is still the solvent of choice for accelerating Diels-Alder reactions. Both the hydrogen-bonding ability and the viscosity of the solvent are thought to play a role.



Diffusion of diene and dienophile through viscous ionic liquid

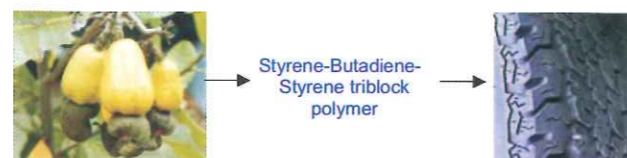
Satav S.S., Karmalkar R.N., Kulkarni M.G., Mulpuri N., Sastry G.N., Formation of linear polymers with pendant vinyl groups via inclusion complex mediated polymerization of divinyl monomers, *Journal of the American Chemical Society*, 128(24), 7752-7753

**Abstract:** Ethylene glycol dimethacrylate (EGDMA) and ethylene glycol methacrylate 4-vinyl benzoate (EGMAVB) were shown to form 1:1 inclusion complexes with cyclodextrin and were characterized by instrumental techniques. Computational analysis showed that the bent conformation of the included divinyl monomer was more stable than its linear conformation. Complexation of the divinyl monomer with the first CD molecule offered substantial stabilization than with the second CD molecule. The vinyl group included in the CD cavity did not participate in polymerization. As a result, solvent

soluble, linear polymers with pendant vinyl unsaturation per repeat unit were obtained. This was unequivocally established by the polymerization of a complex comprising CD and EGMAVB. The unreacted vinyl group can be polymerized in the subsequent step to yield cross-linked products.

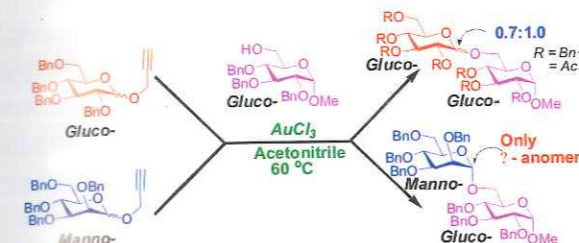
Matmour R., More A.S., Wadgaonkar P.P., Gnanou Y., High performance poly(styrene-*b*-diene-*b*-styrene) triblock copolymers from a hydrocarbon-soluble and additive-free dicarbanionic initiator, *Journal of the American Chemical Society*, 128(25), 8158-8159

**Abstract:** A new hydrocarbon-soluble (additive-free) dicarbanionic organolithium initiator, obtained by a simple halogen-lithium exchange reaction (Gilman's reaction) from a diarylhalide containing a side  $C_{15}$  alkyl chain, has been designed and used to initiate the anionic polymerization of butadiene and styrene. The dilithiated species formed afford well-defined poly(styrene-*b*-butadiene-*b*-styrene) (SBS) triblock copolymers with a high percentage of 1,4-microstructure polybutadiene (91%) and excellent mechanical properties, such as ultimate tensile strength higher than 30 MPa and elongation at a break of 1000%. This represents a breakthrough in the synthesis of SBS polymers, one of the most used thermoplastic elastomers.



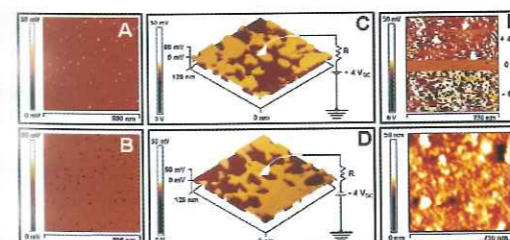
Hotha S., Kashyap S., Propargyl glycosides as stable glycosyl donors: Anomeric activation and glycoside syntheses, *Journal of the American Chemical Society*, 128(30), 9620-9621

**Abstract:** The advantages of stable glycosyl donors for saccharide coupling are many, and we describe herein the utility of propargyl glycosides for anomeric activation and glycoside synthesis exploiting the alkynophilicity of  $AuCl_3$ . Various aglycones were reacted with propargyl glycosides, resulting in the formation of an  $\alpha,\beta$ -mixture of glycosides and disaccharides in good yields.



Bansal V., Poddar P., Ahmad A., Sastry M., Room-temperature biosynthesis of ferroelectric barium titanate nanoparticles, *Journal of the American Chemical Society*, 128(36), 11958-11963

**Abstract:** The syntheses of inorganic materials by biological systems is characterized by processes that occur close to ambient temperatures, pressures, and neutral pH, as is exemplified by biosilicification and biomineralization processes in nature. Conversely, laboratory-based syntheses of oxide materials often require extremes of temperature and pressure. We have shown here the extracellular, room-temperature biosynthesis of 4-5 nm ternary oxide nanoparticles such as barium titanate (BT) using a fungus-mediated approach. The tetragonality as well as a lowered Curie transition temperature in sub-10 nm particles was established, and the ferroelectricity in these particles was shown using Kelvin probe microscopy.

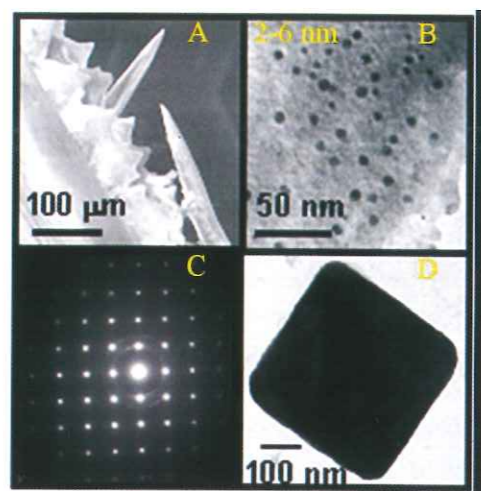


(A-D) Low magnification (A and B) and higher magnification (C and D) SPM images from BT particles obtained in potential mode after application of +4 V (A and C) and -4 V (B and D) external DC bias voltages respectively. (E and F) Potential image of BT particles obtained after sequential application of +4, 0, and -4 V external DC bias voltages to the conductive AFM tip (E) and height image of BT particles without any external bias voltage (F).

Bansal V., Ahmad A., Sastry M., Fungus-mediated biotransformation of amorphous silica in rice husk to nanocrystalline silica, *Journal of the American Chemical Society*, 128(43), 14059-14066

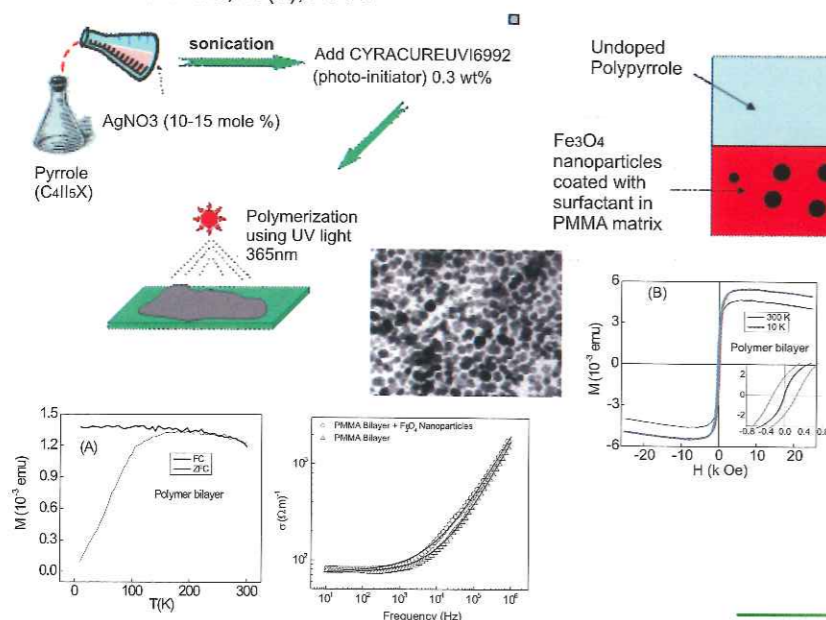
**Abstract:** Rice husk is a cheap agro-based waste material, which harbors a substantial amount of silica in the form of amorphous hydrated silica grains. However, there have been no attempts at harnessing the enormous amount of amorphous silica present in rice husk and its room-temperature biotransformation into crystalline silica nanoparticles. In this study, we address this issue and describe how naturally deposited amorphous biosilica in rice husk can be bioleached and simultaneously biotransformed into high value crystalline silica nanoparticles. We show here that the fungus *Fusarium oxysporum* rapidly biotransforms the naturally occurring amorphous plant biosilica into crystalline silica and leach out silica extracellularly at room temperature in the form of 2-6 nm quasi-spherical, highly crystalline silica nanoparticles capped by stabilizing proteins; that the nanoparticles are released into solution is an advantage of this process with significant application and commercial potential. Calcination of the silica nanoparticles leads to loss of occluded protein and to an apparently porous structure often of cubic morphology. The room-temperature synthesis of oxide nanomaterials using microorganisms starting from potential cheap agro-industrial waste materials is an exciting possibility and could lead to an energy-conserving and economically viable green approach toward the large-scale synthesis of oxide nanomaterials.





A: SEM micrograph showing an edge of a single rice husk flask.  
 B: TEM micrograph of silica nanoparticles synthesized by the exposure of rice husk to the fungus, *Fusarium oxysporum*.  
 C: SAED patterns recorded from silica nanoparticle shown in image  
 D: TEM micrograph of silica nanoparticles synthesized by the exposure of rice husk to the fungus *Fusarium oxysporum* after calcination at 400 °C for 2 hour.

Gass J., Poddar P., Almand J., Srinath S., Srikanth H., Superparamagnetic polymer nanocomposites with uniform Fe<sub>3</sub>O<sub>4</sub> nanoparticle dispersions, *Advanced Functional Materials*, 16(1), 71-75



**Abstract:** Magnetic nanoparticles embedded in polymer matrices are good examples of functional nanostructures with excellent potential for applications

such as electromagnetic interference shielding, magneto-optical storage, biomedical sensing, flexible electronics, etc. Control over the dispersion of the nanoparticle phase embedded in a polymer matrix is critical and often challenging. To achieve excellent dispersion, competition between polymer-polymer and polymer-particle interactions have to be balanced to avoid clustering of particles in polymer nanocomposites. We report the first deposition of magnetic nanocomposite poly(methyl methacrylate)/polypyrrole bilayers from solution using spin-coating. Fe<sub>3</sub>O<sub>4</sub> nanoparticles have been synthesized using a chemical co-precipitation route. Using a combination of dissolving the polymer and mixing fatty acid surfactant coated Fe<sub>3</sub>O<sub>4</sub> nanoparticles, we have demonstrated the formation of nanocomposites with uniform nanoparticle dispersion. Cross-sectional scanning electron microscopy, transmission electron microscopy, and magnetic measurements confirm the excellent dispersion and super-paramagnetic response. Low-frequency impedance measurements on these bilayers are also presented and analyzed.

Giri A.P., Wunsche H., Mitra S., Zavala J.A., Muck A., Svatos A., Baldwin I.T., Molecular interactions between the specialist herbivore *Manduca sexta* (Lepidoptera, Sphingidae) and its natural host *Nicotiana attenuata*. VII.



Changes in the plant's proteome, *Plant Physiology*, 142(4), 1621-1641.

**Abstract:** When *Manduca sexta* attacks *Nicotiana attenuata*, fatty acid-amino acid conjugates (FACs) in the larvae's oral secretions (OS) are introduced into feeding wounds. These FACs trigger a transcriptional response that is similar to the response induced by insect damage. Using two-dimensional gel electrophoresis, matrix-assisted laser desorption ionization-time of flight, and liquid chromatography-tandem mass spectrometry, we characterized the proteins in phenolic extracts and in a nuclear fraction of leaves elicited by larval attack, and/or in leaves wounded and treated with OS, FAC-free OS, and synthetic FACs. Phenolic extracts yielded approximately 600 protein spots, many of which were altered by elicitation, whereas nuclear protein fractions yielded approximately 100 spots, most of which were unchanged by elicitation. Reproducible elicitor-induced changes in 90 spots were characterized. In general, proteins that increased were involved in primary metabolism, defense, and transcriptional and translational regulation; those that decreased were involved in photosynthesis. Like the transcriptional defense responses, proteomic changes were strongly elicited by the FACs in OS. A semiquantitative reverse transcription-PCR approach based on peptide sequences was used to compare transcript and protein accumulation patterns for 17 candidate proteins. In six cases the patterns of elicited transcript accumulation were consistent with those of elicited protein accumulation. Functional analysis of one of the identified proteins involved in photosynthesis, RuBPCase activase, was accomplished by virus-induced gene silencing. Plants with decreased levels of RuBPCase activase protein had reduced photosynthetic rates and RuBPCase activity, and less biomass, responses consistent with those of herbivore-attacked plants. We



conclude that the response of the plant's proteome to herbivore elicitation is complex, and integrated transcriptome-proteome-metabolome analysis is required to fully understand this ubiquitous ecological interaction.



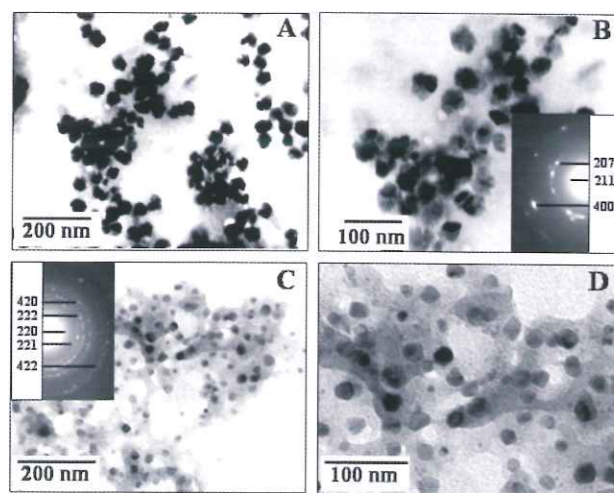
Plant responds to insect damage by producing novel proteins

Bharde A., Rautaray D., Bansal V., Ahmad A., Sarkar I., Yusuf S.M., Sanyal M., Sastry M., Extracellular biosynthesis of magnetite using fungi, *Small*, 2(1), 135-141

**Abstract:** The development of synthetic processes for oxide nanomaterials is an issue of considerable topical interest. While a number of chemical methods are available and are extensively used, the collaborations are often energy intensive and employ toxic chemicals. On the other hand, the synthesis of inorganic materials by biological systems is characterized by processes that occur at close to ambient temperatures and pressures, and at neutral pH (examples include magnetotactic bacteria, diatoms, and S-layer bacteria). Here we show that nanoparticulate magnetite may be produced at room temperature extracellularly by challenging the fungi, *Fusarium oxysporum* and *Verticillium* sp., with mixtures of ferric and ferrous salts. Extracellular hydrolysis of the anionic iron complexes by cationic proteins secreted by the fungi results in the room-temperature synthesis of crystalline magnetite particles that exhibit a signature of a ferrimagnetic transition with a negligible amount of spontaneous magnetization at low temperature.



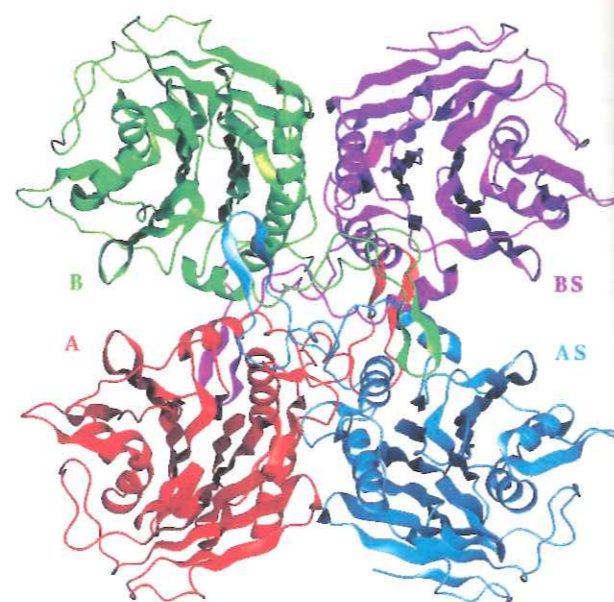
Extracellular biosynthesis of Magnetite Nanoparticles using fungus *Fusarium oxysporum*



TEM micrographs of magnetite (iron oxide) nanoparticles synthesized using fungus *Fusarium oxysporum* before (A & B) and after calcination at 400 °C for 3 h (C & D)

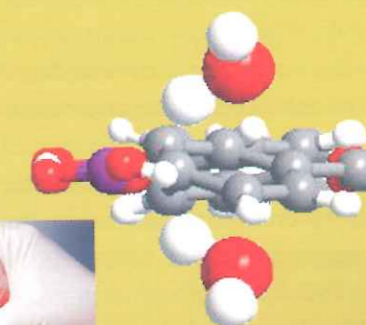
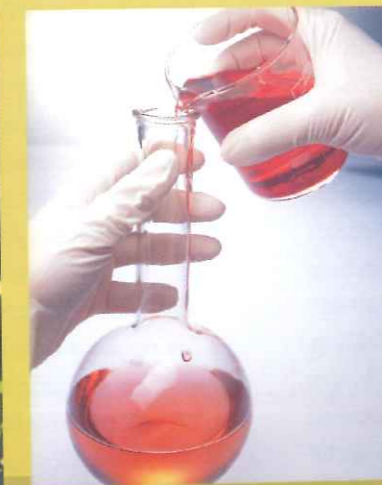
Kumar R.S., Brannigan J.A., Prabhune A.A., Pundle A.V., Dodson G.G., Dodson E.J., Suresh C.G., Structural and functional analysis of a conjugated bile salt hydrolase from *Bifidobacterium longum* reveals an evolutionary relationship with penicillin V acylase, *Journal of Biological Chemistry*, 281(43), 32516-32525

**Abstract:** Bile salt hydrolase (BSH) is an enzyme produced by the intestinal microflora that catalyzes the deconjugation of glycine- or taurine-linked bile salts. The crystal structure of BSH reported here from *Bifidobacterium longum* reveals that it is a member of N-terminal nucleophil hydrolase structural superfamily possessing the characteristic  $\alpha\beta\alpha$  tetra- lamellar tertiary structure arrangement. Site-directed mutagenesis of the catalytic nucleophil residue, however, shows that it has no role in zymogen processing into its corresponding active form. Substrate specificity was studied using Michaelis-Menten and inhibition kinetics and fluorescence spectroscopy. These data were compared with the specificity profile of BSH from *Clostridium perfringens* and penicillin V acylase from *Bacillus sphaericus*, for both of which the three-dimensional structures are available. Comparative analysis shows a gradation in activity toward common substrates, throwing light on a possible common route toward the evolution of penicillin V acylase and BSH.



The tetrameric association of *Bifidobacterium longum* bile salt hydrolase from the crystal structure of the enzyme. The four subunits are shown in different colours

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## 1 BIOLOGICAL SCIENCES

### 1.1 BASIC BIOCHEMICAL SCIENCES

#### 1.1.1 Structure-function studies

##### Lichenase

A bifunctional high molecular weight ( $M_r$  64,500 Da)  $\beta$ -1-3, 1-4 glucan 4-glucanohydrolase was purified to homogeneity from *Thermomonospora* sp., exhibiting activity towards lichenan and xylan. A kinetic method was used to analyze the active site that hydrolyzes lichenan and xylan. The experimental data was in agreement with the theoretical values calculated for a single active site. Probing the conformation and microenvironment at active site of the enzyme by fluorescent chemo-affinity label, OPTA resulted in the formation of an isoindole derivative with complete inactivation of the enzyme to hydrolyse both lichenan and xylan confirmed the results of kinetic method. OPTA forms an isoindole derivative by cross-linking the proximal thiol and amino groups. The modification of cysteine and lysine residues by DTNB and TNBS respectively abolished the ability of the enzyme to form an isoindole derivative with OPTA, indicating the participation of cysteine and lysine in the formation of isoindole complex.

##### Folding/unfolding studies of cellulase

A low molecular weight cellulase 1,4- $\beta$ -D-glucan glucanohydrolase (TSC) was purified to homogeneity from an alkalothermophilic *Thermomonospora* sp. To gain insight into the molecular aspects of unfolding / refolding of enzymes from extremophilic organisms this enzyme was used as the model system. Kinetics of denaturation / renaturation was monitored using intrinsic fluorescence studies. Denaturation studies using the structure - perturbing agent guanidium hydrochloride (GdnCl) indicated that TSC folds through a partially folded state that resembles molten globule. The protein fluorescence measurements suggested a putative intermediate state at 1.8 M guanidine hydrochloride with an emission maximum of 340 nm. The far-UV circular dichroism spectra revealed content of secondary structure similar to the native enzyme. Present investigations were undertaken to understand the folding of TSC using  $\alpha$ -crystallin.  $\alpha$ -Crystallin is a multimeric protein that has been shown to function as a molecular chaperone and shares extensive structural homology to small heat shock proteins. The refolding of GdnCl denatured TSC from its molten globule state (TSC-m

complex) in the presence and absence of  $\alpha$ -crystallin to elucidate the molecular mechanism of chaperone-mediated in vitro folding was studied. The results, based on intrinsic tryptophan fluorescence and the fluorescent hydrophobic probe 1-anilino-naphthalene-8-sulfonate (ANS) binding studies, suggest that  $\alpha$ -crystallin formed a complex with a putative intermediate molten globule like intermediate in the refolding pathway of TSC. Reconstitution of the active TSC was observed on cooling the  $\alpha$ -crystallin TSC-m complex to 4°C. Addition of  $\alpha$ -crystallin to the molten globule-like intermediate of TSC (TSC-m complex) complex initiated the refolding of TSC with 69 % recovery of the biological activity of the enzyme.

The N-terminal sequence of the purified 1,4- $\beta$ -D-glucan glucanohydrolase is GSVINPATRNY. The N-terminal sequence showed 93 % homology with putative secreted cellulose-binding protein of *Thermobifida fusca* YX through BLAST search. It has 72 % homology with secreted cellulose-binding protein of *Streptomyces coelicolor* A3. Multiple sequence alignment of GSVINPATRNY to that of other cellulases showed the presence of conserved glycine, serine, proline, asparagine, and tryptophan.

##### Alkaline xylanase

The three-dimensional structure of a tetragonal crystal form of alkaline xylanase from an alkalophilic *Bacillus* sp. (NCL 87-6-10) with bound and hydrolysed xylotriose has been determined at 2.5 Å resolution. Analysis of this structure along with data from other binding studies has helped in the active site characterization and elucidation of the enzyme-substrate interactions.

##### Aspartic proteases from *Vigna radiata*

Aspartic proteases are the focus of recent research interest in understanding the physiological importance of this class of enzymes in plants. This is the first report of an aspartic protease from the seeds of *Vigna radiata*. The aspartic protease was purified to homogeneity by fractional ammonium sulfate precipitation and pepstatin-A agarose affinity column. It was found to have a molecular weight of 67,406 Daltons by gel filtration chromatography. SDS-PAGE analysis revealed the presence of a heterodimer with subunits of molecular weights of 44,024 and 23,349 Daltons respectively.



The enzyme was pH stable with the amino acid analysis confirming the molecular weight of the protein. The substrate cleavage site as analyzed by using the synthetic substrate was found to be the Phe-Tyr bond. The kinetic interactions of the enzyme were studied with the universal inhibitor, pepstatin A. The interactions of a plant aspartic protease with pepstatin-A, an inhibitor from a microbial source showed competitive one-step mechanism of binding is observed. The progress curves are time-dependent and consistent with tight binding inhibition. The  $K_i$  value of the reversible complex of pepstatin with the enzyme was 0.87  $\mu$ M where as the overall inhibition constant  $K_i'$  was 0.727  $\mu$ M.

The existence of essential aspartic acid and serine residues corroborates with the substrate protection studies and the kinetics of the modified enzyme. Modification studies revealed the presence of an essential cysteine residue for enzyme activity. In the presence of lower concentrations of guanidine hydrochloride, the enzyme lost its structure with concomitant loss inactivity. The partially reversible denaturant induced structural changes, irreversible loss in functionality of the enzyme and the free energy of 8 J/mole associated with the folded enzyme indicated the criticality of aspartic acid residues in the enzyme. Structural determinants and functional studies establish the sensitiveness of the enzyme and point towards a novel alkali induced molten globule state.

##### Penicillin G acylases

Penicillin G acylase (PGA) or penicillin G amidohydrolases hydrolyses penicillin G to phenylacetic acid and 6-aminopenicillanic acid, the latter being used in the manufacture of semi-synthetic penicillins. Though enzyme from *E. coli* has been extensively explored, comparatively lesser information is available about *Kluyvera citrophila* penicillin G acylase. PGA from *K. citrophila* has many features useful for industrial applications such as greater stability towards heat, pH, organic solvents and the ease of immobilization. Hence with the aim of obtaining higher yield we tried cloning *pac* gene.

We have successfully cloned and expressed *K. citrophila* PGA intracellularly as well as extracellularly. The enzyme has been expressed as active secretory protein to overcome the discrepancy in the intracellular precursor

processing. Attempts were made to enhance the production of extracellular enzyme using various inducers and we found that inulin could substitute the conventional and costlier inducer, IPTG, moreover it exhibited four-fold increase in the enzyme production. Biochemical, Biophysical studies on this PGA have been carried out and its structure has been modeled to elucidate the characteristics of its active site. At present efforts to crystallize this enzyme and to study its three-dimensional structure are in progress. The crystal structure of a penicillin G acylase (PGA) from *Alcaligenes faecalis* has been determined at 3.5 Å resolution.

##### Conjugated bile salt hydrolases and penicillin V acylases

Cholesterol is found in the cell membranes of all body tissues. Cholesterol plays a central role in many biochemical processes, but elevated cholesterol levels are known to be associated with cardiovascular diseases. Pharmacological agents such as fibrates, bile acid sequestrants and statins are also available for the treatment of high cholesterol. Although these drugs effectively reduce cholesterol levels, they are expensive and are known to have severe side effects. In recent years, interest has risen in the possibility of using bile salt deconjugation to lower serum cholesterol level in hypercholesterolemic patients and prevent hypercholesterolemia in normal people.

Penicillin V acylase (PVA) is structurally related to bile salt hydrolases and it hydrolyses penicillin V to phenoxycetic acid and 6-aminopenicillanic acid. Compared to the more popular penicillin G acylase-penicillin G combination PVA-penV combination has several advantages to use in the manufacture of semi-synthetic penicillins. We have been carrying out the screening, characterization and three-dimensional structure determination of novel penicillin V acylases and conjugated bile salt hydrolases.

The three-dimensional crystal structures of penicillin V acylases (PVA) from *Bacillus sphaericus* (*BspPVA*) and from *Bacillus subtilis* (*BsuPVA*) and a conjugated bile salt hydrolase (BSH) from *Bifidobacterium longum* (*BIBSH*) have been determined and compared. Biochemical, biophysical and kinetic studies to understand the substrate specificity and to assess the stability of these



enzymes towards denaturation conditions have been carried out. Using modeling techniques the reason behind variation in the substrate specificity and activity shown by these enzymes has been studied. The above observations have been compared with structural data also. These detailed studies have shown that *Bsu* PVA has only PVA activity and *BIBSH* has only BSH activity, whereas *Bsp*PVA shows both PVA and BSH activities. Their active sites are similar and the differences lie in the different lengths and mutations present in their substrate binding loops.

Bile salt hydrolase from *Geobacillus caldxylosilyticus* has been purified to homogeneity using Q sepharose column. Biochemical characterization such as optimum pH and temperature for activity, pH and temperature stability, effect of metal ions, substrate specificity, native and subunit molecular weight of the purified protein has been done. Preliminary screening for crystallization conditions has been carried out simultaneously.

Partially purified enzyme was immobilized using mesoporous silica, SBA-15 matrix and the properties of the immobilized enzyme such as optimum pH, Temperature, pH and temperature stability, Michealis menten kinetics has been studied and compared with that of free enzyme.

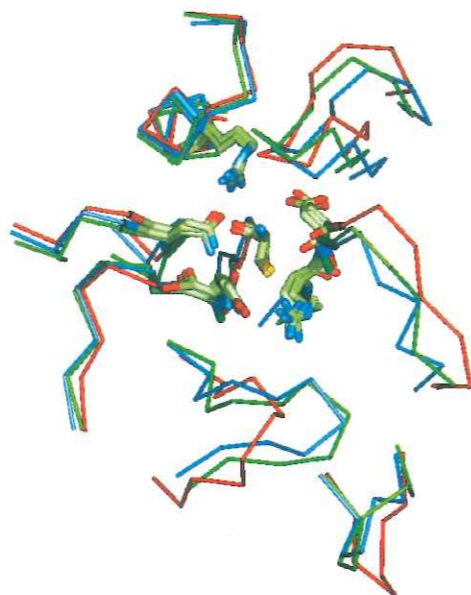
Another novel bacterial source of bile salt hydrolase has been isolated from marine habitat and identified as *Brevibacterium casei*. Enzyme from this organism has been purified to homogeneity.

*Rhodotorula aurantiaca* has been identified as a new source of penicillin V acylase. Enhancement in the cell bound activity of penicillin V acylase from *Rhodotorula aurantiaca* has been achieved through. This intracellular enzyme has been purified and biochemically characterized.

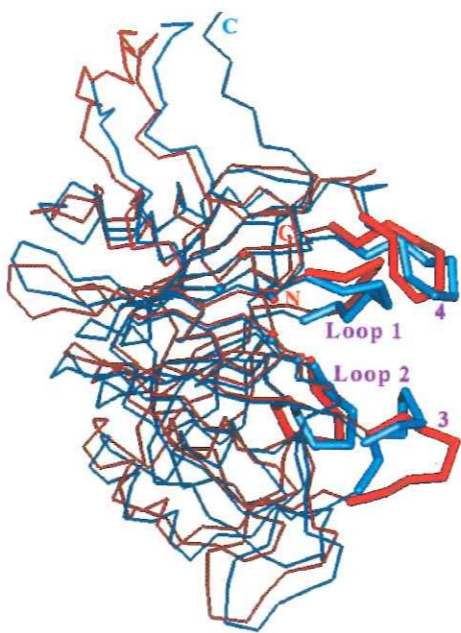
#### Cephalosporin C acylases

Cephalosporin C acylases are a group of enzymes involved in the conversion of cephalosporin C to 7-amino cephalosporanic acid (7-ACA), which is an important precursor molecule for various semi-synthetic cephalosporins. Whole cell immobilization of *Alcaligenes xylooxidans* was carried out using various entrapment matrices such as calcium alginate and gellan gum. Rheological properties of the matrices were also

studied to show the efficacy of the immobilization procedure. Forezyme immobilization amino functionalized SBA-15 was used successfully till the 10<sup>th</sup> cycle without any loss in activity.



Overlap of the active site residues of a true penicillin acylase from *Bacillus subtilis*, a true conjugated bile salt hydrolase from *Bifidobacterium longum* and the enzyme from *Bacillus sphaericus* showing both the above activities.



Overlap of the substrate binding loops of a penicillin V acylase (*Bsu*PVA) and a bile salt hydrolase (BIBSH) to show the difference between them.



#### Lectins

In the progress towards determining the three-dimensional structure of the lectin from chickpea (*Cicer arietinum*), crystals of a heavy atom derivative of iodine was grown and characterized using Patterson analysis. Analyses of the structures of lectins from *Trichosanthes dioica* and *Erythrina indica* are in progress. Purification and characterization of a lectin from *Moringa oleifera* is also undertaken.

#### Structure-function relationship of $\alpha$ -mannosidase from *Aspergillus fischeri*

$\alpha$ -Mannosidase is an important therapeutic target for the development of anticancer agents, apart from the vital role in glycoprotein biosynthesis and degradation. Fluorescence quenching and time resolved fluorescence of  $\alpha$ -mannosidase were carried out to investigate the tryptophan environment. The tryptophans were found to be differentially exposed to the solvent and were not fully accessible to the neutral quencher indicating heterogeneity in the environment. Surface tryptophans were found to have predominantly positively charged amino acids around them as shown by quenching with ionic quenchers. Denaturation led to more exposure of tryptophans to the solvent and consequently in the significant increase in quenching with all the quenchers. The native enzyme showed two different lifetimes,  $\tau_1$  (1.51ns) and  $\tau_2$  (5.992ns). The average lifetime of the native protein ( $\tau$ ) (3.187ns) was not affected much after denaturation ( $\tau$ ) (3.219ns), while average lifetime of the quenched protein samples was drastically reduced (1.995ns for acrylamide and 1.537ns for iodide). The active site tryptophan did not contribute significantly to the fluorescence of the protein. The selective chemical modification of the enzyme showed that apart from Trp and His, presence of carboxylate, Arg and Cys was found to be essential at the active site.

#### 1.1.2 Biotransformation

Sophorolipids are extracellular surface active glycolipids that are produced by the yeasts *Candida bombicola* and *Candida apicola*. The yeast *Candida bombicola* (ATCC 22214) grown on primary carbon source glucose (100g l<sup>-1</sup>) and secondary carbon, arachidonic acid (2 g l<sup>-1</sup>) produced mixture of sophorolipids upto 1.44 g l<sup>-1</sup>. The crude product was a heterogeneous mixture of sophorolipids,

Which are glycolipids of sophorose linked to the fatty acid through glycosidic bond between  $\omega$  and  $\omega$ -1 carbon of arachidonic acid. The derived sophorolipids were isolated by silicagel chromatography using dialysis tubing. The purified sophorolipids were characterized by ESI-MS and FT-IR. Acid hydrolysis of the resolved sophorolipids were characterized by ESI-MS for the presence of 20-hydroxy-5Z, 8Z, 11Z, 14Z-eicosatetraenoic acid (20-HETE) and 19-hydroxy-5Z, 8Z, 11Z, 14Z-eicosatetraenoic acid (19-HETE), compounds of pronounced pharmaceutical importance.

#### 1.1.3 The Cell wall bound peroxidases of *Leucaena leucocephala*

In continuation of earlier work on *Leucaena leucocephala*, the present study focuses to gather confluent information from kinetics, structural and gene expression studies regarding the role of cell wall bound peroxidases in lignification process. Peroxidase cDNA clone ~1.2kb was isolated, using PCR strategies. It was cloned in pGEM-T vector and sequenced. Sequence analysis showed more than 80% homology with existing peroxidase sequences in NCBI database. The coding regions from 3' and 5' race products were amplified using new set of primers and the respective fragments were cloned in anti-sense orientation in pCAMBIA 2301 binary vector. Attempts are in progress to transform tobacco and *Leucaena* using these constructs in *Agrobacterium* strain LBA 4404.

## 1.2 BIOTECHNOLOGY

### 1.2.1 Secondary metabolites, inhibitors and drugs

#### Secondary metabolites from *Calophyllum* and *Garcinia*

Two members of the family *Guttiferae* viz. *Calophyllum* and *Garcinia* occurring along the Western Ghats of India were studied for assessment of chemodiversity, identification of new molecules and potential drugs of therapeutic value. The main anti HIV dipyrano-coumarins, inophyllum A, -B, -C, -D, -P and *calophylloide* were analysed in callus and suspension cultures of *Calophyllum* under various physico-chemical conditions.



Quantitative analysis resulted in fifteen fold increase in the inophyllum content. This is a significant achievement in terms of its potential biotechnological application. Four endophytic fungi were also isolated from the plant material and would be used further for enhancing the production of inophyllums. Genomic diversity of these plants was also studied using ISSR primers. Somatic embryogenesis was achieved last year as in-vitro regeneration method. Regeneration from mature roots was obtained and could be used for mass multiplication of elite plants.



Root organogenesis in *Garcinia indica*: (Top photograph): mother explant with production of shoots on its root (Bottom photograph): Induction of shoots on root explant

### Lectin

A lectin has been purified from the fungus *Fusarium oxysporum*. This lectin has specificity for complex oligosaccharides and recognizes Gal  $\beta$ 1-3-Gal NAc as well as Gal  $\beta$ 1-4-Glc NAc with equal avidity. The binding of sugar moieties to this lectin is enthalpy driven and increased branching as well as multivalency of the glycan structures has profound effect on its affinity for oligosaccharide.

### Taxol

Taxol has been produced from the fungus, *Verticillium* sp. at 10  $\mu$ g/lit culture. Semi synthetic epitaxol has been synthesized by the fungi from 10 DAB III and Phenylisoserine. The taxol has been labeled with fluorescent dyes as well as quantum dots. Fluorescence microscopic studies with these labelled taxol are in progress to understand its mechanism of interaction and uptake.

## 1.2.2 Plant biochemistry and biotechnology

### 1.2.2.1 Molecular approaches to improve the end product quality of Indian wheat

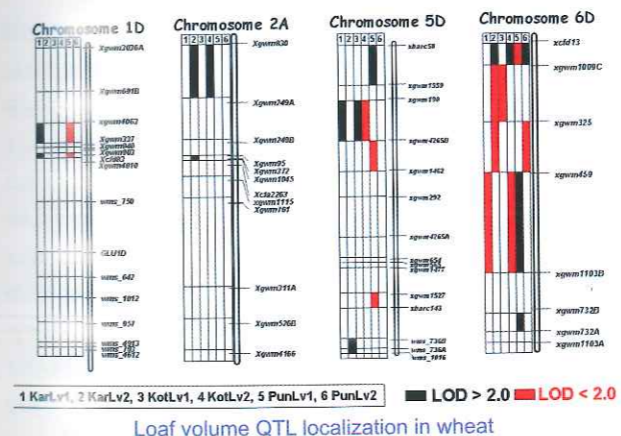
Apart from the household preparations from the wheat flour, the trade communities, millers and bakers are the main end users of wheat. A number of important parameters contribute to the end product quality of wheat and they are grain protein content (PC), grain size, grain hardness (GH) and bread making quality (BMQ). A segregating mapping population was developed at Directorate of Wheat Research (DWR), Karnal, India, from a cross between HI 977 (a wheat cultivar with good BMQ) and HD 2329 (poor BMQ) consisting of 105 individuals was analysed in order to decipher BMQ into its components and also to dissect the chromosomal regions associated with these components.

A total of 30 QTL for Lv were detected and significant QTL were identified on 6B and 6D chromosomes; 1B, 1D, 2A, 3A, 5B and 5D also contributed genetically to Lv. Association between 6B and 6D QTL and variable expression of gliadins on group 6 chromosomes was also speculated. Dissection of Lv through AMMI model revealed significant G x E variance for the trait. In the same population other loaf score related traits as well as yield related traits such as TGW and TW were also mapped. More than 100 QTL contributing to these traits



were identified spanning the wheat genome.

Kernel shape and size characters are important wheat quality traits that contribute to its export potential. Bold kernels of uniform shape command better market price and improve milling yield. Hence development of varieties with large grains and better shape that fit into specific global markets needs has become a major objective of breeding programs. Kernel shape characters like Kernel length (KL) and Kernel width (KW) and TKW are quantitative in nature and are controlled by many QTL. Understanding genetic basis of kernel shape and size has so far been preliminary. Investigations that aim at identifying the number and locations of QTL controlling these traits are, therefore, necessary for genetic dissection of wheat kernel shape and size.



A population of 189 Recombinant Inbred Lines (RILs) developed by Single Seed Descent (SSD) at Punjab Agricultural University (PAU), Ludhiana, from the cross Rye Selection III x Chinese Spring is being used as the mapping population for the identification of markers linked to KL, KW and TKW. Linkage analysis indicated 9 linkage groups belonging to chromosome 1A, 1B, 2B, 2D, 4A, 5B, 5D, 6B and 7A. Single Marker Analysis (SMA) of marker and trait data revealed 15 markers trait association for KL, 7 for KW and 50 for TKW. Markers linked to KL were from chromosome 1A, 2B, 2D and 6B. KW showed marker-trait association on 1A, 2B, 4A and 5B while chromosomes 1A, 1B, 2B, 4A, 5B, 6B and 7A showed association with TKW. Composite Interval Mapping (CIM) performed using QTL Cartographer indicated a significant QTL for KL on chromosome 6B and on chromosomes 1A for TKW at Ludhiana location.

## Development of disease-resistant wheat varieties using molecular marker technology in bread wheat

Leaf rust is the most widespread and frequently occurring disease of wheat affecting its productivity very severely. Genetic resistance is the most economical method of reducing yield losses due to rust. In order to pyramid seedling and adult plant resistance genes in wheat for durable resistance, it is essential to have molecular markers closely linked to these resistance genes. The peninsular zone of India is predominantly marginal, rainfed and semi-arid. Genotype such as NI5439 recommended for this region is adapted to rainfed and low irrigation conditions, is high yielding with one or two irrigations, however is completely susceptible against prevalent races of rusts in this region. It is, therefore, proposed to transfer two leaf rust resistance genes *Lr15* (seedling resistant) and *Lr34* (Adult Plant Resistant) in NI5439 background using molecular markers. Markers linked to *Lr15* on chromosome 2D were identified from the mapping population consisting of 221 F<sub>2</sub> plants developed by crossing Tc x Tc *Lr15*. Four markers gwm102, gwm 988, gwm 4562 and gwm 4901 flanking the *Lr15* gene were identified in which gwm 4562 was the closest at 1.9 cM from *Lr15*. Marker order was observed to be similar to the consensus map of 2D of wheat. The markers for *Lr34* were confirmed in 266 families (F7/F8) from a cross 90RN2491 x WL711. These two rust resistance genes, *Lr15* and *Lr34*, were introgressed into NI5439 by double crossing and were further backcrossed with NI5439. The backcrossed population is screened using the markers for *Lr15* and *Lr34*.

## Increasing the efficiency of production and nutritional value of chickpea

Chickpea is the third most important grain legume crop in the world and first in India. It is grown mostly by poor and marginal soils and is a rich source of high-quality protein. The yield of the crop has been stagnant for many years, due to its susceptibility to various biotic and abiotic stresses. Yield and yield related traits are gaining importance in Indian chickpea breeding program as India is the highest producer of chickpea and aims to become independent in the productivity to meet the demand. Yield in chickpea as in all other crop depends especially



on yield components, which are quantitative in nature and their effect being modified by environment.

Two F9 RIL populations [JG62 X Vijay (JV) and Vijay X ICC4958 (VI)] were developed at MPKV, Rahuri. Yield related traits such as plant height (Pht), plant spread (Psp), branches/plant (Brp), pods/plant (Pdp), Days to maturity (Dmt), yield/plant (Yld) and 100 seed weight (Swt) were recorded consecutively for four years. Different types of molecular markers; RAPD, ISSR, RGA and SSRs were used to construct the intraspecific map. QTLs were identified from these maps using QTL Cartographer Ver 2.5 software and mapped on eight linkage groups. At least two significantly contributing markers for each yield related traits were observed. In the JV population, 41 significant QTLs ( $LOD \geq 3$ ) and 47 suggestive QTLs ( $LOD 2$  to  $3$ ) were identified, whereas in the VI population, 63 significant QTLs ( $LOD \geq 3$ ) and 77 suggestive QTLs ( $LOD 2$  to  $3$ ) were detected for the seven traits. The number of significant QTLs for individual traits ranged from two (Swt) to twelve (Psp) in JV and five (Yld) to fifteen (Psp) in VI populations. All identified QTLs were mapped on their respective position on linkage groups.

#### Genetic diversity of *Symplocos* species

The existence of plants common to Northeastern (NE) and South India (SI) has been interpreted as the outcome of postglacial colonization. To infer the history and postglacial migration routes taken by montane species in India, *Symplocos laurina* Wall., a Pleistocene relict was used as a model system in the present study. Twelve populations comprising 218 individuals representing NE and SI were analyzed using PCR-RFLP with three cpDNA and eight mtDNA primer restriction endonuclease combinations that yielded nine chlorotypes and twenty four mitotypes. Diversity was found to be high for both the genomes (cpDNA  $hT = 0.653$ ; mtDNA  $hT = 0.8503$ ). Although a strong population differentiation (cpDNA  $GST = 0.742$ ; mtDNA  $GST = 0.642$ ) was obtained, phylogeographic structure was not observed for both cpDNA and mtDNA. The haplotype network revealed presence of two main lineages: Northeastern-Western Ghat (NE-WG) lineage and Eastern Ghat (EG) lineage largely without overlapping distributions. There is evidence supporting the hypothesis that these two lineages evolved from the

NE refugium and migrated possibly due to Pleistocene eustatic changes and corresponding climate fluctuation via central India which acted as a transitional refugium after glaciation. The favorable condition on the hilltops of SI allowed rapid expansion of plants from transitional refugia to SI. In contrast, the disjunct *S.laurina* populations presently persisting in EG seem to have experienced many bottlenecks during the course of migration and have, therefore, accumulated a high degree of differentiation and have also maintained a unique store of genetic variation for both the genomes. Our study indicates that postglacial migration and founder events could have played a significant role in the history of montane species of India, which is reflected by their present day population structure.

#### Improved productivity, profitability and sustainability of sheep production

To enhance the prolificacy of Indian sheep breeds, *FecB* gene from prolific Garole breed of Sunderban area was introgressed into Deccani and Composite breed which do not have *FecB* gene mutation as confirmed by PCR-RFLP test. One copy of the *FecB* gene increased litter size per ewe conceived by 0.37 lambs and per ewe lambing by 0.64 lambs in Deccani and crossed ewes. The *FecB* gene was introduced into local small holder flocks in the Deccan plateau region by providing 30 homozygous rams by NARI, Phalatan. Both Fecund Deccani and Fecund Composite were used for introduction of the gene. The performance of the *FecB* gene was monitored within the flocks using the PCR-RFLP test. The gene increased lambing rate significantly but within manageable limits. More lambing and survival data from *FecB* heterozygous ewes need to be collected. Genetic diversity of three Indian domestic sheep breeds namely, the Garole, Deccani (represented by the Lonand, Sangamneri, Kolhapuri, Sangola and Madgal strains) and Madras Red, was assessed using 15 microsatellites markers. Two hundred and eighty seven (about 27-62 individuals per breed) animals were genotyped to ascertain their historical relationships by applying recent statistical methods. All the breeds displayed high within breeds genetic diversity, reflected by high mean allelic diversity and heterozygosity, and were genetically distinct ( $FST: 0.20 \pm 0.03$ ). Both the genetic distance based methods, nearest neighbor



clustering (constrained) and Principal Components Analysis (PCA) distinguished the three breeds with the Deccani strains clustered together while the Garole and Madras Red formed distinct and separate clusters. A Bayesian clustering approach identified the Garole breed as one lineage, whereas the Deccani population was subdivided according to the strain except for the Lonand and Sangamneri strains, which clustered together. Interestingly, the Madras Red population was split in two clusters. Overall, a pattern of isolation by distance was evident ( $r = 0.99$   $P < 0.001$ ) suggesting limited dispersal and extensive philopatry of the breeds studied. The diversity pattern was concordant with geographical origin and supports the traditional classification system.

#### 1.2.2.2 Secondary metabolites and metabolic pathway analysis

##### Fatty acid pathway analysis from Linseed

Linseed/Flax is the richest and cheapest agricultural source of Alfa linolenic acid (ALA), which is an Omega 3 fatty acid. It is planned to understand and characterize the pathway of Omega 3 fatty acid synthesis in flax. Linolenic acid trait is controlled by two independently inherited genes, namely LuFAD3A and LUFAD3B, which encode microsomal desaturases (Delta-15 desaturases) capable of desaturating linoleic acid (LA) to ALA. Using bioinformatics tools, these two FAD3 genes were isolated from an Indian flax variety NL115, cloned in pGEM-T vector system and sequence characterized. These sequences were then used to design primers to study gene diversity at these particular loci in various Indian flax varieties, having wide variation in their ALA content. Further molecular analysis of the genes is in progress.

##### Revealing secrets of mango flavour

Alphonso mango grown in coastal belt of Maharashtra is considered as the "King of Mangoes" and is popular for its flavour and colour throughout the world. It is known that the environment that reigns during the fruit development enforces the alteration in the quality of ripe fruit. It would be interesting to study the fruit chemistry that is changed by the environment along with the study of influencing environment itself. Such an approach would uncover the secrets underlying the complex

biological processes and biological interactions with the environment.

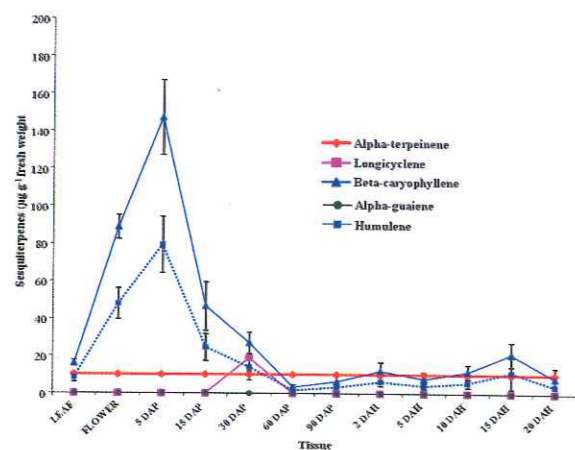
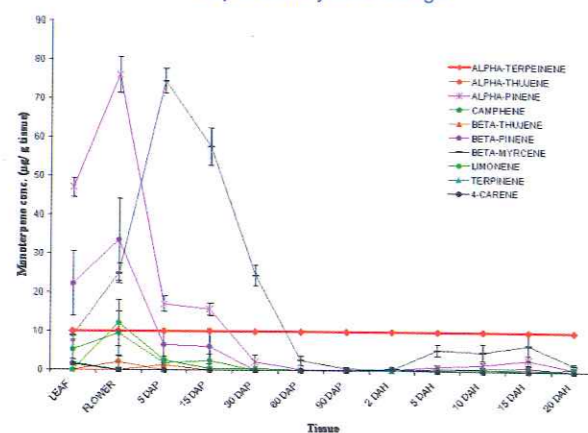
Alphonso fruit takes about 90 days to mature after the fruit-set and further 15 to 20 days to ripe at  $28^{\circ}C$ . Fruits of various developing and ripening stages were used for GCMS analysis. Along with the fruit tissues, leaf and flower tissues were also analyzed. In this analysis, very low and unpleasant flavored cultivar Sabja was used as a negative control. Over 50 compounds could be tracked through the development and ripening of the Alphonso fruit. E-Ocimene dominated all the profiles followed by Z-ocimene,  $\beta$ -caryophyllene,  $\alpha$ -humulene and  $\alpha$ -pinene. Monoterpenes and sesquiterpenes lowered during the process of ripening. Fatty acid levels were observed to be elevated in the metabolically accelerated stages of fruit development and ripening. Aldehydes did not have any common profile. Esters represented by furanones and lactones, were totally absent during the development and were found to be synthesized de novo during the process of ripening; their concentrations declined during the late ripening period. Raw as well as ripe Sabja fruits were found to be terpene rich and totally devoid of esters.  $\alpha$ - and  $\delta$ -guaiene,  $\tau$ -muurolol and  $\alpha$ -cadinol were found confined to Sabja fruit. Results suggest that the flavor of the alphonso is a combination of freshening sap scent and the ripening induced fruity odor. Sap flavor is the major ingredient and contributes by the addition of principal volatile chemicals, the mono and sesqui-terpenes. The sweetness or the fruitiness is gained as an outcome of the metabolic changes during the post-harvest period. This fruitiness can be attributed to the ester components of the blend. This also explains why Sabja fruit retains unpleasant turpentine flavor even on ripening.

Along with the qualitative and quantitative profiles of various Alphonso flavorants, expression profiles of various flavor and non flavor genes have been revealed in the present investigation. Terpenoids being the most abundant flavorants in Alphonso, the genes from terpene biosynthesis pathway were targeted. In plants, two different pathways are engaged in terpene biosynthesis till the formation of the main building block, isopentenyl diphosphate (IPP). Methylerythritol phosphate (MEP) pathway (or 1-deoxy-D-xylulose (DOX) pathway) in the chloroplast synthesizes IPP for mono- and diterpenes,



where as the mevalonic acid (MVA) pathway in the cytosol, produces IPP for sesquiterpenes. Further mono-, di- and sesquiterpenes are synthesized from this IPP through geranyl diphosphate (GPP) and geranyl geranyl diphosphate (GGPP) and farnesyl diphosphate (FPP) synthesis, respectively. Mango fruits of various developing and ripening stages make an array of tissues that is chemically inconsistent; therefore, a comprehensive RNA isolation method was required in order to maintain the uniformity in the RNA templates. For this purpose a method was developed that could be applied to a wide range of complex plant tissues. The qualitative RT-PCR were performed in order to identify an array of transcripts from the terpene biosynthesis pathway. Detail analysis of these genes is in progress.

Terpene analysis in mango



### 1.2.2.3 Host pathogen interactions Transcript profiling during host-pathogen interactions with reference to chickpea and *F. oxysporum f. sp. ciceri*

Differential expression of chickpea genes was studied from resistant and susceptible varieties in response to *Fusarium oxysporum f. sp. ciceri* race1 infection. Many gene transcripts that were upregulated in the resistant cultivar upon FOC1 infection were identified. Of the genes upregulated in resistant cultivar during pathogen attack, WRKY and 14-3-3 were identified for the first time in chickpea, though their role in defense is described and understood in other plant species. Previously described defense genes in host-pathogen interactions like NBS-LRR, chitinase, hydrolase, ATPase, and gamma glutamyl-cysteine synthetase were observed to be upregulated in resistant cultivar upon FOC1 infection. Interestingly, LTR and non-LTR types of retrotransposons were also seen to be upregulated in chickpea roots during pathogenic stress. The host-pathogen interaction was marked by few more genes whose identity could not be established, either due to the smaller size of the obtained sequence or they could be new genes hitherto undescribed.

Most resistance proteins are receptor-like protein kinases of the nucleotide-binding site-leucine-rich-repeat (NBS-LRR) class and composed of different combinations of conserved elements. In this study at least three NBS-LRR like transcripts were identified. Full-length 14-3-3 genes from chickpea variety resistant to FOC infection were also isolated and cloned. 14-3-3 genes are present as a fairly large family in eukaryotes especially in plants. Two isoforms of the 14-3-3 genes in chickpea (Cal433-1 and Cal433-2) were identified and hypothesized for presence of more isoforms. The Cal433-1 gene was of epsilon type suggesting it to be of primitive origin, while Cal433-2 was of non-epsilon types, which are known to be more evolved. Of the two isoforms Cal433-2 appeared to be positively associated (upregulated upon FOC1 infection) with the resistant cultivar during FOC1 infection while the Cal 433-1 was observed to be positively associated with the susceptible cultivar during FOC1 infection. Cal 433-1 could possibly be involved in stomatal opening and probably, the TDF, CaFri51, an aquaporin, is therefore, found expressed at



higher levels in susceptible cultivar.

On the other hand Cal 433-2 was disease responsive and involved in signal transduction pathway, triggering the cascade of molecular responses leading to resistance. Cal 433-2 could possibly act via ATPase activation through the accumulation of reactive oxygen species (ROS), which was supported by the fact that gamma glutamyl-cysteine synthetase, a key enzyme in ROS scavenging was also upregulated during pathogen attack. Interestingly, a TDF (CaFri36) encoding ATPase like protein was identified, which was upregulated during pathogenic stress.

### 1.2.2.4 Development of insect tolerance in crop plants

We have adopted proteinase inhibitor strategy to inhibit the *Helicoverpa* gut proteinases and pod borer larval growth. Many nonhost plant species have been identified and characterized for the same.

### Winged bean proteinase inhibitor for *H. armigera* resistance

Dry mature seeds of winged bean (*Psophocarpus tetragonolobus* L., DC.) (WB) contain several proteinase inhibitors of Kunitz type and Bowman-Birk type serine proteinase inhibitors. Two putative Kunitz-type chymotrypsin inhibitor genes (WCI2 and PtCI5) were isolated from winged bean (*Psophocarpus tetragonolobus* (L.) DC). While WCI2 has previously been identified, PtCI5 represented a new member of the WCI family. These genes were used to develop constructs for plant transformation. The binary vector pBINAR was provided by Dr. M.T Tegeder (SBS, WSU, USA) while pVicGalS\_hp was provided by Dr. Kevin Mcafee (USDA, ARS, WSU, USA). These vectors carry nptII gene linked to nos promoter and terminator for kanamycin resistance as plant selection marker. The PtCI-5 gene (ORF 850 bp) without introns was identified and isolated from mature seeds of winged bean and was cloned earlier in pGEMT Easy vector. This gene was cloned into the binary vectors driven by constitutive CaMV 35S promoter (pBINAR) or seed specific pea vicilin promoter (pVicGalS\_hp) and nos terminator. The plant vectors were mobilized into *A. tumefaciens* strain Agl-0 by triparental mating using pRK220 as helper plasmid and used for cocultivation and genetic transformation of

chickpea plant. The 850bp ORF of PtCI-5 gene was harvested from pBINAR and pVicGalS\_hp, and used as a gene specific probe for confirmation.

### Tomato proteinase inhibitors: Potential growth inhibitor of *H. armigera*

The inhibition potential of crude tomato PIs against *Helicoverpa armigera* gut proteases (HGP) was demonstrated. Analysis of trypsin inhibitor (TI) and HGP inhibitor (HGPI) distribution in various parts of tomato plant showed that flowers accumulate about 300 and 1000 times higher levels of TI while 700 and 400 times higher levels of HGPI as compared to those in leaves and fruits, respectively.

Three novel isoforms observed on native PAGE were separated by ion-exchange chromatography. Initial characterization of each native isoform showed that isoform A has 3 PI species of same charge but different masses, isoform B had only one PI species and isoform C had one PI species. Based on the protein sequence data, primers were designed to identify and isolate these *lepi* genes. Isolation and sequencing of the organ specific *lepi* gene(s) would reveal the genetic variations (if any). Semi-quantitative RT-PCRs using gene specific primers showed strong expression of *lepi* genes in flowers than any other organ of tomato plant. This supports our earlier biochemical data. Furthermore, the response of these genes to elicitor (MeJA, ABA, Ethylene, SA) and induction (mechanical wounding and insect spit application) treatments would indicate their potential role in defending tomato plant against *H. armigera* attack.

### Capsicum proteinase inhibitors and their interaction with insect gut proteinases

Novel forms of Pin-II type proteinase inhibitor cDNAs (CanPis) having three or four inhibitory repeat domains (IRD) were isolated from the developing green fruits of *Capsicum annum*. Deduced amino acid sequences of the CanPis showed up to 15% sequence divergence among each other or reported inhibitors. Amino acid sequence analysis of these CanPis revealed that the three IRD PIs have trypsin inhibitory sites, while four IRD CanPis have both trypsin and chymotrypsin inhibitory sites. Four CanPis, two having three IRD (CanPI-3 and CanPI-4) and the other two having four IRD (CanPI-7



and CanPI-9) were cloned in *Pichia pastoris* for expression of recombinant CanPIs. Recombinant CanPIs showed 90% inhibition of bovin trypsin (TI) while chymotrypsin inhibition (CI) varied with the number of chymotrypsin inhibitory sites in the CanPIs. Recombinant inhibitors exhibited over 70% inhibition of gut proteinases of *Helicoverpa armigera*. *H. armigera* larvae fed with recombinant CanPIs incorporated in artificial diet individually, showed 35% larval mortality, severe larval and pupal weight reduction as compared to larvae fed on control diet. Of the four Can Pis, CanPI-7, with two sites for TI and CI, showed consistent antagonistic effect on *H. armigera* growth and development. We conclude that CanPIs containing diverse IRDs are the best suited for developing insect resistant transgenic plants.

#### Expression studies of *H. armigera* gut proteinases

*Helicoverpa armigera* is one of the severe polyphagous lepidopteran insects, which infest important crops like cotton, chickpea, pigeonpea etc. Plasmid vectors were pET-32a (+) (NOVAGEN) containing genes coding for trypsin and chymotrypsin individually transformed to competent *E.coli* cells, positive colonies selected for expression of proteases. Expressed recombinant proteases in the form of inclusion bodies were isolated and recombinant protein containing histidine-tag subjected to affinity column chromatography. Column purified proteins were further attempted for refolding and activation of recombinant proteinase carried out to check its catalytic function. Cloned pET-32a (+) vector containing genes for trypsin (clone SR24) and chymotrypsin (clone SR117) were transferred to competent *E.coli* BL 21 DE 3 strains and transformed cells selected on Ampicillin (100 µg/ml) -LB plate. Positive colonies were confirmed by checking appropriate size of the inserts (801bp for trypsin and 971bp for chymotrypsin) by double restriction enzyme digestion using enzyme pairs *EcoRV-XhoI* for trypsin and *EcoRV-NotI* for chymotrypsin clone. One of the positive colonies containing appropriate insert was inoculated in LB-Ampicillin (100 µg/ml) broth and protease gene expression achieved by induction with addition of 0.4mM IPTG in the media when the cell density reaches to O.D value 0.4 at 600nm. Inclusion bodies containing recombinant protein were isolated by disrupting cells by

sonication followed by the centrifugation. Inclusion bodies suspended in Tris-buffer were made to pass through affinity column (Ni-NTA-Agarose) previously equilibrated with 100mM Tris-Cl pH 8.5 containing 300mM NaCl and 8M urea. In column six His tagged Trx-trypsin is trapped by Ni<sup>+2</sup> ions. Affinity bound His-tagged proteins were eluted by treating with elevated concentration of Imidazole. Refolding of recombinant trypsin was achieved by containing 300mM NaCl. The dialyzed sample was concentrated and quantity of expressed protein was estimated to be ~40 mg/L culture. Molecular weight of the recombinant pro-trypsin was determined by SDS-PAGE, which showed a prominent band of ~43.7kDa since trypsin (~25.7 kDa) is fused with thioredoxin (~18kDa), a conjugate protein.

#### 1.2.3 Metabolic Engineering Metabolic engineering of phenylpropanoid pathway in plants

Metabolic engineering of the phenylpropanoid metabolic pathway of plants has the potential to modify the content and the composition of the plant lignins. A change in the syringyl/ guaiacyl (S/G) ratio of the plant lignins, would make lignin removal from lingo-cellulose materials easy and environmentally less hazardous. Regulated expression of the caffeoyl CoA 3-O-methyl transferase (CCoAOMT), cinamyl alcohol dehydrogenase (CAD), cinamoyl CoA reductase (CCR), coumaryl CoA ligase (4-CL), coniferin- glucosidase (CBG) and the coniferyl aldehyde 5 hydroxylase (CAld5H) genes, individually or in various combinations, by antisense, co-suppression or RNA interference technologies is a possibility. It necessitates isolation of the genes and then their use in various constructs to develop and recover transgenics with either reduced lignin content or altered lignin composition.

Two full length genomic and cDNA clones of CCoAOMT were cloned, sequenced and characterized. They showed more than 85% homology at nucleic acid level and more than 90% homology at amino acid level. Full length genes were cloned in expression vector pET30(b) within restriction sites Nde I and Xho I so as to express CCoAOMT protein with C terminus HisTag. The recombinant CCoAOMT protein was expressed in *E. coli* strain BL-21 and its purification was done using nickel chelated column and also from inclusion bodies.



Polyclonal antibodies were raised in rabbits which will be used for immunocytolocalization to study spatial and temporal expression. Two partial promoters of CCoAOMT were also isolated, cloned and sequenced. They showed all the essential elements of core promoter. QRTR PCR studies showed that expression of CCoAOMT 1 gene is negligible in seedlings of one month age, but CCoAOMT 2 gene is expressed maximum in leaf with rachis, followed by root and least in stem. After isolation of full length genes of CAD, 4CL, CCoAOMT, CCR, CAld5H and CBG, UTRs of these genes were also isolated for differentiating among gene family. 4CL, CAD and CCR genes were cloned in expression vectors for isolation of proteins and development of polyclonal antibodies. Transformation of *Leucaena* and tobacco is being studied using *Agrobacterium* and biolistic gun approach with anti-sense and sense construct of the above genes.

#### 1.2.4 Nanobiotechnology

In vitro synthesis of nanoparticles of Ag and Au has been achieved using the enzymes Nitrate reductase and sulfite reductase. The reactions require the presence of  $\alpha$ -NADPH, hydroxyquinone and phytochelatin as capping agent. Sulfite reductase has also been used for the synthesis of CdS and CdSe quantum dots. These fluorescent nanoparticles have been coupled to proteins without any activation using the capping peptide.

#### 1.2.5 Pest management Molecular studies on the $\alpha$ -amylases of the rice pest *Scirpophaga incertulas*

*Scirpophaga incertulas*, commonly known as yellow stem borer, is a predominant monophagous pest of rice, which causes 5% to 30% loss of the rice crop. The larvae of *S. incertulas* complete their growth and development within the stem by feeding on the stem parts due to which the normal growth of the tillers is affected resulting in the 'dead hearts' or 'white-heads' condition. In India, infestation by this pest is a serious problem in almost eight states. Since the larvae complete a major part of their life-cycle within the stem, they are not easily accessible to sprayed pesticides. Moreover, no completely known source of resistance has been identified in spite of screening all the germplasm that is available at the International Rice Research Institute at

the Philippines, and the tolerance to this pest that has been observed in a few rice varieties has been found to be polygenic in nature. Hence conventional breeding strategies to incorporate resistance into rice varieties that are susceptible to *S. incertulas* are not practical. Development of transgenic rice plants has successfully achieved using genes encoding *Bacillus thuringiensis* crystal proteins. Though presently 100% mortality of *S. incertulas* larvae grown on such transgenics has been observed, there always exists the possibility of the larvae developing resistance to the Bt toxins as has been observed in a few other insects. Hence, in order to prevent any resistance being developed and to attain durable resistance, it is important to pyramid different genes into the same rice variety such that the product of each of the incorporated genes acts on different physiological and biochemical processes of the larvae, by a mechanism independent and different from each other.

Two forms of alpha-amylases have been identified in the gut of this rice pest, both of which are completely inhibited by inhibitors from wheat. The optimum pH of these alpha-amylases was confirmed to be pH 8.0 with 90% activity at pH 9.0. At pH 10.0 the activity was 69% of the optimum activity at pH 8.0. The optimum temperature was found to be 40°C with 72 % of activity at 50°C. The activity declined sharply at 60°C. The mode of action of the crude amylases was detected by hydrolyzing soluble starch for different intervals of time. TLC of the hydrolysed products showed the presence of sugars ranging from glucose to maltohexose. At 24 h maltose and glucose were the predominant products, indicating the enzyme to be endo in action. The molecular weights of the two forms were determined to be 40,000 daltons and 39,890 daltons, respectively.

The gene encoding one of the alpha-amylases was cloned using 3' and 5' RACE, using primers based on conserved regions of insect alpha-amylases. The gene is 1506 bp long, with a complete open reading frame encoding a protein of 502 amino acids, including the signal peptide. The gene sequence has been submitted to Gene Bank with the accession number EF672102. The signal peptide is 15 amino acid long. Cleavage of the signal peptide would leave a mature protein of length 487 amino acids with a predicted molecular weight of 54,955 daltons and theoretical pI of 5.39. The deduced amino



acid sequence shows significant homology to other insect alpha-amylases. Initial separation of the inhibitors from wheat into four peaks was achieved using Sephadex G100 gel permeation chromatography. From a practical point of view of developing transgenics, only the peak with molecular weight of about 16 kilo-daltons was further purified using HPLC and three peaks showing inhibitory activity towards the alpha-amylases from *S. incertulas* have been identified. The interaction of these three peaks with the cloned alpha-amylase gene product is being studied.

#### Interactions of aspartic protease inhibitor with insect mid-gut aspartic protease

An aspartic protease inhibitor (API) of Mr 1363 Da from a newly isolated strain of *Bacillus licheniformis* was reported earlier. API inhibited aspartic protease pepsin competitively. Digestive proteolytic apparatus of insects is remarkably plastic to study protease inhibitor interactions in highly complex plant pest systems which allow target pests to hydrolyze the inhibitors with non target proteases. The choice and development of appropriate, suitable inhibitors is a primary determinant in the success or failure of any pest control strategy. New, broad spectrum inhibitors of natural origin are currently considered for the improvement of protease inhibitor based pest control strategies. To evaluate the potency of API against insect aspartic proteases, aspartic protease from *Plutella xylostella* (Diamond backmoth) which is an insect pest of cruciferous vegetables was purified. The enzyme exhibited a Mr. of 46.1 kDa on SDS-PAGE with an optimum pH and temperature of 3.4 and 37°C respectively. The enzyme hydrolyzed hemoglobin with a  $K_m$  value of 538  $\mu$ M. The kinetic analysis of enzyme-API interaction suggested the competitive mode of inhibition with  $IC_{50}$  and  $K_i$  values of 44.0  $\mu$ M and 55.0  $\mu$ M respectively. Further, the studies are in progress to develop API as a biopesticide.

#### Chitin //chitosan contents of different fungal isolates

Chitin comprises 22-44% of cell walls of fungi. In comparison with marine sources, chitin production from industrial fungal waste is negligible, but the mucoraceous fungi, that contain chitosan, a deacetylated form of chitin, can be used for

its commercial production intended for sophisticated applications.

The mucoraceous fungal species contain chitosan as one of the main cell wall components. Different fungi were collected from NCIM for the estimation of chitin-chitosan contents in their cell walls. As zygomycetous fungi have higher amount of chitosan in their cell walls, eleven different strains were used for the analysis number of other fungi also show increased per cent of chitosan in their cell walls for the self defence. Therefore the cultures like *Ustilago* were also be studied. *Benjaminiella poitrasii* is a zygomycetous dimorphic fungus being investigated extensively to understand the process of differentiation. Large scale (100 g biomass) chitosan extraction from *B. poitrasii*, *Rhizopus stolonifer*, *Gongronella butleri* for further characterization with respect to purity, and percentage deacetylation using spectrophotometric and Solid state NMR analysis was carried out. Further media were optimized for the increased biomass with high level of chitosan contents in *B. poitrasii*. The biochemical correlation in the enzymes involved in the chitin synthesis and further modification of chitin to chitosan was also studied. A novel method of chitin deacetylase treatment of chitin to increase the per cent deacetylation was standardized. The per cent deacetylation obtained for *B. poitrasii* chitosan was more than ninety.

#### Development of a mycoinsecticide against *H. armigera* in pulses

Under the Indo-Swiss Collaboration in Biotechnology (ISCB) studies were undertaken to develop a mycoinsecticide for the control of *Helicoverpa armigera* on pulses in April 2000. The project started with the isolation of different entomopathogenic fungi, mainly belonging to genera; *Metarhizium*, *Beauveria* and *Nomuraea* which were tested for their effectiveness against *H. armigera* under laboratory conditions. With a view to the introduce the mycoinsecticide in to the market. In the second project phase, large scale field trials (on hector scale), in pulses with *M. anisopliae* formulations were carried out. Significant control of the larval population of *H. armigera*, and a consequential reduction in pod damage and increase in grain yield (5.4 larvae/5 plants, 23 % pod damage, 930 Kg/ha) in comparison with the untreated control (10.25 larvae/5



plants, 43 % pod damage 617 Kg/ha) was seen. *H. armigera* is also an important pest in cotton. Interestingly, initial trials carried out in 2006 have shown that the mycoinsecticide based on the strain M34412 is a better control than chemical control by endosulphan. Thus the mycoinsecticide might develop in to an alternative control measure for *H. armigera* in cotton. Experiments were carried out to investigate the potential loss of virulence of biocontrol strain *M. anisopliae* M34412 after subsequent in vitro subcuturing on artificial media this phenomenon is well known for other fungal biocontrol organisms and demands a strategy for the provision of back-up strains. Three strains (M34311, M81123, M91629) with properties close to those of strain M34412 were identified as back up strains. Experiments for the optimization of conidia production on a large scale and formulation studies for product development are currently in progress.

#### Enzyme complex from *M. verrucaria* as a biocontrol agent

*Myrothecium verrucaria* is one of the potential fungal organisms that produces very high levels of mycolytic and cuticle degrading enzyme activities. The studies on the production of conidia and/or yeast-like cells of *M. verrucaria* in the submerged fermentation were carried out. Such type of unicellular living propagules which can slowly secrete the cell wall degrading enzymes during their germination will be useful for the seed coating. The scale up studies with 100 L fermentor by varying nutritional parameters were also undertaken with the help of HiTech Bio Laboratories, Pune. The chitinase activity up to 0.90- 0.95 U/ ml was obtained using cheaper sources of chitin after 7 days. With respect to the downstream processing the different methods for the concentration of the crude broth were studied. The thermostability, UV and soil stability of the enzyme activities were studied with and without the addition of protectants like glycerol, sorbitol and other polyols. To make the cost effective production of enzyme the solid state fermentation for the enzyme production was carried out using jawar with and without chitin. The field trials to control soil borne fungal pathogens and an insect pest with the enzyme preparation are in progress.

#### Polyamines and dimorphism in *Y. lipolytica*

*Yarrowia lipolytica* is a nonpathogenic ascomycetous fungus studied to understand its dimorphic behavior. The polyamines putrescine, spermidine and spermine are ubiquitous aliphatic polycations required for cell growth and differentiation. In fungi, changes in the polyamine contents have been associated with a variety of morphological changes. Ornithine decarboxylase (ODC) is the key regulatory enzyme involved in the biosynthesis of polyamines. *Yarrowia lipolytica* NCIM 3589 is a marine isolate isolated from the Arabian sea. It however does not behave like the earlier reported strains of *Y. lipolytica* with respect to mycelium formation and requires low oxygen tension to induce mycelia. It has been reported that yeast cells degraded aliphatic fraction of crude oil when supported with nitrogen and phosphorus at a temperature optimum of 30°C under aerobic conditions. The ability of the strain to degrade oil, both in sea water and fresh water makes it a suitable candidate for bioaugmentation trials both in marine and fresh water environments.

#### Dimorphism in *B. poitrasii*

A saprophytic zygomycete *Benjaminiella poitrasii* has been identified to understand the role of NADP-dependent glutamate dehydrogenases in the morphological (unicellular yeast to hypha) transition, its taxonomical relatedness with human or plant pathogens, if any and to design antifungal strategies. Among the ammonium assimilating enzymes, such as NAD-/NADP-glutamate dehydrogenases (GDH), glutamine synthase (GS) and glutamate synthase (GOGAT), in case of *B. poitrasii* GDH (1 NAD-GDH and 2 NADP-GDH) enzymes were shown to have biochemical correlation with the morphological (yeast-mycelium) transition. The role played by NADP- GDH independently in *B. poitrasii* morphogenesis is being studied at genetic level by isolating and characterizing specific GDH genes, monomorphic and GDH minus mutants too. The ultimate goal is to understand the contribution of GDH enzymes in the fungal morphogenesis of different plant and human pathogens and to use GDH as a novel target to develop antifungal agents.

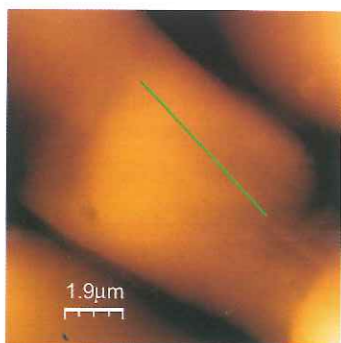
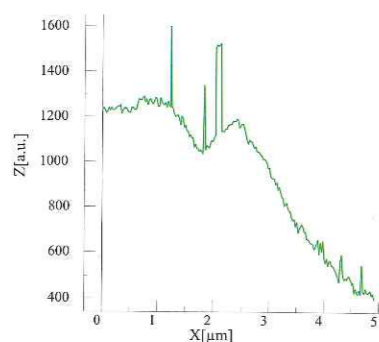
Furthermore, yeast- hypha transition was also studied by monitoring changes in the cell surface of *B. poitrasii* using atomic force microscopy (AFM). AFM height



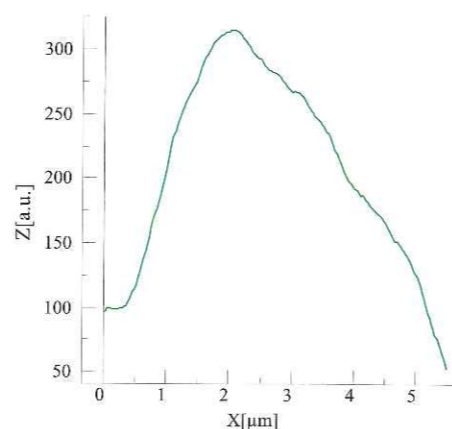
images of yeast surface showed grainy structure, when stained with Fluorescein Isothiosyate (FITC) labeled Wheat Germ Agglutinin (WGA) and which were observed to be made up of chitin. Average roughness ( $R_a$ ) was found to decrease marginally from Y-H transition in complex (organic nutrient) media whereas the  $R_a$  increased dramatically in transition from Y-H in minimal (inorganic salts) media. In particular, results of AFM imaging showed significant difference in Y-H transition in the presence of organic and inorganic nitrogen sources. In organic nitrogen the transition led to smooth hyphal surface, whereas in the presence of inorganic nitrogen hyphal surface was found to be rough and showed tubular structure on its surface. Overall, this study has highlighted the usefulness of AFM in the studies of fungal morphogenesis, *per se*.



Grown in minimal medium



Grown in complex medium



Changes in surface structure of hypha

### 1.2.6 Production of microbial biomass: Single cell protein production

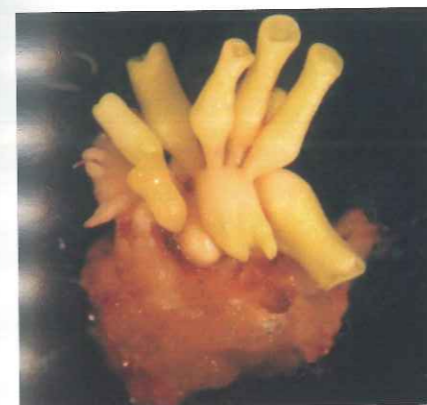
Single cell protein (SCP) can be used as an alternative to conventional proteins like casein, soyabean meal, egg protein or meat protein in animal feed. In this project, yeast and fungal strains from NCIM and bagasse which is a by-product of sugarcane industry, having low protein content is used as carbon source for SCP production. Bagasse is rich in fermentable carbohydrates (39% hexosan and 15-30% pentosan and 4-18% lignin). Simple method like steam treatment was used as a pretreatment method so that hemicellulose portion of the bagasse can be used as a substrate along with cellulose for microbial biomass production. *Penicillium janthinellum* culture produced 46% protein at 28°C and in 48 h. in a simple medium using bagasse hydrolysate (2%) as carbon source, ammonium sulphate as nitrogen source. Xylanase activity (100-151 IU/ml) is obtained as a by-product. *Candida utilis*, *Candida tropicalis*, *Candida guilliermondii* and *Saccharomyces cerevisiae* cultures also produced SCP in the same medium with 38-54% protein content. Cultures from NCIM showing maximum RNase activity were selected for reducing RNA content of the SCP produced by fungal and yeast cultures in first part. High RNA content is a major problem of SCP production which limits its use in animal feed. After reducing RNA content, then it is regarded safe to use as animal feed.



## 1.3 PLANT TISSUE CULTURE

### 1.3.1 Basic studies In vitro morphogenesis and genetic transformation in peanut

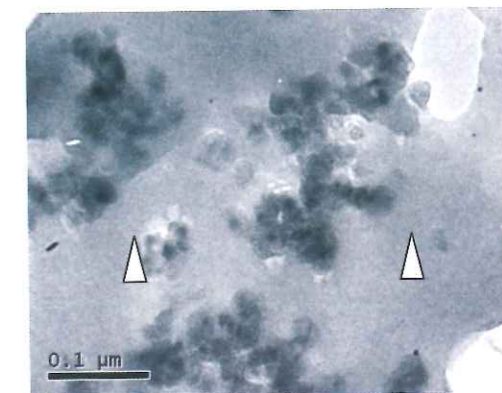
In peanut, regeneration protocols via somatic embryogenesis were established. However, the plant recovery is poor due to morphological abnormalities in these embryos. Attempts are being made to manipulate the cultures at initial stages of embryo development to obtain physiologically and morphologically normal somatic embryos with high conversion frequency in SB-11, a cultivated variety of peanut. Using determined organogenic buds as initial explants, somatic embryos were produced. Preliminary evidences proved modulation of the pathway from organogenesis to embryogenesis and was confirmed histologically. The plants derived from somatic embryos were hardened in green house to maturity. This system is now being used for standardization of transformation protocols using *Agrobacterium*.



Development of somatic embryos from mature zygotic embryo axis of peanut

### Production of nanoparticles in living tissues

To explore the possibility of an environment friendly method for recovering metal from mining wastes and a new alternative to produce nanoparticles, production of nanoparticles was demonstrated, in alfalfa plants cultured in silver containing medium. Presence of metallic silver in the plant was detected using EDS. The silver nanoparticles were detected in the plant organs by TEM. These methods are being extended to the plants that are growing on metal mining dumps to identify the nanoparticle producers if any.



Silver nanoparticles appear as black dots in TEM photograph of alfalfa leaves.

### 1.3.2 Micropropagation of *Pongamia* and *Semecarpus*

*Pongamia pinnata* has potential in production of biodiesel. Protocols for micropropagation of *Pongamia* from different explants of seedlings and mature trees were standardized. Clonal fidelity within the propagules was demonstrated using ISSR techniques. The methods were extended to the in vitro raised plantlet surviving in soil. The study confirmed the need for micropropagation technique over the seed raised plants to obtain multiples of a specific genotype.

Tissue culture raised *Pongamia* plants growing in a private farm near Pune

### Micropropagation of marking nut

The plant, marking nut (*Semecarpus anacardium*), has potential in production of biodiesel and in production of compounds of medicinal value. Clonal propagation of this plant is important for germplasm preservation as it is disappearing fast due to over exploitation for the medicinal value of the seeds and bark. Protocols were standardised for clonal propagation of this plant from seedling explants and the plants are growing in green house. This protocol is now being extended to the mature tree derived explants. A successfully induced *novo* caulogenic buds in the cotyledon explants was done.





Semecarpus shoot culture

#### Micropropagation and DNA fingerprinting of selected grape varieties and rootstocks

In this multi-institutional project involving Pune-based National Research Centre for Grapes (NRCG) and Agharkar Research Institute (ARI), the main objective of the programme at NCL was to develop and refine *in vitro* plant regeneration protocols of selected rootstocks and varieties of grapevine. Four commercially important varieties of grape (Red globe, 2A Clone, Crimson Seedless and Italia), and two rootstocks (110R and 1103P), which have shown field tolerance to drought and salinity were selected for micropropagation studies. Experiments were carried out to optimize conditions for micropropagation stages like shoot initiation, multiple shoot induction, proliferation and elongation of shoots, *in vitro* and *ex vitro* rooting of shoots, hardening of plantlets and production of tissue culture plants. Four grape cultivars and two rootstocks significantly differed in their optimum requirement of basal medium and growth regulators for different stages of *in vitro* propagation. Two routes of propagation were developed. In one route, bud break and rooting was induced in single node segments from field grown vines and whole plants were established on potting. Induction of bud break and simultaneous rooting at base of nodal explants provide an opportunity to have established plantlets within two months.

In second route, axillary buds were subjected to induce multiple shoots, which were subsequently rooted *in vitro* or *ex vitro* by auxin pulse treatment and plantlets were established. Total number of tissue culture raised plants produced and supplied to NRCG Pune was as follows: Red Globe (785), 2A-Clone (817), Italia (542), Crimson Seedless (509), 110 R (461), 1103P (134).



Stages of micropropagation of grapevine cultivars: Shoot initiation in TS (A), 2A-clone (B), Crimson seedless (C) and Italia (D); Direct rooting in Crimson seedless (E), 2A-clone (F), Red Globe (G); Multiple shoot induction in Crimson seedless (H, I), Red Globe (J); Elongation of *in vitro* shoots in Crimson seedless (K); Rooting in shoots of 2A-clone in agar medium (L), rooted shoots of Crimson seedless in agar medium (M); *Ex vitro* shoot of Crimson seedless (N); Hardened plants of 2A-clone (O).

#### Biodiversity conservation and characterization of *Iphigenia*

Six species of *Iphigenia* genus namely *I. stellata*, *I. indica*, *I. pallida*, *I. magnifica*, *I. sahyadrica* and *I. mysorensis* are endemic to the peninsular India. The plant species are distributed in well-separated and distinct geographical locations from the north of Raigadh district of Maharashtra State to the south in the Shimoga district of the Karnataka State. The main objective of this study was to collect *Iphigenia* species from their wild, ecologically distinct and well separated habitats and generate reproducible methodologies for *in vitro* regeneration.



Different combinations of BAP in combination with NAA, KIN and TDZ were tried for regeneration of corms but only single shoot was obtained. The shoots were hardened and transferred in pots. For embryogenesis the hormones like 2,4-D, 2,4,5-T, Picloram and Dicamba were used. The hormone 2,4,5-T showed callus formation after 3-6 weeks (C). Then callus got converted into somatic embryos. In control, initially seed germinated, a single shoot with callus was formed which then multiplied into multiple plants (B). The Picloram medium also produced somatic embryogenesis (A,D).

Regeneration of *Iphigenia*

#### Micropropagation of *Acacia* hybrid

*Acacia* hybrid is a tropical leguminous tree species widely planted in Southeast Asia, India and the southern provinces of China for reforestation and soil rehabilitation of degraded land. In recent years, it has become a preferred fiber source for the paper and pulp industry because of its rapid growth, high pulp yield, high fiber quality and its ability to thrive in degraded soils. The plant is used as biomass mainly for paper and pulp industries. Apical and nodal explants were collected from the identified mother trees, surface sterilized and cultured on different media. Cultures were established and multiplied. Various physical and chemical parameters have been standardized. The shoot cultures have been up scaled, rooted and plants have been successfully hardened. A few plants have been field planted. At present, more than 1000 plants in green house are ready for field planting. Protocol is now being extended to selected genotypes.

#### Micropropagation of *Casuarina*

*Casuarina equisetifolia* Forst. (Australian or Whistling pine) is an evergreen, xerophytic tree used for sand stabilization, shelterbelts, soil rehabilitation, fuel wood, timber production, animal fodder and field crop protection. The impact of the recent tsunami was reduced in the coastal areas of Tamil Nadu where *C. equisetifolia* were planted as shelterbelts. As a multipurpose agro forestry tree species, *Casuarina* is efficient nitrogen fixer and provides a wide range of social, economic and environmental benefits. A micropropagation protocol for rapid multiplication of *C. equisetifolia* has been standardized. Extensive work has been carried on standardizing the season of collection, type of explants, sterilization treatment, basal media and growth regulators. Auxiliary proliferation and elongation of shoots have been obtained. These shoots were rooted and plantlets were successfully hardened.

#### Mycorrhizal association with tissue culture raised *Casuarina* plants

Studies were carried out on the association of mycorrhiza with tissue culture raised plants of *Casuarina equisetifolia* Forst using mycorrhizal infected roots (MIR) entrapped AM fungi in Ca-alginate. The methodology adopted to inoculate AM fungi by MIR Ca-alginate beads and inoculation of local *Frankia* strain was found to be efficient, since 1) both mycorrhizal and *Frankia* nodules were observed in the host roots, 2) increase in plant survival during hardening phase, 3) increase in root surface due to efficient colonization, and 4) increase in biomass. It has been concluded that *Glomus mosseae* is the efficient AMF strain for better survival rate of micropropagated *C. equisetifolia* plants. A protocol has been standardized for mycorrhizal association in *Casuarina* sp. Further studies to check whether improved plant growth obtained after mycorrhizal association is due to change in micronutrient assimilation were also carried out. Plant samples were tested for elements like  $Fe^{3+}$ ,  $Cu^{2+}$ ,  $Zn^{2+}$  and  $Mg^{2+}$  by ICP-spectrometric method. The results obtained showed increased elemental uptake. This may be the reason for increased survivability of AM inoculated plants and better performance of host plants under AM fungal association.



### Regeneration studies in Eucalyptus

*Eucalyptus tereticornis* Sm. is an economically important species, the wood is useful as a raw material for paper and pulp industry. Direct shoot regeneration has been obtained from leaf explants of *E. tereticornis* on modified MS medium supplemented with BAP. Regenerated shoots were rooted on half strength MS salt medium supplemented with IBA. The regenerated plants were hardened successfully.

### Micropropagation of Jatropha

*Jatropha curcas* L. is an economically important plant and is considered as a source of biodiesel and also reclamation of marginal lands. It is cultivated as an oil seed crop. Seeds of this plant contain 40-50% smudging oil k/a curcas oil that is an efficient substitute fuel for diesel engines. Due to its tremendous potential as a source of biodiesel, at national level Jatropha mission has been taken up for large-scale plantation of these plants through seeds, micropropagation.

Studies on micropropagation of *Jatropha* and development of protocol are being carried out with special emphasis on source of explant, season of collection, isolation and identification of the contaminants, different trials for control of contaminants, culture establishment, multiplication and rooting. Success has been achieved in establishing germ free cultures and shoot cultures are growing for more than three cycles. Studies on protocol development for multiplication and rooting are in progress.

### Demonstration plots on horticulture and forest tree species

Extensive work on development and refinement of micropropagation protocols for economically important plants at NCL, have led to development of micropropagation technologies which have been tested for technocommercial feasibility by the way of conducting large number of field verifactory trials, benefit to cost ratio analysis and technology transfer to industries. On this background, with a view to generate awareness about the superiority of tissue culture raised propagules among the farmers / user agencies, small scale demonstration plots using tissue culture propagules for horticulture crops, and forest tree species have been established under this project for banana, turmeric,

ginger, chlorophytum, patchauli, teak and bamboo. It was observed that tissue culture raised plants showed higher growth as compared to conventional plants. Growth of banana var. mahan was best amongst the banana tissue culture raised plants. While in turmeric, the average yield was approximately double as compared to the conventional plants. It was observed that the height of tissue culture raised trees was more than that of local variety. Tissue culture raised teak trees grew straight and had fewer branches; hence the commercial bole realization will be more. Tissue culture teak trees had fewer branches on the lower portion and thus expenses of labour for pruning can be saved. The problem of nodes was also less. Thinning was performed in 2005 and wood density analysis results are encouraging.

### 1.3.3 Phytoremediation Industrial waste minimization and clean-up

Phytoremediation strategy is an environment friendly approach for minimization of metal contamination. To identify plants for phytoremediation of land degraded due to industrialization the tissues collected from three identified tree species of manganese mine dumps, Gumgaon near Nagpur were analysed. Manganese content in these tissues was compared with the tissues collected from NCL and other sites away from manganese mines. *Holoptelia integrifolia* leaf and stem tissues accumulated high amount (eight times and thirteen times, respectively of control) of manganese whereas accumulation of this metal in cassia and neem were approximately three times only. In all three species manganese was higher in leaves compared to stems. The *Holoptelia* plant growing in the dump could be a potential hyperaccumulator. Cadmium tolerance and cadmium stress induced changes were tested using in vitro system in peanut seedlings. Metal content in different parts of the seedling, the data generated from enzyme estimations, and thiobarbituric reacting substances (TBARS) leads to the conclusion that cadmium causes lipid peroxidation leading to cell and plant death.

Sanquelim and Codli mine dumps of SESA Goa were surveyed for naturally growing high iron tolerant plants. The plants *Trema orientalis*, *Acacia auriculiformis*, *Macaranga peltata* and *Alstonia scholaris* were identified on the dumps. Estimation of iron content demonstrated accumulation of iron in the different parts of some of these plants



Iron Ore Dump



Soil Texture



*Alstonia scholaris*



*Trema orientalis*

### Application of in vitro techniques to determine metal tolerance in oil producing plants

Jojoba (*Simmondsia chinensis*) a potential source of liquid wax with a wide range of industrial uses can thrive in unfavorable conditions and produce products of commercial interest. Thus, it is a species of choice for phytoremediation and value addition to the wastelands. Using plant tissue culture techniques experiments were conducted to determine its potential to survive in cadmium and copper rich soil. The shoot growth in culture was more sensitive towards Copper. Increased lipid peroxidation in presence of these metals indicated stress. Tolerance of *Jatropha* seeds towards various metals (Cu, Cd, Cr, Fe, Mn, and Zn) was tested. Seedlings were highly sensitive towards presence of cadmium followed by chromium and copper. It survived in medium containing high manganese, iron and zinc.

### 1.3.4. Biotechnology and genetic improvement of turmeric

Turmeric (*Curcuma longa* Linn.), a spice and coloring agent, is fast becoming an important medicinal plant. With this change in status, an increase in its demand is expected. Biotechnological and genetic improvement efforts are necessary for increasing production, profitability to farmers and foreign exchange earnings. Induction of polyploidy (turmeric being a triploid, to induce hexaploidy) was attempted. In the previous year the concentrations normally employed (0.05-0.3% for different durations 3, 6, 9 and 24 hrs) were tried. Deep seated meristem, covered by many layers of leaf-sheaths was a barrier. This year higher concentrations



(0.4%, 0.5% and 0.6%) in 2% DMSO for short duration (3 hrs) were tried in three commercially important varieties viz. Krishna, Salem and Thekkurpetta. There were some indications of successful induction of polyploidy. In one of the treatments (fresh sprouts immersed in 0.5% colchicine in 2% DMSO, exposed to sunlight in the morning hours 9 am to 1 pm) all the treated buds showed signs of induced polyploidy (smaller, rounded and leathery leaves). On growing in the field nearly half the plants flowered (normally one in 100,000 plants flower). However, there was no seed-set. Being a vegetatively propagated crop the polyploids can be multiplied, field-tested, and if found superior can be used for commercial cultivation.

#### 1.4 BIOCHEMICAL ENGINEERING

##### Neera

Under this program, further pilot plants were built for two locations, one in Saronda Gujarat and the other in Dahanu, Maharashtra to test the efficacy of improved shelf life of Neera using a process developed at NCL.

##### Biomass from *Lactobacilli*

A technical service was undertaken for isolation of lactic acid bacteria from natural sources for use as probiotics. The strains were isolated and characterized for their growth, nutritional requirements and viability under various techniques of cryo-preservation.

##### Aqueous two phase separations.

A number of modified polymers from natural material like guar and tamarind Kernel powder were prepared and their properties for use as aqueous phases elucidated.

##### Cloning, Expression and Production of haeme-proteins by yeast in fermenters for combating nutritional iron deficiency

The incidence of iron deficiency in the Indian population, especially in the rural population is very high. Iron deficiency anaemia is one of the most common nutritional disorders worldwide. NCL had initiated a multi-institutional project for Cloning of the Human Haemoglobin in *Saccharomyces* (NCCS, Pune) and Lactoferrin (NDRI, Karnal) gene in an effective GRAS Yeast Expression system that gives high yield of intracellular haemoglobin/lactoferrin. Lactoferrin was

cloned and expressed in *Pichia pastoris* and *Saccharomyces cerevisiae* and tested at laboratory scale.

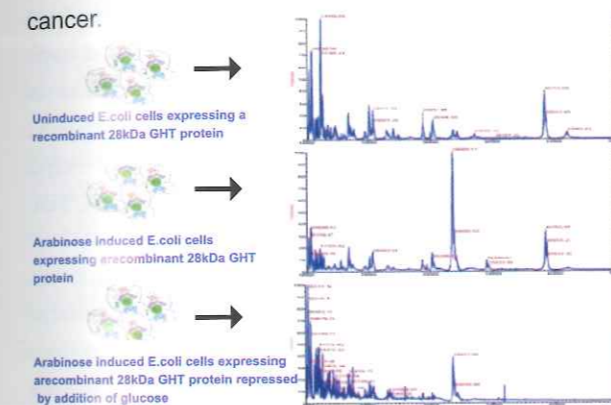
#### 1.5 PROTEOMICS AND MASS SPECTROMETRY

##### ICM-MS tool to screen drugs in vivo for regulation of protein expression

The Intact Cell MALDI-MS (ICM-MS), a mass spectrometry technique, has been used for rapid identification and characterization of clinically important microorganisms, including bacteria, fungi, viruses, and spores. ICM-MS has been established for low molecular weight compounds and was recently extended to the analysis of proteins. Change in expression (synthesis) of specific proteins and their activity is associated with the development of any disease. For example during cancer development proteins involved in cell proliferations are upregulated e.g. MAPKs, EGFR, cyclins etc. Similarly, during inflammation cyclooxygenase-2 activity is increased. Therefore, understanding the regulation of such proteins is important in view of controlling the disease. ICM-MS offers a very high potential in monitoring protein expression and drug discovery. In view of this, a method was demonstrated with a potential for the rapid screening of drugs that regulate the protein expression directly from an intact cell by laser desorption / ionization, by ICM-MS using *Escherichia coli* cells expressing a recombinant glutathione-S-transferase (GST) gene under an arabinose-inducible promoter, as a model system. Using ICM-MS analysis, a 28kDa peak corresponding to the recombinant GST was detected under the arabinose-induced condition. Furthermore, the regulation of GST protein expression was studied using glucose as an alternative metabolite. Glucose decreased the intensity of arabinose induced GST synthesis suggesting that the technique can be used for screening the drugs in vivo. The ICM-MS technique when compared to other techniques such as SDS-PAGE, Western blotting, ELISA etc., offers a simple procedure for sample handling, gives specific and accurate patterns of mass spectra, has the potential for autosampling and the rapidity of analysis combine to meet virtually all the performance criteria required for high-throughput drug screening. Therefore can be used to discover novel drugs against specific.



protein expressions in different diseases and can be extended to eukaryotic system or mammalian cell lines for in vivo screening of drugs against specific targets. Recently, this technique has been used for classifying subpopulation of *Moraxella catarrhalis* based on outer membrane proteins using ICM-MS, suggesting this technique can also be easily extended to study the regulation of cell surface receptors such as EGFR, VEGFR, GPCRs, which are important drug targets of cancer.



ICM-MS analysis of E. coli cells expressing a recombinant GST protein under the control of the arabinose promoter was not include (a), include with 0.2% arabinose (b) repressed with 0.02% glucose (c)

##### Taxonomical characterization of some *Rhizobial* species by ICM-MS

For some time the Rhizobiaceae family was treated as one group consisting of five genera-*Rhizobium*, *Bradyrhizobium* and *Azorhizobium* along with *Agrobacterium* and *Phyllobacteria*, based on 16S rRNA typing. However, interpretation of certain studies based on 16S rRNA sequences can not fully convince inter-generic or inter-specific relatedness of *Rhizobium*. For example whether *R. galigae* is closer to *A. vitis* or *A. rubi*, is ambiguous. Whereas few other findings of 16S rRNA does show unambiguously that *R. galigae* is closer to *A. vitis* and *A. rubi* than it is to *R. leguminosarum*. Therefore, taxonomical classification based on 16S rRNA is a matter of debate. Recent developments in mass spectrometry have given hopes for analyzing biological macromolecules. One such technique is ICM-MS, which has been used to differentiate different microbial strains especially in clinical microbiology. In this technique intact bacterial cells in their dynamic state are co-crystallized with matrix and exposed to laser for ionization and desorption of cell surface molecules. This technique examines the chemistry of the cell surface molecules, yielding spectra consisting of a series of

peaks ranging from the mass to charge ratio ( $m/z$ ) of 50010,000 Da. Each peak corresponds to a molecular fragment released from the cell surface during laser desorption. The peaks obtained from different microbial strains may be chemically different, as the cell surface molecules vary from species to species. These ionized molecules may be mixture of small peptides, teichoic acids, oligosaccharides and lipids. Using ICM-MS, an attempt has been made to bring out similarities and differences among some *Rhizobium* species and a species of *Agrobacterium* based on specific mass:charge ( $m/z$ ) values. *Rhizobium* species isolated from the root nodules of selected leguminous plants were analysed by ICM-MS. The spectra were acquired in the range of 50010,000 Da yielding several peaks specific to each species. The number of peaks were more in the range of 5001200 Da. Dice similarity coefficient analysis of  $m/z$  values indicated that *Rhizobium* species isolated from *Trigonella foenum-graecum* and *Pisum arvense* showed more similarity than any other species. *Agrobacterium* species did show a few common  $m/z$  values in comparison with other *Rhizobium* species. This clearly shows that *Agrobacterium* is closely related to *Rhizobium*. Eventually, ICM-MS technique offers clear, distinct, and consistent results for replicates, in less than an hour's time, therefore this technique has high potential in molecular taxonomy.

##### Study of papaincystatin interaction by intensity fading MALDI-TOF-MS

Molecular recognition involves specific interaction between ligand and protein, leading to biological processes such as enzyme catalysis, cell signaling etc. Information on proteinligand interactions are accumulating at a faster pace through different experimental techniques. Mass spectrometry has become one of the important techniques especially after the development of soft ionization techniques such as electrospray ionization (ESI) and matrix assisted laser desorption ionization (MALDI). The potential of mass spectrometry (MS) for the direct analysis of complex biological samples has been extensively demonstrated. In particular, electrospray ionization ESI-MS has been shown to be very useful for the study of enzyme kinetics, and has become an excellent technique complementary



to photometric, fluorometric and radiometric assays. ESI-MS has low tolerance toward sample contaminants especially salts and buffers.

Analysis with matrix-assisted laser desorption/ionization time-of-flight MALDI-TOF-MS, is rapid, sensitive and amenable for high throughput studies. Quantitative analysis with MALDI-TOF-MS has been challenging task due to significant variations in ion signals. Several parameters must be taken into account such as sample preparation, appropriate matrix, homogeneous co-crystallization of matrix and sample, pH of the solution, shot to-shot reproducibility, signal suppression effects, fluctuation in laser power and non-linear detector response and a right internal standard. In addition to these factors, for studying protein/ligand interactions, inability of the MALDI-TOF-MS to maintain the integrity of the protein/ligand complex, and to detect them in a high mass range, makes the job more challenging. In view of this, recently an interesting application of MALDI-MS called 'Intensity fading (IF) by MALDI-TOF-MS was described to study protein/ligand interactions, which is very powerful technique and amenable for high throughput screening. Here the relative intensities of combinatorial library or extract of natural product is monitored in the presence or absence of target protein by MALDI-MS. In the presence of target protein the relative concentration of the ligand that binds to the target decreases and therefore its relative intensity decreases or fades in MALDI spectrum. The technique is highly sensitive and has remarkable ability to detect non-covalent protein/ligand/protein interactions. In this investigation an attempt has been made to study the protein/ligand interaction by intensity fading (IF) MALDI-MS using papain and cystatin as model system for protein/ligand interactions. The intensity fading of cystatin was monitored using various concentration of cystatin ranging from (1 to 8.6  $\mu$ M) in presence of target protein, papain. The results indeed indicate that the intensity of cystatin decreases upon addition of papain. Furthermore, for the first time IF-MALDI-MS was used for determining the number of binding sites for cystatin on papain by Scatchard analysis.

## 1.6 ENTOMOLOGY

### 1.6.1 Basic entomology

#### Effect of lufenuron on the red rust flour beetle, *T. castaneum*

In our continuing efforts at identifying product(s) in controlling the most notorious stored product pest worldwide, the red rust flour beetle, *Tribolium castaneum*, the effect of lufenuron (Match<sup>®</sup> 5% EC), an acylurea belonging to the benzoylphenylurea group, on this pest and its biological activity and residual life in treated and milled wheat was investigated. It was observed that even at sub-lethal concentrations of lufenuron (LC<sub>10</sub>, LC<sub>20</sub> and LC<sub>40</sub>) there was a drastic effect on certain biological and reproductive end points on the different developmental stages of *T. castaneum*. Further, residue analysis of levels of lufenuron by GC-MS of treated and milled wheat revealed that the residual levels could control the larval stages of this pest for a period of 90 days. Interestingly, the levels of residue found were well within the maximum residue limit (MRL) set by international agencies on other food commodities. These findings, opens up a new vista for its possible application in protecting stored product commodities against *T. castaneum*. However, large scale field trials for information on degradation as well as the effects on the population dynamics of the insect should be considered before they can be incorporated in operational stored product's protection protocol.

### 1.6.2 Chemical ecology

Study on chemoreception in lepidopteran larvae is an ongoing research programme aimed at elucidating mechanisms of sensory perception of chemicals besides sensory transduction. Electroantennograms recorded from males and females of the potato tuber moth, *Phthorimaea operculella* revealed a broad range of response to plant volatile compounds. The fatty acid derivatives comprising essentially green leaf volatile components elicited significantly higher responses in females compared to oxygenated and hydrocarbon monoterpenes. Dose-response studies indicated differences between the sexes and concentrations suggesting existence of sexual dimorphism.



### 1.6.3 Applied entomology

4-Methyl-7-hydroxy coumarin is considered as a lead molecule for biopesticide. Its five derivatives including mono- bromo- and tribromo- derivatives synthesized by the collaborator were bio assayed against two species of mosquitoes: *Culex quinquefasciatus* and *Aedes aegypti*. The lowest LC<sub>50</sub> values were found 1.49 ppm and 2.23 ppm, respectively, against IV instar larvae of *C. quinquefasciatus* and *A. aegypti*. Among the derivatives, acetic acid 3,6,8-tribromo-7-hydroxy-4-methyl-chromen-2'-oxo-2H-chromen-7-yl ester showed remarkable ovicidal activity. Significant reduction of 80-85% hatching of eggs of both mosquito species was observed at the highest dose of 100ppm. The hatched larvae showed 100% mortality in the successive instars.

The larvicidal activity of ethanol, chloroform and hexane extracts of *Sterculia guttata* seeds was investigated against the IV instar larvae of Dengue fever vector, *A. aegypti* and filarial vector, *C. quinquefasciatus*. All extracts exhibited 100% larval kill within 24 hrs exposure period at 500 ppm concentration. Petroleum ether fraction of ethanol was found to be most promising. Its LC<sub>50</sub> was 21.55 ppm and 35.52 ppm against *C. quinquefasciatus* and *A. aegypti*, respectively (This work was done in collaboration with T.R. Ingle Research laboratory, S.P. College, Pune).

### Use of essential oils in pest control

Certain essential oils in known proportions were found to be active against some stored product pests (viz. *Sitophilus oryzae* and *Callosobruchus chinensis*) and vectors of human diseases (viz. *Aedes aegypti* and *Culex quinquefasciatus*). Besides, the same were found to be effective against certain plant pathogenic microbes (viz. *Fusarium oxysporum*, *Helminthosporium sp.*, *Sclerotium rolfsii*, *Curvularia lunata* and *Alternaria solani*). The combinations of these oils were formulated into emulsified concentrates and their effectiveness confirmed under laboratory conditions.

### Interaction and performance of *A. mylitta* on its host plants with special reference to *S. robusta*

In our continuing efforts to document the annual cycle of changes in primary and secondary metabolites as well as the nitrogen and carbon content in the three host plants (viz. *Terminalia tomentosa*, *T. arjuna* and *Shorea robusta*) with a view to correlate it with the performance of the tasar silkworm, *Antheraea mylitta* are being pursued. Extraction and quantification of flavonoids in *S. robusta* has been completed. Besides alkaloids, the lipids of the three host plants have also been completed. With respect to the nitrogen and carbon content quantification has been completed in *S. robusta* and *T. arjuna*.

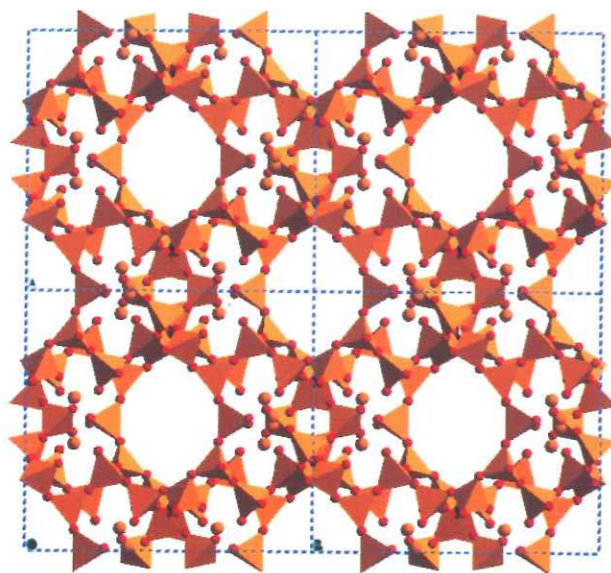


## 2 CATALYSIS

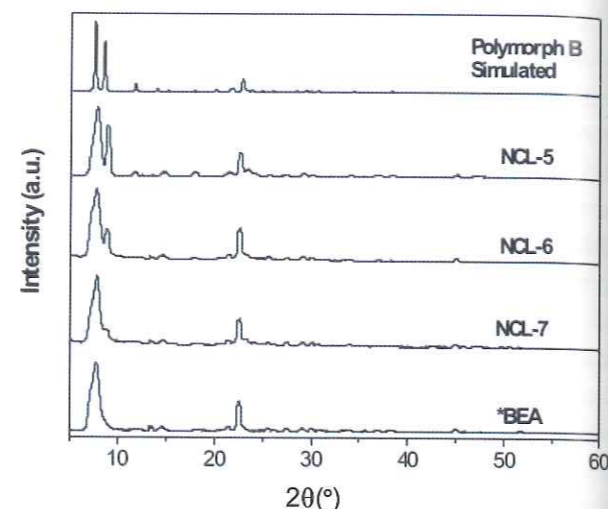
### 2.1. NEW MATERIALS

#### 2.1.1: Novel zeolite structures of BEA/BEB family

The synthesis of all-silica analogs of polymorph B-enriched zeolites of the BEA family denoted as NCL-5, NCL-6 and NCL-7 was realized hydrothermally at lower water content in fluoride medium using perchloric acid as promoter and tetraethylammonium hydroxide as template. The phase composition of the structures was derived using simulated patterns for the random intergrowths of polymorph A and -B using DIFFaX Code. The stacking direction *c'* is perpendicular to the *a'b'* plane of the layer. The pore architecture of zeolite NCL-5 is shown in figure. The phase composition of polymorph B derived using DIFFaX code was found to be 90-95 %, 70-75 % and 60-65 % in NCL-5, NCL-6 and NCL-7, respectively. The gradual decrease of polymorph B concentration in these samples showed a correlation with the decrease in water / SiO<sub>2</sub> molar ratio in synthesis gel. FTIR spectral analysis of NCL-5 has also confirmed the significant enrichment of polymorph B with tortuous channel structure in NCL-5 compared to all-silica-beta.



The pore architecture of zeolite NCL-5



Powder X-ray diffraction patterns of NCL-5, NCL-6 and NCL-7 and BEA (Standard Si-Beta) along with simulated pattern for pure polymorph B

#### 2.1.2 Fabrication of zeolite membranes

Even though zeolites have been known and utilized for numerous applications for decades, the concept of zeolite membranes is relatively novel and the technology not fully developed. Attaining a maturity in zeolite membrane technology demands a lot of effort in developing new methodologies of preparation and understanding their effects on the membrane characteristics. Few problems are identified with the conventional preparation methods and efforts have to be made to overcome these difficulties. One of the main drawbacks of the conventional method which involves simple *in-situ* crystallization of the zeolite over macroporous supports like oxides, steel and carbon is the loosely bound membrane, its thickness and brittleness. In case of oxides like alumina and silica, due to the electrostatic repulsion of the negatively charged support and the zeolite particles under synthesis conditions, the anchoring of the particles on to the support is not strong enough. Hence these types of membranes have limited use in separation or reactor purposes. However, this problem can be solved if the support surface charge is reversed prior to keeping in contact with the zeolite gel. Methods currently available to reverse the support charges are not cost effective for any real applications.



Very recently, the idea of using ionic polymers which are cheaply available to reverse the support charge has been implemented. Under zeolite gel conditions (pH ~11), the surface of the support is negative and the zeolite colloidal particles also are negative. Hence a cationic polymer like poly-dimethyl-diallyl-ammonium chloride is used so that it is anchored on to the negatively charged surface reversing the charge to positive. Now, zeolite colloidal / gel particles can easily attach themselves onto the positively charged surface and a subsequent hydrothermal synthesis and calcination at higher temperatures of the order ~500 °C will help in forming the thin film and burning away the polymer.



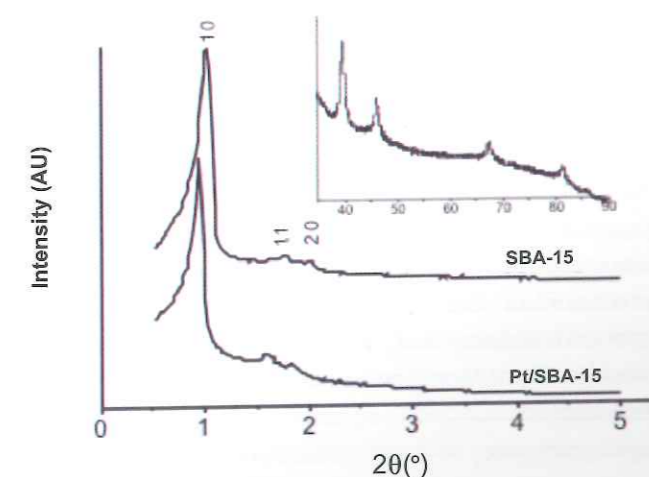
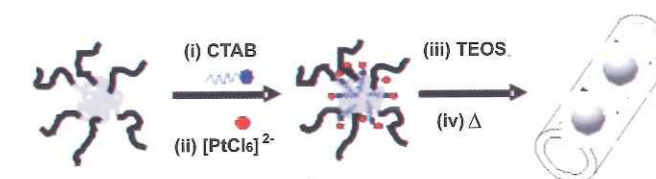
SEM of silicalite-1 membrane over alumina support

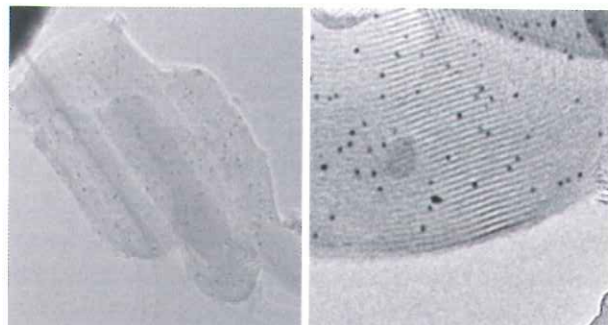
#### 2.1.3 A novel *in-situ* method for incorporating metal nanoparticles within mesoporous compounds

The advantage of using mesoporous compounds as supports in heterogeneous catalysis is the highly porous interpenetrating channel systems without any capillary effect diffusion limitations, within which nanoparticles can be located. This is expected to give a better control of particle size, morphology and even modified surface properties, which can be exploited for various applications even beyond catalysis. Incorporation of metal particles into mesoporous compounds is usually achieved by simply adding metal salt precursors to the oxide precursor gel or wet impregnation of metal salt on already formed mesoporous compounds. These methods have the disadvantage of uncontrolled growth of metal particles on the walls since no preventive

measures are taken to ensure that the metal precursors are isolated within the channels.

In an attempt to have better control over the size, amount and location of Pt particles in SBA-15, we have developed a new, simple and convenient *in-situ* one pot method of dispersing the metal salt precursors within template polymers modified with ionic surfactants in a controlled manner. The ionic surfactants are expected to be dispersed within the polymer micelle structure with the ionic head groups decorating the corona and the hydrophobic tail groups penetrating the core. Added to this polymer-surfactant composite, metal precursor ions diffuse into the corona depending on various factors viz. ageing time, surfactant and precursor concentration etc. Later calcination of this material leads to a dispersion of metal nanoparticles of fairly uniform size distribution. This method provided an easy and efficient way to have an enhanced control over fine-tuning of the particle sizes at the same time ensuring that they are localized within the mesochannels.

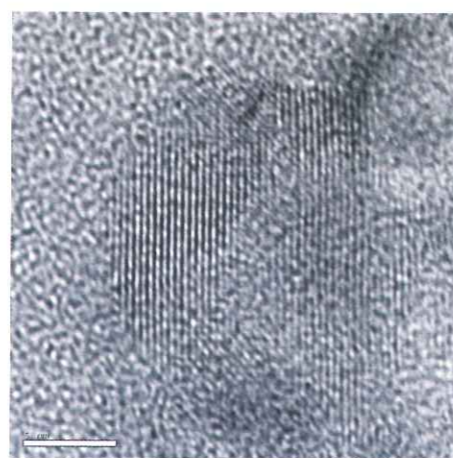
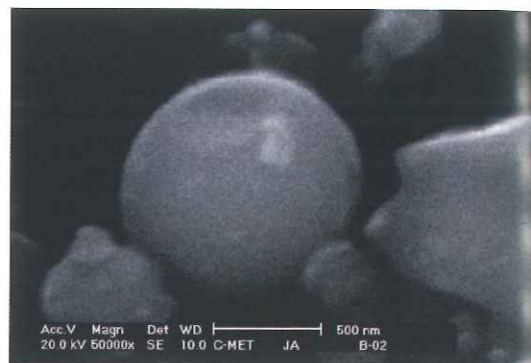




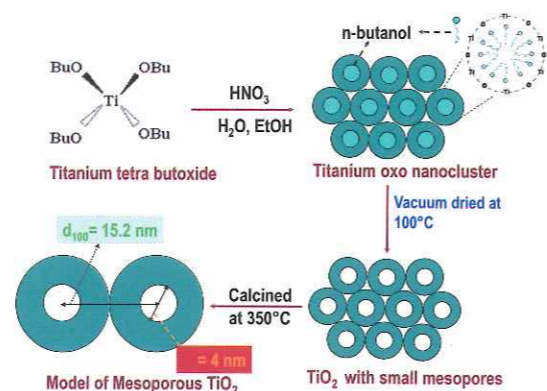
Schematic representation of the localization of precursor salts within the channels; XRD patterns of the Pt incorporated material compared with the parent showing a slight swelling (inset Pt particles); TEM images showing the presence of nanoparticles of size 6-9 nm located exclusively within the mesochannels

#### 2.1.4. Template free synthesis of mesoporous TiO<sub>2</sub>

Mesoporous silica is well known in the literature and employed for many catalytic reactions, however very few reports are available on mesoporous titania. Recent efforts at NCL led to the preparation of mesoporous titania in a nanocrystalline framework and anatase phase with a fairly high wall thickness, which is an essential requirement to make the material more stable and intact under harsh reaction conditions. A simple sol-gel procedure was adopted to prepare nanocrystalline mesoporous titania without any templating agent and it possesses a reasonably high surface area (~200 m<sup>2</sup>/g) and a large pore wall thickness (11.3 nm) than that of meso-TiO<sub>2</sub> prepared by known methods with surfactants. The meso-TiO<sub>2</sub> materials were characterized by structural, spectroscopic and textural properties. Spherical shape particles in a range of few hundred nanometers are obtained in the template free method. Bundles of hexagonal array of mesopores were clearly observed in TEM demonstrate the formation of mesoporous titania. Systematic characterization provided definite and direct indications toward the mechanism of formation of meso-TiO<sub>2</sub> in the template free method.



SEM (top) and TEM (bottom) of mesoporous TiO<sub>2</sub> showing spherical particle and lattice fringes

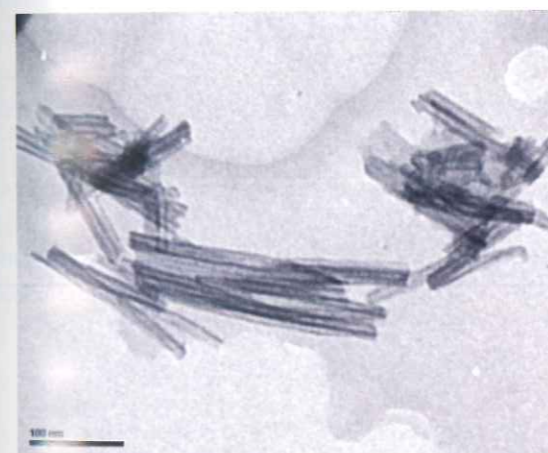


A schematic model to demonstrate the various stages of formation of mesoporous TiO<sub>2</sub> through template free sol-gel method



#### 2.1.5 Titania nanotubes

Well-aligned titania nanotubes have been synthesized by subjecting TiO<sub>2</sub> to a hydrothermal treatment under alkaline medium. Two different precursor samples were employed for this purpose, a mesoporous titania sample obtained by hydrothermal treatment to Ti(IV) tetra isopropoxide using tartaric acid as structure directing agent and another a commercial titanium dioxide sample. The composite samples having gold (1-2 wt %) dispersed over these TiO<sub>2</sub> nanotubes were synthesized so as to obtain highly efficient photocatalytic materials for photo-oxidation of volatile organic compounds. The physico-chemical properties and the catalytic activity of these samples for vapor phase photocatalytic oxidation of organic compounds were monitored.

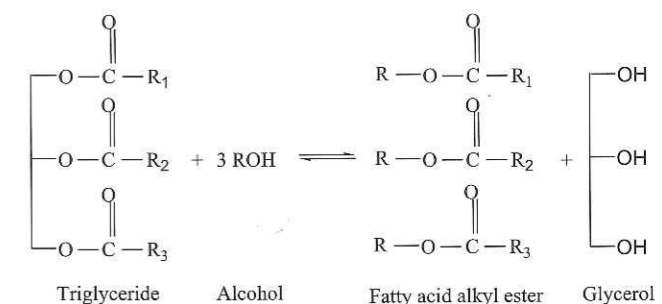


TEM pictures of TiO<sub>2</sub> nanotubes and gold containing composites

## 2.2. FUELS AND ENERGY

### 2.2.1. Biodiesel and biolubricants

Biodiesel is a biodegradable, cleaner burning, renewable alternative to petrodiesel. It consists of mono alkyl esters of long chain fatty acids produced from vegetable oils or animal fats by transesterification with methanol or ethanol. Biodegradable biolubricants are produced when longer chain alcohols (octanol, for example), instead of methanol / ethanol are used. Biodiesel leads to ~25% reduction in the emission of harmful pollutants like carbon monoxide, sulfur oxides, and other particulate matter. However, the presently used alkali process is not environmentally friendly and co-produces huge amounts of spent alkali wash consuming large quantities of very precious water. Therefore, application of solid catalysts instead of homogeneous alkali based catalysts and use of unrefined, non-edible oils and waste cooking oils instead of expensive refined, edible oils in biodiesel and lubricants production would make manufacture of biodiesel economically and environmentally attractive.



Transesterification of triglycerides with alcohols. R<sub>1</sub>-R<sub>3</sub> = Fatty acid alkyl groups, R = C<sub>10</sub> or C<sub>2</sub> (biodiesel) and C<sub>6</sub>-C<sub>8</sub> (biolubricant) alkyl groups

A suitable, solid, stable catalyst system is developed, where non-edible oils with high contents of free fatty acids can be used to produce not only biodiesel but also biolubricants. Further, the catalyst systems can be used in batch or continuous mode including continuous fixed bed operations. Another advantage of the versatile catalyst systems is that a range of oils including jatropha, karanja and unrefined rubber seed oil (containing large amounts of free fatty acid, FFA) can be used for producing biodiesel and biolubricants, where both transesterification (of the triglycerides) and esterification (of the FFAs) are accomplished by this solid catalyst in a single reactor.

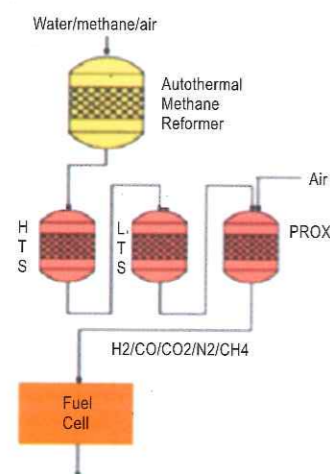


The biodiesels and biolubricants produced meet the standard specifications. The solid catalysts developed are reusable and active even when significant quantities of water are present (unrefined oils).

Another significant advantage of this heterogeneous catalytic process for producing biodiesel and biolubricants is that the glycerol, which is co-produced is highly pure and does not require extra-efforts for purification and recovery.

### 2.2.2 Hydrogen generation for PEM fuel cells

Hydrogen gas is the preferred fuel for PEM fuel cells because of its high energy density (per kilogram) and the low environmental impact. A fuel processor is used to generate hydrogen for PEM fuel cells. It mainly consists of three parts: (i) Auto Thermal Reforming (ATR) section, wherein syn gas is produced from a primary fuel such as natural gas, LPG or ethanol. (ii) Water gas shift (WGS) section, in which CO in syn gas (8-12 vol%) is converted to hydrogen and CO<sub>2</sub> by reacting it with water, and (iii) PROX (preferential oxidation) section, in which residual CO in the reformat, followed by WGS step is oxidized to CO<sub>2</sub> to bring it down its concentration level to < 20 ppm. It is desired that the ATR catalysts should be able to handle multiple fuels, so that the fuel processor is versatile to handle any of the fuels available locally. NCL started working on an 'all' honeycomb monolith based-ATR based-fuel processor that will have quick start and load following characteristics along with better thermal efficiencies.



Flow chart of proposed ATR based fuel processor

### Development of ATR catalysts

Major progress was made towards development of ATR catalysts in terms of catalysts that work at high space velocities and high hydrogen yields. We have developed more than one formulation of precious metal (Rh, Pt and Pd) based ATR catalyst for reforming of natural gas and LPG. A laboratory set-up was assembled for testing and evaluation of ATR catalysts. Catalysts supported on novel mixed oxides work at very high gas hourly space velocities (25,000-80,000 h<sup>-1</sup>) and at low steam/carbon ratios (as low as 1.2). An exclusive facility was created for testing and evaluation of monolith based ATR catalysts. The syn gas generated from the reactor is analyzed using an on-line GC that can separate and estimate all gas components present in the reformat.



Laboratory assembly for ATR catalyst testing

Results of ATR of methane using NCL catalyst

O <sub>2</sub> /C	H <sub>2</sub> O/C	CH <sub>4</sub> conv (%)	Reformat composition (vol%)				
			H <sub>2</sub>	N <sub>2</sub>	CO	CO <sub>2</sub>	CH <sub>4</sub>
0.65	1.20	99.63	7.87	44.69	10.53	6.84	0.06
0.63	1.20	99.33	8.85	43.50	10.40	7.13	0.12
0.61	1.20	98.44	0.56	41.74	10.37	7.06	0.27



These catalysts were also evaluated using various oxygen/nitrogen ratios for a possible enhancement of H<sub>2</sub> concentration in the reformat. Another formulation of precious metal catalyst was also developed employing perovskites as supports.

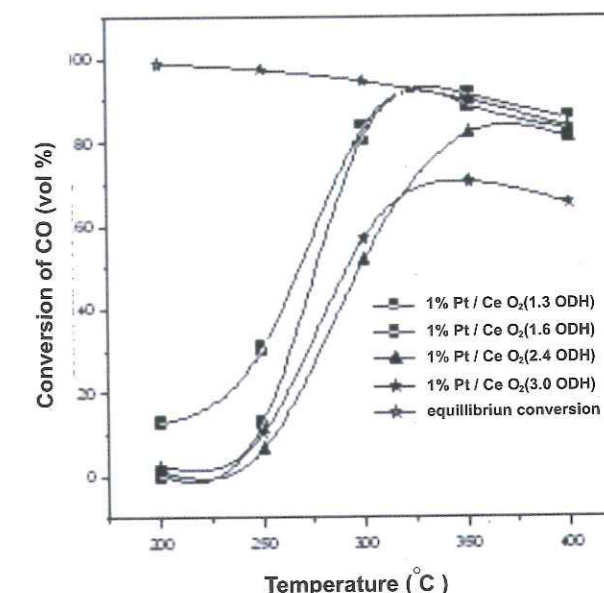
### High performance for water gas shift reaction catalysts

Followed by ATR, the CO in the reformat is converted to H<sub>2</sub> and CO<sub>2</sub> by reacting it with water either in single stage, using a mid temperature shift (MTS) catalyst or in two stages, using high temperature shift (HTS) followed by low temperature shift (LTS). Commercially available catalysts are not suitable at high space velocities (>3000 h<sup>-1</sup>) and are not suitable for on-off cycles. On top of it, the LTS catalysts are also pyrophoric. Hence, NCL has embarked on the development of precious metal based catalysts, which are non-pyrophoric and handle high space velocities. On successful completion of their screening as particulates, the formulations that are found to be good will be transferred on to honeycomb monoliths as wash coats. These honeycomb based catalysts will be tested using realistic reformates of an autothermal reformer. A reactor suitable for this purpose was designed and assembled.



Reactor for testing of WGS monolith catalysts

Pt-based catalysts were prepared by supporting them on various CeO<sub>2</sub> based mixed oxides and evaluated them for water gas shift activity using simulated gas mixtures that contain H<sub>2</sub>, N<sub>2</sub>, CO, CO<sub>2</sub> and water. These catalysts were prepared by various routes to obtain high surface area supports as well as very good Pt metal dispersion. These are highly active at around 300°C and at high space velocities.

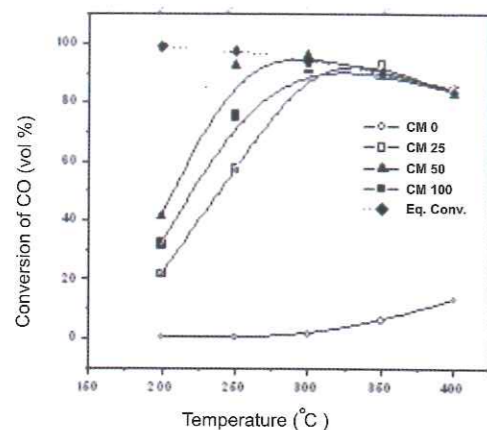


WGS results on various combustion synthesized Pt-CeO<sub>2</sub> catalysts

In addition, two sets of copper (non-precious metal) based-spinels, i.e., Cu-Zn-Mn-O and Cu-Mn-O catalysts containing various atomic ratios of metals were prepared and tested for low to medium temperature shift applications. Out of the catalysts in this series, one particular composition gave excellent results. Its long term stability and on stream durability is being tested. The WGS results of these catalysts at various temperatures and space velocities are shown in figure. Unlike the copper based commercial catalysts (LTS and MTS), the Cu-Mn-O spinels were found to be highly active even at high space velocities.

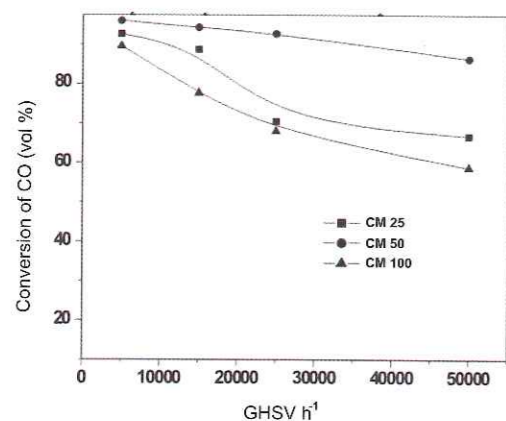


Feed : 39.3%H<sub>2</sub>, 34.9%N<sub>2</sub>, 10.4% CO, 15.4% CO<sub>2</sub>, GHSV 5000 h<sup>-1</sup>



WGS activity of Cu-Mn-O catalysts at different temperatures.

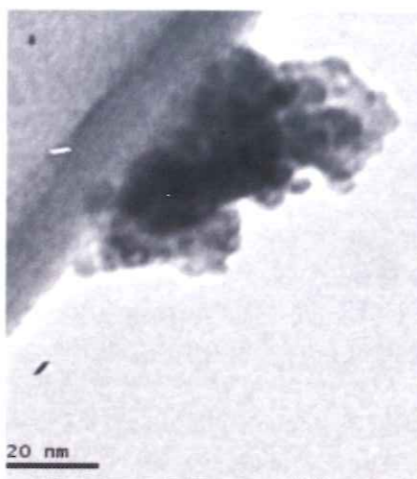
Feed : H<sub>2</sub> 39.3%, N<sub>2</sub> 34.9%, CO 10.4%, CO<sub>2</sub> 15.4%; temp 300°C



WGS activity of Cu-Mn-O catalysts at various space velocities.

### 2.3 HYDROGEN GENERATION VIA VISIBLE LIGHT INDUCED SPLITTING OF WATER

The work is aimed at development of efficient photocatalytic systems for production of hydrogen via dissociation of water using visible light. A well-dispersed cadmium sulfide (CdS) catalyst on a hydrophobic polymer support exhibited high activity for visible light-driven hydrogen production by photocatalytic splitting of water. It maintained a significantly long active life because of its hydrophobic nature. The catalyst comprises uniform CdS crystallites of 2-5 nm size, coated at loadings of 5-17 wt% over a polymeric support (polystyrene) having a rough and porous texture.



TEM of supported CdS nanoparticles on PET

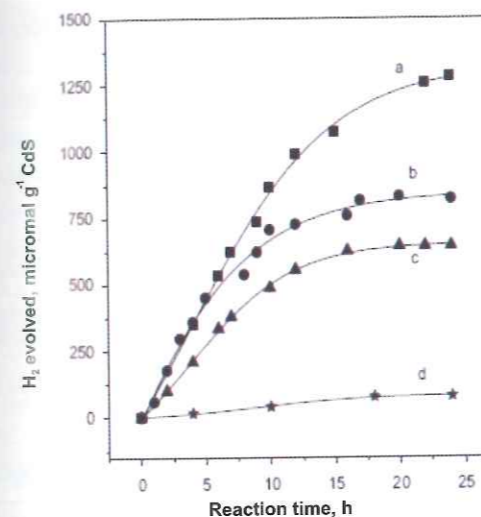


(higher magnification)

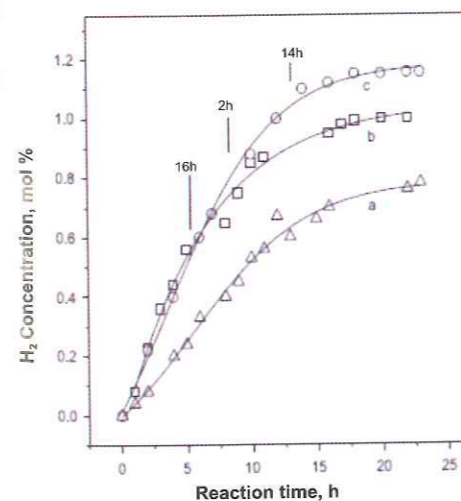
The photocatalytic activity of this supported CdS catalyst, as well as that of an aqueous suspension of CdS powder, was monitored for the visible light-induced evolution of H<sub>2</sub> from water in the presence of hole scavengers S<sup>2-</sup> and SO<sub>2</sub><sup>3-</sup>. While the rate of hydrogen evolution was found to increase with loading, a reverse trend was observed for the amount of H<sub>2</sub> produced per unit mass of CdS. Furthermore, much smaller quantities of hydrogen were evolved under the identical test conditions when an equivalent amount of bulk CdS powder was directly suspended in water. These results clearly demonstrated the vital role played by the particle size and dispersion in the photocatalytic splitting of water for hydrogen generation. In the experiments conducted over the period of several days, with random breaks in



photo-irradiation but no in-between catalyst activation, the evolution of hydrogen was found to stop at the stage when sacrificial agents S<sup>2-</sup>/SO<sub>2</sub><sup>3-</sup> were completely oxidized. The reaction was revived again when the aqueous solution was replaced by a fresh lot. It can therefore be concluded that the slow activity loss of CdS/polyester is related to the formation of S<sub>2</sub>O<sub>2</sub><sup>6-</sup> and/or SO<sub>2</sub><sup>4-</sup> species produced on photo-oxidation of the sacrificial agents, rather than to the degradation of the photocatalyst.



Amount of hydrogen evolved per g of CdS during photocatalytic splitting of water using PET supported samples with different CdS loadings. Curve (a) 5 wt%, (b) 10 wt% and (c) 15 wt%. Curve (d) shows the comparative activity of a bulk CdS sample.



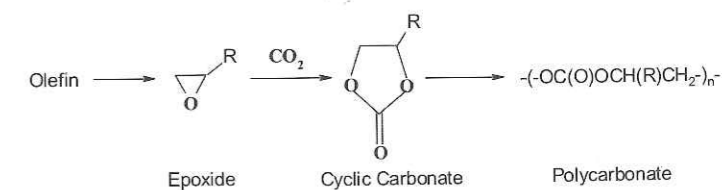
Hydrogen yield during photocatalytic splitting of water over CdS(x)/P catalysts with different loadings of CdS. Curve (a) 5 wt%, (b) 10 wt% and (c) 15 wt%.

### 2.4 UTILIZATION OF RENEWABLE AND SUSTAINABLE FEED STOCKS

Utilization of renewable feed-stocks such as CO<sub>2</sub> and biomass has been gaining considerably importance in recent years due to depletion of petroleum-based reserves and more awareness about the environment. NCL has taken up initiatives in this direction under the sponsorship of CSIR. The highlights of the works undertaken and achievements are given below:

#### 2.4.1 CO<sub>2</sub> as renewable feedstock for the synthesis of polycarbonate precursors

Cyclic and dialkyl carbonate precursors of polycarbonates are conventionally manufactured using toxic chemicals like phosgene. Their synthesis utilizing carbon dioxide, a greenhouse gas and renewable feedstock, (instead of phosgene) is eco-friendly. Carbon dioxide is inexpensive, non-flammable, ubiquitous and highly abundant. This environmentally benign process is already in commercial practice. In most of the commercial processes homogeneous catalysts are used. Replacement of a homogeneous catalyst by more efficient, reusable, heterogeneous catalysts makes the manufacturing process more attractive and economical. A CSIR-Network project was undertaken to develop a more efficient solid catalyst for producing cyclic carbonates.

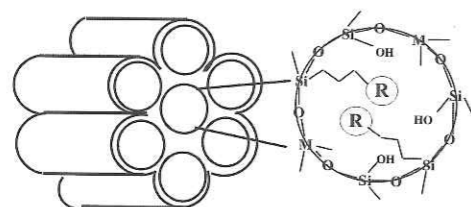


Amine modified silica based mesoporous solid catalysts like Ti-SBA-15-pr-Ade were found to be highly active and selective. These solid catalysts are more advantageous and do not require use of additional co-catalyst/promoter. They are reusable and reaction occurs even at mild conditions. A range of cyclic carbonates was synthesized by insertion of CO<sub>2</sub> into the oxirane ring of different epoxides. Even bulky cyclic carbonates like styrene carbonate could be synthesized in high yields over Ti-SBA-15-pr-Ade catalysts.





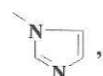
To understand the causes for the enhanced catalytic activity of Ti-SBA-15-pr-Ade catalysts, acid-base properties and adsorption characteristics were determined and found that epoxide adsorbs on acidic Ti functionalities while CO<sub>2</sub> is activated at basic adenine groups. The simultaneous activation of both epoxide and CO<sub>2</sub> on the catalyst surface is the reason for the enhanced catalytic activity of these organic-inorganic, hybrid, solid catalysts.



Lewis acid functionality (M): Ti<sup>4+</sup>, Al<sup>3+</sup>

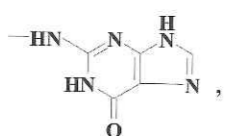
Lewis base functionality (R):

-NH<sub>2</sub>,

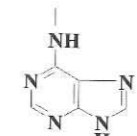


Amine

Imidazole (Im)



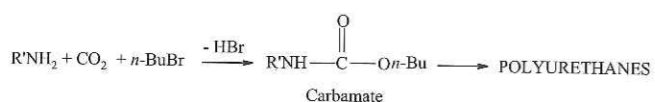
Guanine (Gua)



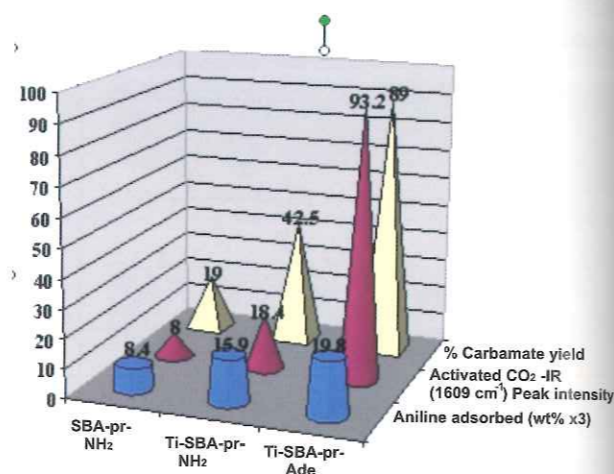
Adenine (Ade)

#### 2.4.2 Synthesis of polyurethane precursors utilizing CO<sub>2</sub>

Alkyl and aryl carbamate precursors of polyurethanes were commercially synthesized by using either phosgene or CO. Both these feedstocks are toxic/hazardous. Utilization of CO<sub>2</sub> instead of phosgene/CO in the synthesis of carbamates, as depicted below, over solid catalysts was undertaken.

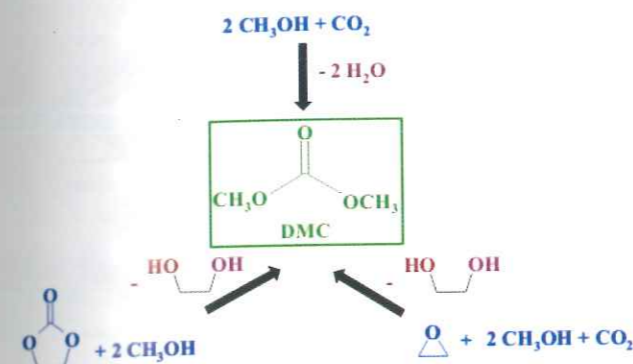


Mesoporous, bifunctional catalyst, Ti-SBA-15-pr-Ade was also found highly active and selective to form a range of alkyl and aryl carbamates by the reaction of amines, CO<sub>2</sub> and alkyl halide at mild temperatures and pressures. Comparative studies on different solid catalysts indicated that higher the amount of amine as well as CO<sub>2</sub> adsorption higher was the yield of carbamate.



#### 2.4.3 Efficient, eco-friendly catalytic route for producing dialkyl carbonates

Dialkyl carbonates, especially dimethyl carbonate (DMC), find important applications in "green" chemical synthesis as raw material and reagent for carbonylation and methylation reactions, replacing toxic-phosgene and dimethyl sulfate, respectively. DMC is the precursor for manufacture of engineering polymers such as bis-phenol-A polycarbonates. It finds application also as an octane booster, solvent, electrolyte in lithium ion batteries, lubricant fluid etc. The conventional manufacturing processes of DMC via oxidative carbonylation and phosgenation of methanol are hazardous. Some possible eco-friendly routes for the synthesis of DMC include a) direct carboxylation methanol with CO<sub>2</sub>, b) reaction of epoxides, CO<sub>2</sub> and methanol, and c) transesterification of cyclic carbonates with methanol.



The yield of DMC is higher in the third option. This route catalyzed by homogeneous catalyst has been adopted recently in the manufacture of bis-phenol-A polycarbonate. A solid catalyst-based process has advantages over a homogeneous catalyst-based process. However, the yield and selectivity of DMC over the known solid catalysts are considerably low (below 60%).

Some highly efficient solid HPA as well as solid Fe-Zn double metal based materials were discovered as transesterification catalysts for the efficient synthesis of DMC from cyclic carbonates and methanol. A range of dialkyl carbonates were synthesized in high yields by transesterification of cyclic carbonates with alcohols. DMC, for example, was produced with 100% selectivity and isolated yield of more than 86% over these solid catalysts. Unsymmetrical carbonates could also be synthesized by using different alcohol mixtures. Structural and spectroscopic studies revealed that Lewis acidic sites are the possible active sites in the transesterification reaction.

### 2.5 ENVIRONMENTAL CATALYSIS

#### 2.5.1 Sulphur resistant DeNOx for diesel automobile exhaust

As our continued efforts for developing sulphur tolerant deNOx catalyst for lean burn engine exhaust using selective catalytic reduction (HC-SCR) technology using hydrocarbon as reductant, Ag/Al<sub>2</sub>O<sub>3</sub> catalyst, having Ag nanoparticles in the range of 25-30 nm, was found to be quite active (>92 % NO conversion at 330 °C with 77 % hydrocarbon conversion and 100 selectivity for nitrogen). The sulphur tolerance studies showed decrease in NO conversion to 60% and hydrocarbon conversion to 34 % in presence of 80 ppm SO<sub>2</sub>. When this catalyst was

modified with addition of SiO<sub>2</sub> (1 and 2.5 %) the sulphur tolerance increased compared to Ag/Al<sub>2</sub>O<sub>3</sub> however at slightly higher temperature (370 °C). Further modification in the catalyst composition for getting low temperature deNOx activity showed promising results for Ag/Al<sub>2</sub>O<sub>3</sub> modified with CeO<sub>2</sub>, which showed 70% NO conversion at 300 °C in absence of hydrogen and 85% NO conversion at 200 °C in presence of hydrogen. Au/Al<sub>2</sub>O<sub>3</sub> catalyst is also showing promising results at low temperature (at 300 °C 70% NO conversion). Detailed catalyst characterization and optimization of the catalyst composition is in progress.

#### 2.5.2 Photocatalytic activity of mesoporous titania and corresponding goldmodified nanocomposites

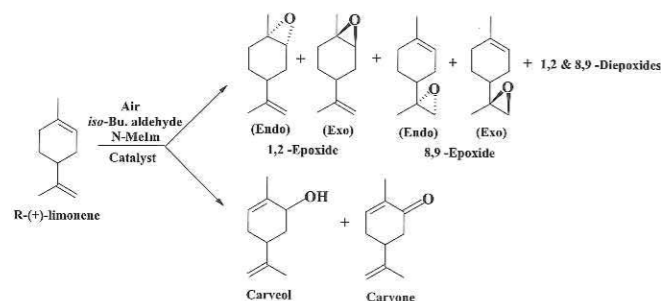
Nano-structured titanium dioxide with a mesoporous texture was synthesized by following a simple hydrothermal procedure, using tartaric acid as a templating agent. 1- to 2 wt% of gold was incorporated into this titania, either during the hydrothermal process or by post-synthesis wet-impregnation. Samples were characterized for their physicochemical properties and also for their photocatalytic activity towards mineralization of volatile organic compounds. The inclusion of small quantity (~1 wt%) of gold during the hydrothermal step followed by calcination at an optimized temperature in range 575-625 K gave rise to quite efficient catalyst, which contained part of the gold in titania network and the rest in form of ~1nm size gold clusters dispersed in the pores of the host matrix. In the case of samples prepared by impregnation and also those containing larger loadings of gold, the surface area was found to be lower and at the same time the gold crystallites of larger size were located prominently at the external surface. *In situ* Fourier-transform infrared spectroscopy studies were conducted to monitor the molecular species over catalyst surface that serve as transient species in this photocatalytic process. The mechanistic routes of photocatalytic oxidation of organic compounds and the important role of the nano-structured gold crystallites in the catalytic activity were proposed based on these experiments.



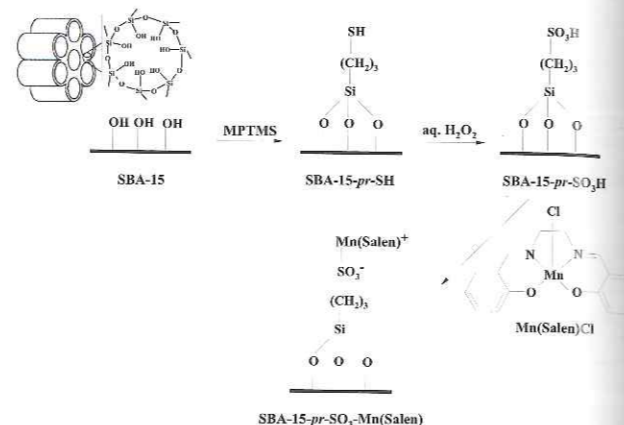
## 2.6. SPECIALTY CHEMICALS

### 2.6.1 Chemo, regio and stereoselective oxidation of terpenes

Limonene epoxide is a key raw material in the synthesis of pharmaceuticals, fragrances, perfumes and food additives. Conventionally, it is manufactured by oxidation of limonene with stoichiometric amounts of peracids. As this process is not ecofriendly, attempts are in progress to develop more suitable solid catalysts for this reaction. Oxidation of limonene, in general, yields a variety of products. Epoxides will be the selective products if oxidation occurs at olefinic positions. If the oxidation takes place at allylic positions, the products will be carveol and carvone. In addition, limonene has two olefinic bonds (1,2 and 8,9) and the oxidation can take place at either or both of these sites.

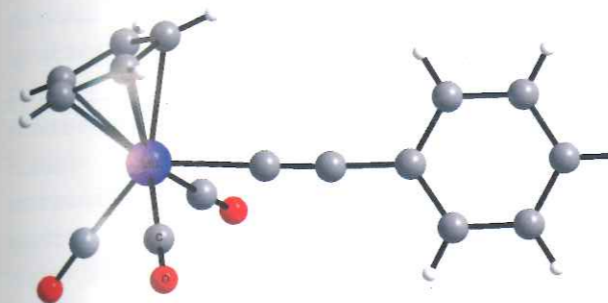


Further, two types of diastereomers (*endo* and *exo*) are expected for each of the epoxide products. Most of the known solid catalysts show significantly low limonene conversions and epoxide selectivities (20-30%); carveol, carvone and polymeric products are formed in large quantities. They require expensive oxidants such as alkyl hydroperoxides and  $H_2O_2$ . It is found that aerial oxidation of R-(+)-limonene over Mn(Salen) complexes immobilized on sulfonic acid-functionalized, mesoporous SBA-15 molecular sieves yields selectively the *endo*-1,2-epoxide of limone. The *endo*-diastereomer is formed with a diastereomeric excess of 39.8%. A change in the oxidation state of Mn from +3 in the "neat" complex to +2 when immobilized on the sulfonated surface is a probable cause for the observed enhancement of catalytic activity.



### 2.6.2 Highly reactive molybdenum acetylide catalyst for oxidation

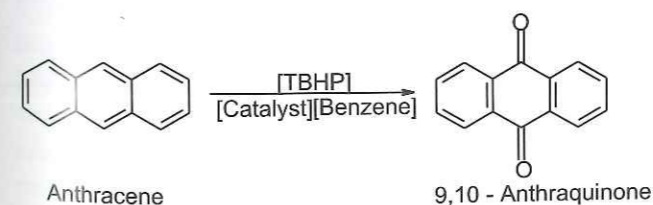
Dihydroxylation of olefins in a single-step is to selectively produce cis-diols is of significant interest. In this regard, a molybdenum acetylide complex, as homogeneous oxidation catalyst, was developed as an efficient catalyst for cis-dihydroxylation of various olefins. This catalyst has definite advantages over conventionally used dihydroxylation catalyst,  $OsO_4$ , such as non toxic, needs no co-oxidants hence no byproduct formation. Hydrogen peroxide acts as efficient and environmentally benign oxidant. Interestingly though this is homogeneous catalyst, it can be recycled very efficiently without loss in conversion or selectivity. This catalyst is also efficient for selective oxidation of sulphides to sulphoxides or sulphones depending on the reaction parameters. Oxidation of alcohols to aldehydes can also be carried out using this Mo-acetylide complex. This catalyst has potential to be used for chiral oxidation reactions by replacing nonchiral Cp ligand by chiral Cp ligands. Structure of the acetylide complex has been determined using single crystal X-ray diffraction analysis. Detailed characterization of catalyst, catalytically active species and reaction intermediate has been carried out and based on the characterization, mechanism for cis-dihydroxylation of olefins using Mo-acetylide complex has been proposed.



Structure of  $(C_5H_5)Mo(CO)_3(-CCPh)$

### 2.6.3 Selective oxidation of anthracene using efficient inorganic-organic hybrid materials

Inorganic-organic hybrid materials were synthesized by immobilization of molybdo vanadophosphoric acids onto mesoporous silica such as MCM-41, MCM-48 and SBA-15 through an organic linker. The 12-molybdo-vanadophosphoric acids of the general formula  $H_{3+x}P_{12}Mo_{12-x}V_xO_{40}(x=0-3).nH_2O$  such as  $H_4[PMo_{11}VO_{40}]32.5H_2O$ ,  $H_5[PMo_{10}V_2O_{40}]32.5H_2O$ , and  $H_6[PMo_9V_3O_{40}]34H_2O$  (represented as V1PA, V2PA and V3PA, respectively) were prepared and immobilized onto mesoporous silica. It was found that the structure of the polyoxometalate was retained upon immobilization over mesoporous materials. These inorganic-organic hybrid materials were tested for their catalytic activities in the liquid-phase oxidation of anthracene with 70% aqueous *tert*-butylhydroperoxide (TBHP) oxidant in benzene. Among the catalysts, V2PA immobilized onto amine-functionalized SBA-15 was highly active in the oxidation of anthracene (turn over frequency, TOF = 21 mole anthracene converted per mole catalyst per hour) with TBHP oxidant in benzene at 80°C and gave 100% selectivity to 9,10-anthraquinone. Catalyst leaching studies indicated the absence of leaching into reaction medium and the catalyst truly functioned as heterogeneous catalyst in the oxidation reaction.

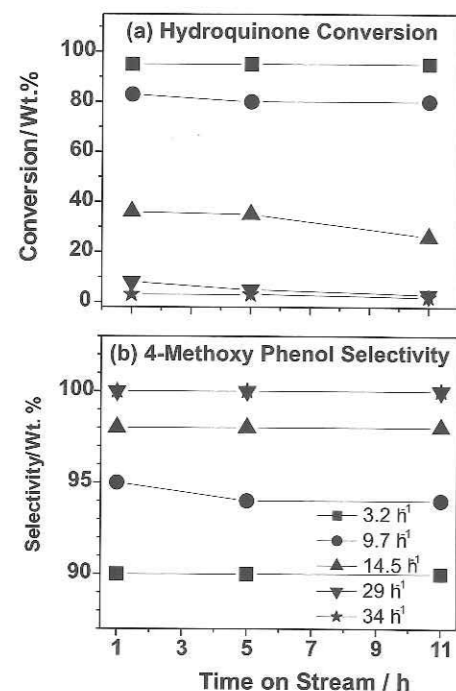


### 2.6.4 Mesoporous silica supported molybdenum oxide nano particles

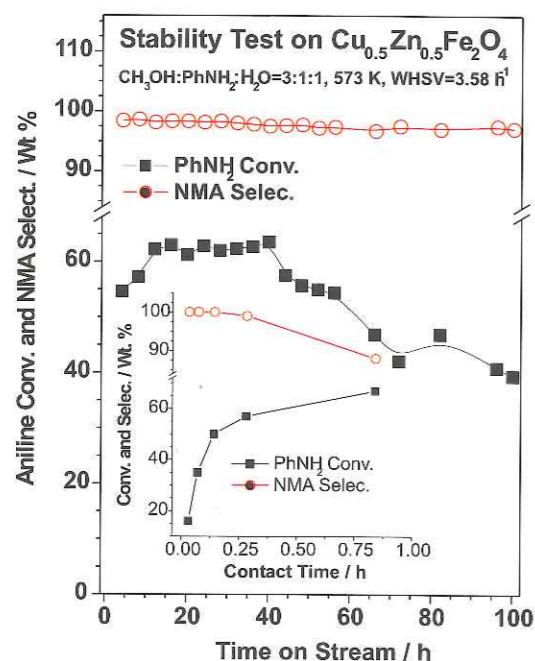
A series of solid acid catalysts,  $MoO_3/SiO_2$  with different Mo loadings using sol-gel technique was developed. These catalysts have very high surface area (720  $m^2/g$ ) and the support is mesoporous in nature (pore size 40-80 Å) without using any template for synthesis. The  $MoO_3$  particles are in the range of 0.6 to 1.5 nm along with some  $MoO_3$  clusters on the surface. The acidity was found to increase with increase in the Mo loading from 1 to 20 mol %. 20 %  $MoO_3/SiO_2$  was found to be highly acidic with 0.94 mmol/g ammonia desorbed with presence of Lewis as well as Brønsted acidic sites. Nitration of aromatics have been carried out using 20%  $MoO_3/SiO_2$  with 99.9 % selectivity for mononitrobenzene. The catalyst life has been tested for more than 1000 h without appreciable loss in conversion in case of benzene nitration. Pharmaceutical drug tinidazole has been synthesized using 20 %  $MoO_3/SiO_2$  as bifunctional catalyst which involves condensation step as well as oxidation step. Use of acetic acid in condensation step as well as tungstic acid or ammonium molybdate in oxidation step in conventional process could be eliminated totally when  $MoO_3/SiO_2$  was used.

### 2.6.5 Selective production of methoxyphenols from dihydroxybenzenes

The O-methylated dihydroxybenzenes (DHB - catechol, resorcinol and hydroquinone) and phenols are widely used in the production of variety of fine chemicals and valuable synthetic intermediates. Selective catalytic production of methoxyphenols from DHBs is an interesting and challenging problem from the process as well as kinetic control point of view. Selective O-methylation of DHBs to methoxyphenols was carried out with dimethylcarbonate on MgO and alkali metal (Li, K and Cs) ions loaded MgO between 523 and 603 K. Catalytic activity and product selectivity varies with respect to DHB substrates. Selectivity for O-methylated products increases with increasing basicity of alkali ions; however, K-MgO shows a high and stable activity towards methoxyphenols suggesting an optimum basicity requirement. Selectivity for methoxyphenols obtained from three substrates increases in the following order: catechol < resorcinol < hydroquinone. Very high selectivity (>90%) observed even at high space velocity.



Space velocity dependence of (a) hydroquinone conversion and (b) 4-methoxy phenol selectivity at 583 K on K(5)-MgO with DMC:hydroquinone = 2:1 feed mixture.



Time on stream and weht hour space velocity (inset) dependence of aniline conversion and NMA electivity on  $\text{Cu}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$  at 573 K

The mode of interaction of substrates on the catalysts surface influences the reactivity and product selectivity. High selectivity of 4-methoxy phenol suggests a perpendicular orientation of the hydroquinone aromatic ring to the catalyst surface. It is likely that the low reaction temperatures employed (< 603 K) controls the reaction kinetically and favors high methoxyphenols selectivity from DHBs.

### 2.6.6. Methylation of aniline over $\text{Cu}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$

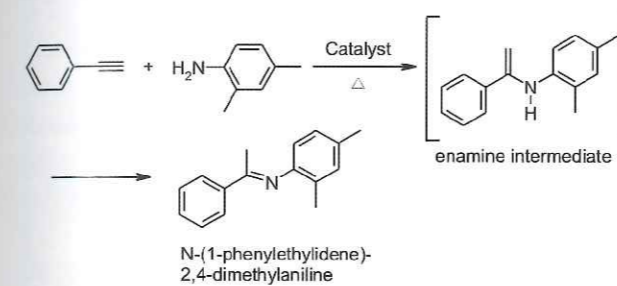
Normally the mono methylation of amino group in aniline(s) is industrially achieved by kinetic control. However, our recent systematic studies on catalytic methylation of aniline and aniline substrates on  $\text{Cu}_{1-x}\text{Zn}_x\text{Fe}_2\text{O}_4$  materials demonstrate the selective production of N-methylaniline(s) (NMA). Aniline methylation with a feed composition of  $\text{CH}_3\text{OH}:\text{PhNH}_2:\text{H}_2\text{O} = 3:1:1$  between 513 and 633 K produced NMA selectively on all the Cu-containing catalyst compositions. Particularly  $\text{Cu}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$  composition shows stable activity up to 100 h in addition to high catalytic activity. It is demonstrated that while the  $\text{Cu}^{2+}$  is responsible for methylation activity,  $\text{Zn}^{2+}$  enhances the overall stability of the catalyst system, although ZnO and  $\text{ZnFe}_2\text{O}_4$  shows no significant activity. Photoelectron spectroscopic investigations revealed the degree of  $\text{Cu}^{2+}$  reduction is minimum on the  $\text{Cu}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$  composition. Temperature programmed reduction studies indicated that the reducibility of  $\text{Cu}^{2+}$  to Cu could happen well above 573 K, the reaction temperature. Stable activity observed on  $\text{Cu}_{0.5}\text{Zn}_{0.5}\text{Fe}_2\text{O}_4$  is attributed to the highly heterogeneous distribution of metal-ions and no  $\text{Cu}^{2+}$  sees another  $\text{Cu}^{2+}$  in the immediate neighborhood and hence the Cu-reduction is avoided. Above heterogeneous distribution also indicated an important role of zinc, as an "active spacer cum stabilizer" and hinders the reduction of active  $\text{Cu}^{2+}$  and contributes to prolonged activity.

### 2.6.7 Hydroamination of terminal alkynes with aromatic amines

Hydroamination reaction offers a very attractive route for the synthesis of alkylated amines and their derivatives without any by-product formation. AISBA-15 was synthesized by isomorphous substitution of aluminium into the framework of SBA-15. Hydroamination of



phenylacetylene (PhAc) with 2,4-xylydine has been used as a test reaction which gave N-(1-phenylethylidene)-2,4-dimethylaniline without any by-product formation.  $\text{CuAISBA-15}$  and  $\text{CuAIMCM-41}$  showed around three times higher activity in hydroamination of PhAc compared to Cu-clay and Cu-beta, which is because of moderate Lewis acidity of  $\text{Cu}^{2+}$  present in mesoporous supports. The performance of the  $\text{CuAISBA-15}$  was also determined with different alkynes and amines to know the general applicability of the catalyst in hydroamination

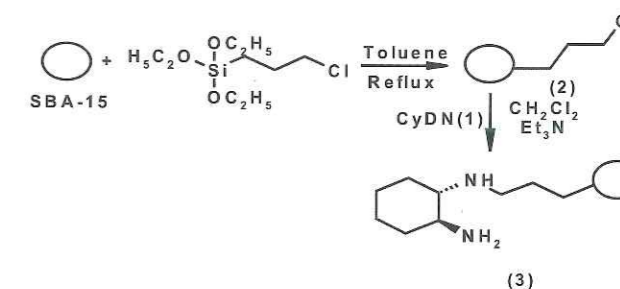


Hydroamination of phenylacetylene with 2,4-xylydine

### 2.6.8. Asymmetric catalysis

#### Immobilized chiral diamino ru complex as catalyst for chemo- and enantio-selective hydrogenation

Chiral cyclohexyldiamine based Ru triphenylphosphine complex has been immobilized over mesoporous silica SBA-15 and used in the chemo- and enantioselective hydrogenation of prochiral and  $\alpha, \beta$ -unsaturated ketones and imines to corresponding products. <sup>31</sup>P NMR, SEM, TEM, XRD, N<sub>2</sub> sorption measurements and FTIR analysis supported the retention of the complex over mesoporous silica. This catalyst was found to catalyze preferentially the hydrogenation of C=O over coexisting conjugated C=C linkages in the hydrogenation of  $\alpha, \beta$ -unsaturated ketones with high turnover frequencies and gave excellent enantioselectivities in the hydrogenation of prochiral ketones compared to its homogeneous analogue. It also showed good activity in the hydrogenation of less reactive imines to secondary amines.



#### Asymmetric transfer hydrogenation of ketones

Asymmetric transfer hydrogenation of acetophenone was carried out using  $\text{Ru}(\text{benzene})\text{Cl}_2/\text{L-ephedrine}$  as a catalyst system and KOH as a base under sonochemical activation and without sonochemical activation (silent conditions). The reaction proceeded smoothly with significant rate enhancement (5-10 times) by ultrasound promotion without significantly affecting the enantioselectivity. Transfer hydrogenation of various ketones such as 4-isobutyl acetophenone, 6-methoxy-2-acetyl naphthalene, and substituted acetophenone derivatives was carried out with good conversion (46-98%) and ee in a range of 40 to 69%.

Screening of various ketones for transfer hydrogenation at room temperature and under sonochemical activation

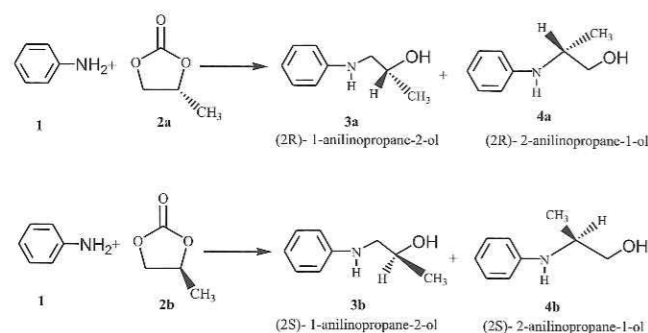
Sr no	Ketone	Sonication		Without sonication	
		Conv. (%)	ee (%)	Conv. (%)	ee (%)
1	Acetophenone	91	69	92	69
2	4-Bromoacetophenone	98	48	98	51
3	4-Methylacetophenone	72	61	79	64
4	4-Chloroacetophenone	98	51	97	51
5	4-Nitroacetophenone	60	39	47	41
6	4-Methoxyacetophenone	46	60	51	62
7	2 Acetyl 6-methoxy naphthalene	60	56	63	55
8	4-Isobutylacetophenone	80	62	83	63

Reaction conditions:-ketone,  $2.5 \times 10^{-3}$  mol; catalyst-Ru-p-cymene,  $1.26 \times 10^{-5}$  mol; IPA 25 cm<sup>3</sup>; KOH,  $1.2 \times 10^{-4}$  mol; Ligand(ephedrine)- $5.1 \times 10^{-5}$  mol, 25°C  
 Reaction time: sonochemical reaction: 12 minutes; without sonication: 2 hr



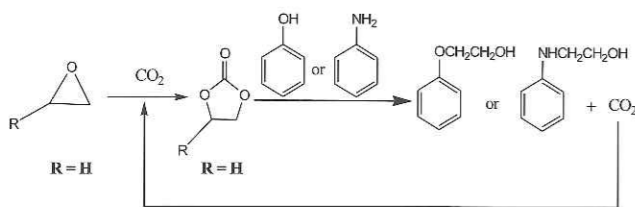
### Chiral amino alcohols

Chiral  $\beta$ -amino alcohols were synthesized from chiral R or S 1,2-propylene carbonate and aniline with ee of 98%. Excellent yields of chiral  $\beta$ -amino alcohols were obtained using zeolite catalyst, in a typical case ~ 91% isolated yield of 3a + 4a or 3b + 4b were realized.

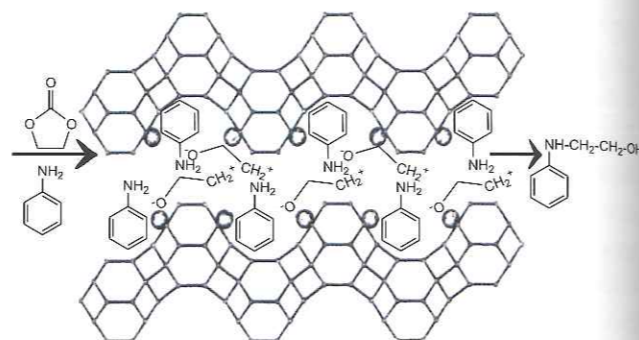


### 2.7 BENIGN SYNTHESIS OF ETHYLENE CARBONATE, PHENYL ETHERS AND AMINO ALCOHOLS

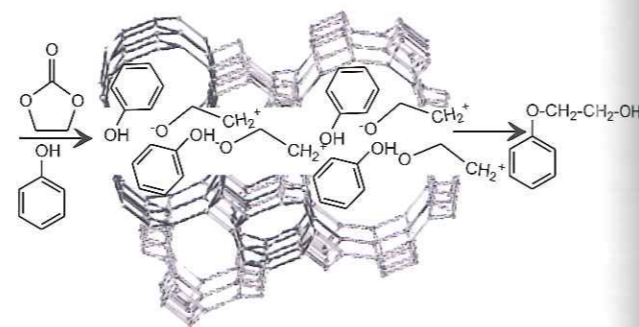
An integrated two-step approach to synthesize mono phenyl ethers and beta-amino alcohols from cyclic carbonate via carbon dioxide addition to epoxide using solid base catalyst was developed. Carbon dioxide in principle can be recycled back to generate cyclic carbonate.



The reaction of beta amino alcohol formation from cyclic carbonate and aniline was studied using in-situ DRIFT technique. The DRIFT spectra showed that aniline is adsorbed in the pores of NaY zeolite and ethylene carbonate reacted with activated aniline to form beta-amino alcohol. A similar mechanism is postulated for mono ethylene glycol phenyl ether formation from phenol and ethylene carbonate catalyzed by KL zeolite.



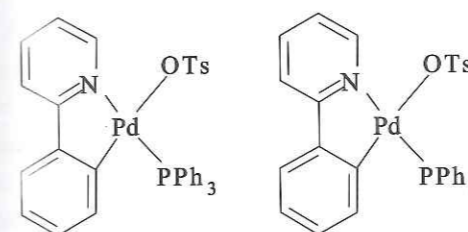
Cross-section through the interconnecting cavities of the Y zeolite, showing the Si/Al framework, sodium ions (Shaded circles, ionic radii) and aniline molecule (van der waals radii)  $\text{NH}_2$  group tilted in super-cage and mechanism of alkylation in super cage of Na-Y



Cross-section through the interconnecting cavities KL zeolites, showing Si/Al framework, sodium cations and phenol molecules adsorb in cage and mechanism of hydroxylation

### 2.8 BROMINATION-HECK-CARBOXYLATION PROCESS FOR IBUPROFEN SYNTHESIS

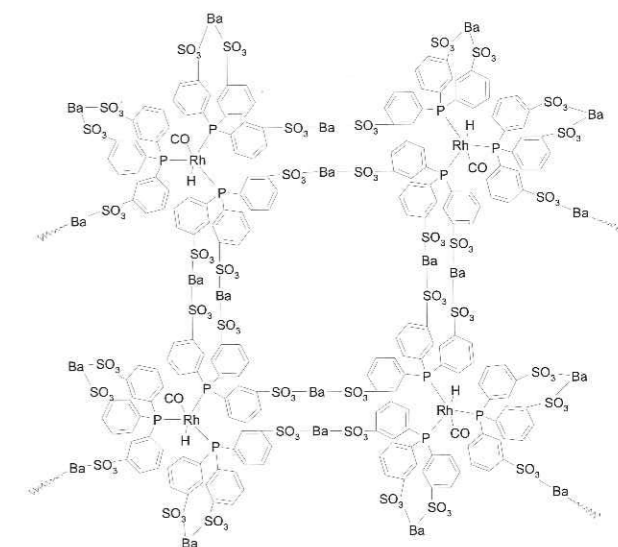
Various novel NC palladacycles have been prepared and structures of the Pd complexes prepared are presented below. Comparison of the activity of palladacycles with literature reports clearly showed that the catalysts prepared are highly active and selective for the vinylation reaction with high turn over numbers in a range of 2500-3000. Vinylation of 2-bromo-6-methoxy naphthalene and 4-isobutylbenzene has been carried out using palladacycle catalysts and high (98%) conversion and high selectivity to the desired product was obtained. Palladium supported on cellulose catalyst prepared by IICT also showed good activity and ~90% conversion of 2-bromo-6-methoxy naphthalene with 95% selectivity to VMN was obtained in 5 h reaction time, indicating good activity of the catalyst.



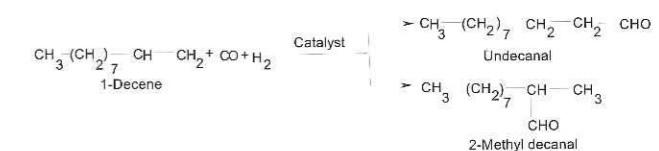
Carbonylation of 4-isobutylstyrene was investigated in detail using homogeneous  $[\text{Pd}(\text{pyca})(\text{PPh}_3)(\text{OTs})]$  complex as catalyst. Catalyst concentration was very crucial in catalyst activity as well as selectivity. At lower catalyst concentration, polymerization of IBS was a competing reaction leading to lower selectivity of Ibuprofen (40%). With increase in catalyst concentration, polymerization reaction was suppressed and 98% selectivity to Ibuprofen was obtained. Polymerization of IBS can be catalyzed by TsOH, which is a promoter for the carbonylation reaction and hence, use of higher loading of catalyst (20 mg) is essential for high selectivity to Ibuprofen. As observed in the catalyst concentration effect, higher IBS concentration also leads to polymerization and lower selectivity to Ibuprofen. Hence, optimum concentration of IBS ( $0.63 \text{ kmol.m}^{-3}$ ) is necessary for obtaining high selectivity to Ibuprofen. Best results were obtained in a temperature range of  $105\text{--}115^\circ\text{C}$ . Higher temperatures resulted in polymerization of IBS leading to lower selectivity to Ibuprofen. Effect of promoter:catalyst ratio was investigated in a range of 25-100. In this study ratio of promoters used (LiCl and TsOH) was kept constant at 1:1. It was observed that the yield of Ibuprofen increased with increasing promoter: catalyst ratio and best results were obtained at ratio of 100.

### 2.9 HYDROFORMYLATION

Supported ossified catalysts for the hydroformylation of higher olefins have been developed. Kinetics of hydroformylation of decene using the supported ossified  $\text{HRh}(\text{CO})(\text{TPPTS})_3$  catalysts has been investigated. These catalysts have been found to be more active than all reported heterogenized catalysts for the hydroformylation of higher olefins. The activity observed for decene hydroformylation using this catalyst was only a third that of the homogeneous catalyst.



Hydroformylation of decene in a biphasic medium using Rh-sulfoxanthphos catalysts has been demonstrated. A linear to branched ratio in the range of 32-40 is obtained. The kinetics of this reaction in presence of a co-solvent has been investigated and shows similarities with homogeneously catalyzed hydroformylation.



### 2.10 HYDROGENATION

Catalysts for the selective hydrogenation of aromatic and aliphatic acids to alcohols, and optimization of reaction conditions to achieve highest selectivity has been developed. The kinetics of hydrogenation of benzoic acid to benzyl alcohol and lauric acid to lauryl alcohol have also been investigated. Catalyst has been developed for the selective partial hydrogenation of benzoic acid to benzaldehyde with about 50% selectivity at conversion levels of 60%. At lower conversion a much higher selectivity to benzaldehyde is obtained. The hydrogenation of dicarboxylic acids like terephthalic acid, isophthalic acid and phthalic acid gave numerous products by chemoselective hydrogenation of the carboxylic acid group.



### 2.10.1 Continuous hydrogenation process for butane- and butanediols

Hydrogenation 2-butyne-1,4 diol ( $B_3D$ ) in presence of a catalyst is an industrially important reaction for the manufacture of 2-butene-1,4-diol ( $B_2D$ ) and butane-1, 4 diol ( $B_1D$ ). The olefinic diol,  $B_2D$  is a starting material for the manufacture of the endosulfan, vitamins A and  $B_6$  while,  $B_1D$  has a wide range of applications in the polymer industry and as a raw material for the manufacture of tetrahydrofuran. Since both  $B_2D$  and  $B_1D$  are large-scale commercial products, it would be most desirable to have a continuous hydrogenation of  $B_3D$  to give either  $B_2D$  or  $B_1D$  selectively or a desired mixture of  $B_2D$  and  $B_1D$ . A catalyst and a bench scale continuous process continuous hydrogenation of ( $B_3D$ ) over supported platinum catalyst to give ( $B_2D$ ) and ( $B_1D$ ) without formation of any other side products was developed. In case of continuous hydrogenation, higher selectivity (66%) to  $B_2D$  could be obtained and the selectivity pattern was completely different from that found in case of batch slurry operation in which  $B_1D$  selectivity was very much higher (83%) than the  $B_2D$  selectivity (17%). Another interesting feature was that by varying the contact time, the selectivity to both  $B_2D$  as well as  $B_1D$  could be varied over a wide range which is an attractive option to obtain the desired products mix of  $B_1D$  and  $B_2D$  depending on the fluctuation in the market demand.

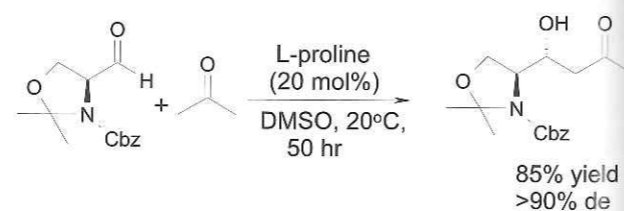
### 2.10.2 Ring hydrogenation of naphthalene compounds in supercritical $CO_2$ medium

Catalytic hydrogenations of solid substrates having high melting points such as aromatic compounds in organic solvents using supported metal catalysts have wide ranging applications in chemical processes; however, the separation of pure products from solvents is critical. Moreover, eliminating the use of organic solvents is highly desirable for environmentally benign processing. Supercritical carbon dioxide ( $T_c = 304.2\text{ }^\circ\text{C}$  and  $P_c = 7.4\text{ MPa}$ ) is a prominent candidate for alternative solvent because of its nontoxic and non-flammable properties. Decahydronaphthalene (decalin) is proposed as a new mobile hydrogen storage medium for proton exchange membrane fuel cells. Effective hydrogenation of naphthalene is important for producing decalin as a hydrogen storage material. Also, the ring hydrogenation

of aromatics is useful for the production of a high performance diesel fuel. Therefore catalytic stereoselective hydrogenation of naphthalene and other aromatics was investigated in supercritical carbon dioxide medium. A very high selectivity to cis-decalin could be obtained in sc  $CO_2$ , due to minimization of flipping of the transition state. This work was carried out in collaboration with Research Center for Compact Chemical Process, National Institute of Advanced Industrial Science and Technology (AIST), Japan.

### 2.11 ORGANO CATALYSIS

Recently, enantioselective organocatalysis has emerged as a powerful synthetic means that can lead to the development of new methods for diverse chiral molecules. In organocatalysis, the main focus is on the use of small organic molecule such as *proline* and its derivatives as an organo-catalyst for different asymmetric reactions. Direct diastereoselective aldol reaction of various amino aldehydes with different ketones and further extension to the synthesis of core "backbone" of sphingolipids and phytosphingosines which are important biologically active molecules, was undertaken. Intermolecular direct aldol reaction in diastereoselective fashion using Garner aldehyde and acetone with  $dr > 90$  in 85% yield was successfully carried out.



Similarly, several other aldol products were also prepared starting from various amino aldehydes using diastereoselective approach. A novel catalytic route involving organocatalyst has been developed for the diastereoselective synthesis of 2-amino-1,3,5-hexane triols with  $de$  (diastereoselective excess)  $> 95\%$  using L-proline catalyzed Aldol reaction. The  $de$  was established by high resolution proton and  $^{13}\text{C}$  NMR.



## 3 CHEMICAL ENGINEERING SCIENCE

### 3.1 Process development and catalysis

Clean synthesis of styrene carbonate by ionic liquid confined in silica spheres of micron/ submicron size range Supported ionic liquid catalysis is a concept which combines the advantages of ionic liquids with those of heterogeneous support material. Majority of supports were silica based, several studies focused on polymeric materials including membranes. Catalyst was synthesized by physical confinement or encapsulation of ionic liquids (with or without metal complex) in a silica gel matrix through sol-gel process. In this method ionic liquids with large molecular size for e.g., C8MIMCl (octyl methyl imidazolium chloride) could be confined into the silica gel nano-pores. TEM and XRD showed silica gel matrix was amorphous with non uniform mesoporous structure. Styrene oxide carboxylation mediated by carbon dioxide using this catalyst, gave 99% yield of styrene carbonate with productivity of 0.0161 g of styrene carbonate/g catalyst/h/atm of  $CO_2$  at  $100\text{ }^\circ\text{C}$  (during reaction IL entrapped in silica matrix was found to coat over silica surface).

### Catalyst development for continuous hydrogenation of butynediol and for diastereoselective Aldol reaction

A catalyst and a bench scale continuous process for the hydrogenation of butynediol was developed, which highlights the results on tuning of selectivity of butene- and butane diols. Both are commercial products and by a proper choice of the feed conditions such as liquid and/or  $H_2$  flow rates,  $H_2$  pressure, the product mix could be obtained in any desired ratio depending on the market demand. No other side products were observed for the catalyst developed in our laboratory. A novel catalytic route involving organic catalyst has been developed for the diastereoselective synthesis of 2-Amino-1, 3, 5-hexane triols with  $de > 95\%$  using L-proline catalyzed Aldol reaction. The  $de$  was established by high resolution proton and  $^{13}\text{C}$  NMR. Catalytic stereoselective hydrogenation of aromatics was investigated in supercritical carbon dioxide medium. A very high selectivity to cis-decalin could be obtained in sc  $CO_2$ , due to minimization of flipping of the transition state. The hydrogenated products of fused aromatic are being

explored as excellent organic hydrides for hydrogen storage useful for fuel cells. This work was carried out jointly with a research group in Japan.

### Studies for the chemical immobilization of penicillin acylase using polymeric membrane

Penicillin acylase (penicillin amidohydrolase, EC3.5.1.11) cleave the acyl chain of penicillin to yield 6-amino penicillanic acid (6-APA) and the corresponding organic acid. Biotechnological applications of penicillin acylase involved mainly in the industrial production of semisynthetic penicillins and cephalosporins, which remain the most widely used group of antibiotics. In addition, penicillin acylase is useful as biocatalysts in many potentially valuable reactions such as protection of amino and hydroxyl groups in peptide synthesis, as well as in the resolution of racemic mixtures of chiral compounds.

Under this project, different studies were carried out to search a novel ligand for the immobilization of penicillin acylase using a novel cellulose based polymeric membrane invented by us. Almost twenty different ligands were studied, except DEAE and polyethylimine all were not studied earlier for the immobilization of penicillin acylase. The relatively higher activity of the immobilized enzyme was obtained on four ligands. These ligands were selected for enzyme stability study. Five cycles of enzyme activity of the immobilized enzyme on the respective ligands was carried out. The ligand was selected for the further study which showed 60% immobilized enzyme activity after the completion of 5 cycles. The effect of different substrate concentration (10 to 200 mM) on the immobilized enzyme activity was studied using 10 ml process volume. The enzyme was immobilized on the selected ligand coupled to the membrane having surface area  $13.4\text{ cm}^2$ . The immobilized enzyme showed  $45.6\text{ mM Km}$  and  $394\text{ U Vmax}$  towards the substrate penicillin G  $K^+$  salt. The scale up studies were carried out using membrane reactor with 250 ml process volume. The enzyme was immobilized on the selected ligand coupled to the membrane having surface area  $72\text{ cm}^2$ . At the higher processing volume the immobilized enzyme showed  $65\text{ mM Km}$  and  $253\text{ U Vmax}$  towards the substrate penicillin G  $K^+$  salt. The average buffer flux of the enzyme immobilized membrane was  $162.85 \pm 5.7\text{ LMH}$  whereas



sample flux was  $104.54 \pm 24$  LMH. The results indicate that the novel ligand used for the immobilization of penicillin acylase on polymeric membrane is suitable for large scale operations:

### Demonstration of catalytic hydrogenation of H-acid intermediate

H-acid is an intermediate for dyes and is manufactured in large quantities for indigenous consumption and export. The manufacturing involves iron-acid reduction of 1 nitro 3,6,8 naphthalene trisulphonic acid and it generates large quantity of iron sludge) 4T/T of H-acid produced as waste which is hazardous and difficult to dispose of. The research aims at the development and demonstration of a catalytic hydrogenation process which will totally eliminate generation of iron sludge.

## 3.2 SEPARATION SCIENCE AND ENVIRONMENTAL ENGINEERING

### 3.2.1 Reaction kinetic and separations

Our research interests encompass adsorption, ion-exchange, hybrid processes, and kinetics of reactions. In adsorptive separation, the adsorption of organic isomers (cresols, cymenes), ground water decontamination (removal of fluorides/ selenium), desulfurization of transportation fuels (diesel, petrol), separation of acids from dilute solutions and mathematical modeling and simulation were studied.

### Adsorption of aromatic isomers

Cresols and cymenes are industrially important intermediates the isomers of which have close boiling points. The adsorption of these compounds on synthetic clays was studied during the year. By suitable chemical modifications it was possible to identify layered double hydroxides (LDH) having high adsorption capacity for these aromatic isomers. The results of experimental studies revealed that the adsorption of these isomers was very sensitive to the chemical composition of the LDH and the solvent used.

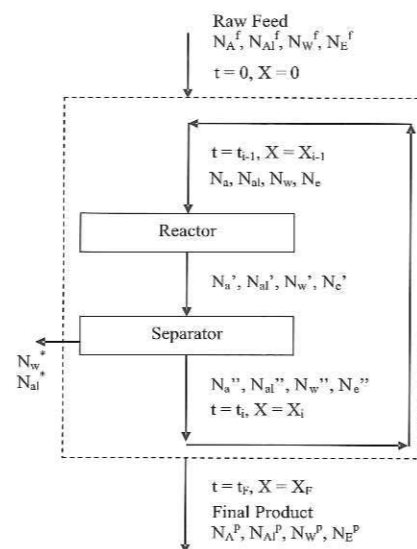
### Fluoride/selenium decontamination from water

Anionic clays with varying amounts of bi-valent and tri-valent metal ion ( $M^{2+}$ ,  $M^{3+}$ ) were synthesized and tested for their fluoride/ selenium adsorption capacity. The influence of type of metal ions, metal ion ratio, pH of

water, presence of other ions and surface charge of the LDH on the adsorption of fluoride and selenium were studied. It was possible to improve the adsorption efficiency of the clay by appropriate surface modification and use of support.

### Hybrid processes

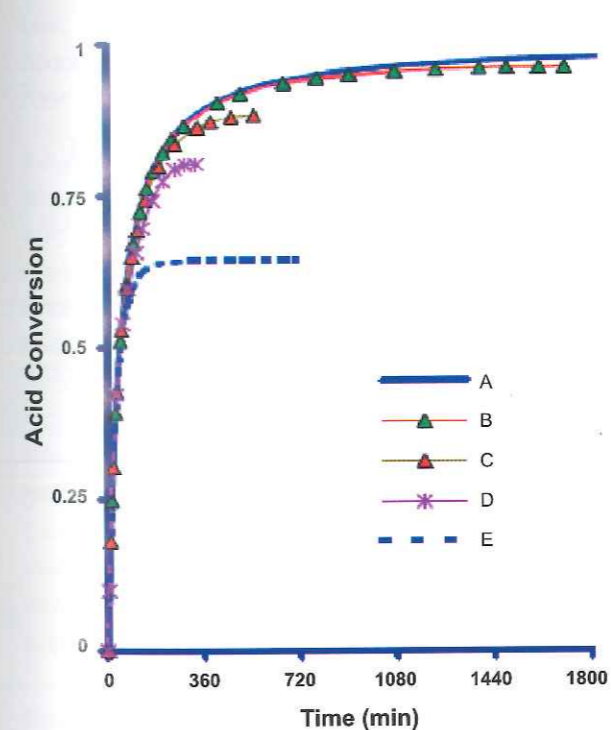
Hybrid processes integrate more than one unit operation / process for operational simplicity and /or enhancement in product yield. During the year we worked on a program on reactions in membrane reactors, which combine reaction and separation into a single unit. As a part of the program we worked on the development of polymer/inorganic membranes that work as the separating medium and catalyst, and the design of membrane reactors. Although the focus is on applications that can use pervaporation membranes for esterification reactions, the membrane reactor facility can be used for any type of liquid-phase reactions. A pervaporation membrane reactor (PVMR) was modeled using a two-step model given below:



Schematic representation of the sequence of steps in two-step model.



The analysis showed that the PVMR performance was similar to that of the batch reactor when both the reactors were in the kinetic phase. However, the performance of the PVMR was superior to that of the batch reactor when both were in the intermediate/ equilibrium phase of the reaction. In these regions, the PVMR performance was influenced/ limited by the membrane flux and selectivity. The analysis showed that the membrane flux affected the PVMR performance in the intermediate region and the membrane selectivity affected the performance in the equilibrium phase. Further, the limitations introduced by



The effect of membrane selectivity on the performance of a membrane reactor (membrane flux:  $2.15 \text{ kg/m}^2\text{h}$ , area:  $3.5 \text{ m}^2$ , alcohol to acid feed ratio (molar): 1, membrane selectivity: A: 10000, B: 1000, C: 100, D: 25, E: conventional batch reactor)

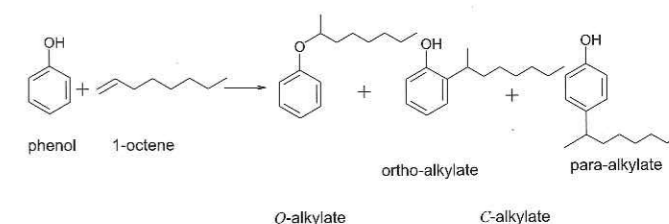
a low-flux membrane could be overcome by appropriate selection of the membrane area and that due to poor selectivity could be compensated to a certain extent by adjusting the feed ratio.

This work was carried out under the project from Department of Science and Technology, New Delhi titled "Membrane reactors for specialty chemicals".

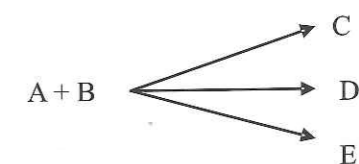
### Kinetics of chemical reactions

In continuation of the previous work of studying the kinetics of organic reactions and using this as a tool for understanding the reaction behavior and its relation to the catalyst characteristics, we studied the alkylation of phenol and Claisen rearrangement over zeolite catalysts, during the year.

A comparative study is presented of the liquid phase alkylation of phenol with 1-octene over different zeolite catalysts: H-beta (BEA(15), Hmordenite (MOR(11) and H-USY (FAU(15)). A wide spectrum of monoalkylated products, identified as isomers of phenyl octyl ether (O-alkylate) and octyl phenol (C-alkylate), was formed in the reaction. The reaction was studied in detail over BEA(15) and included the influence of process variables such as temperature, reactant mole ratio, catalyst amount and alkali metal (K) poisoning on its performance in the alkylation reaction.



(a)

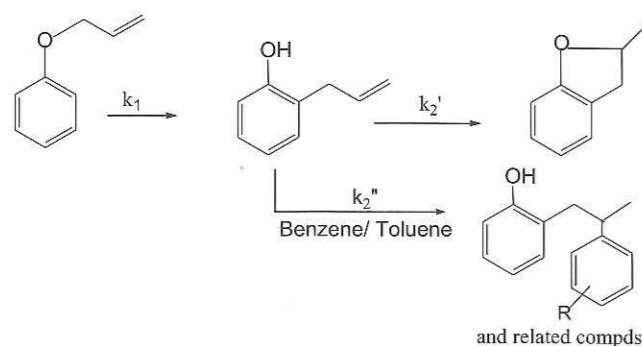


(b)

Major products in the alkylation of phenol with 1-octene, (b) schematic representation of the simplified reaction path



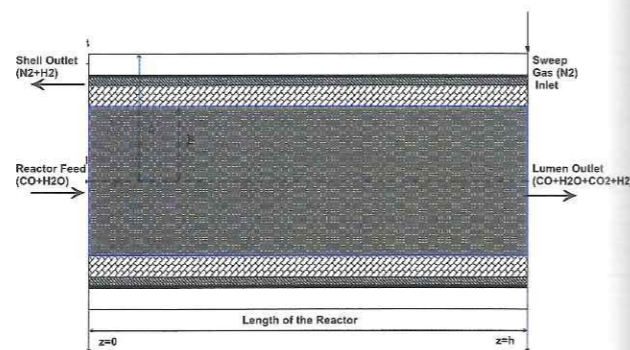
A kinetic analysis of the reaction over BEA(15) was also carried out assuming a second order parallel reaction mechanism. The activity of the different catalysts for the reaction followed the order: BEA(15) > FAU(15) > MOR(11). The poisoning of BEA(15) with potassium resulted in a decrease in the catalyst activity concomitant with a decrease in the number of strong acid centres in the catalyst. The Claisen rearrangement of allyl phenyl ether (APE) to *o*-allylphenol was investigated over zeolites beta (BEA), mordenite (MOR) and Y (FAU) with different Si/Al ratios. Over the zeolite catalysts, the allylphenol cyclized to produce 2,3-dihydro-2-methyl benzofuran. Larger catalyst loading, higher reaction temperatures and longer run duration favored the formation of the ring compound. Conversion was small over MOR and FAU although they possessed higher acidity (as measured by the temperature programmed desorption of ammonia) compared to BEA. Studies using BEA revealed that the nature of the solvent influenced the reaction rate. The order of reactivity in the solvents was, benzene > EDC (1,2-dichloroethane) > toluene > TCE (1,1,2,2-tetrachloroethane) > ACN (acetonitrile). The intermediate allylphenol reacted with the aromatic solvents to produce byproducts when benzene and toluene were used as solvents. A kinetic analysis assuming first order series and parallel reactions was carried out.



Products of Claisen rearrangement of allyl phenyl ether over zeolite beta

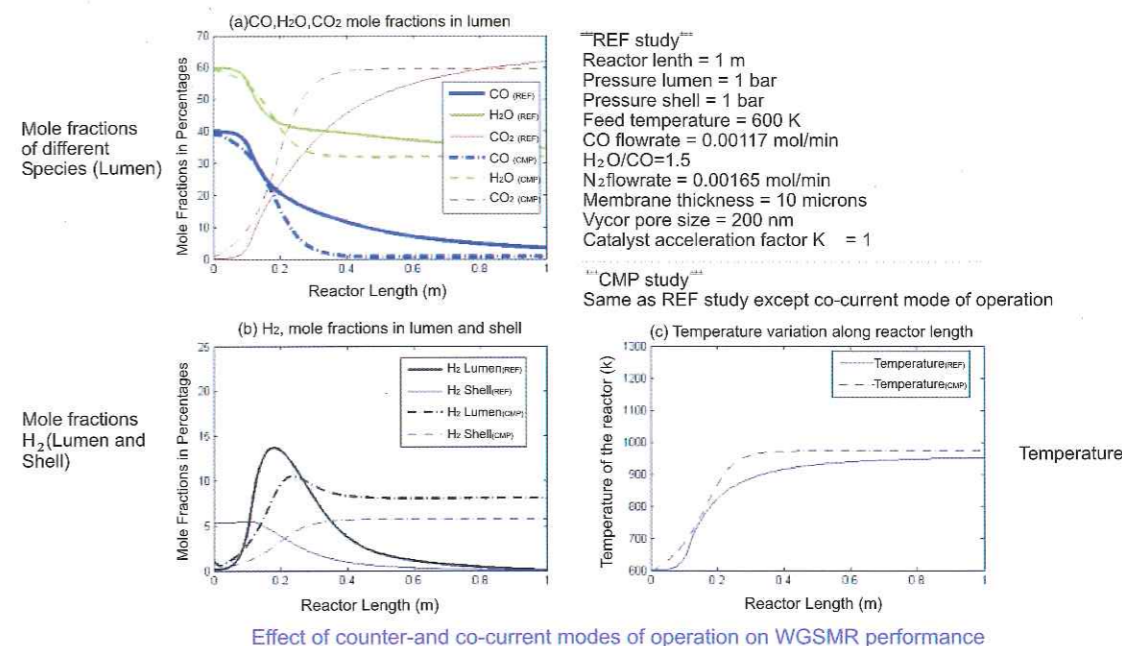
### Modeling the water gas shift membrane reactor

A general mathematical model for the water gas shift membrane reactor (WGSMR) separating  $H_2$  from the other chemical species present, namely,  $CO$ ,  $CO_2$ ,  $H_2O$ , has been developed. Both situations involving counter-current and co-current flow of sweep gas in the shell side of the membrane have been modelled. An algorithm that solves the mass, energy and momentum balance equations has been coded. Simulation studies have been carried out using the code to study the effects of mode of operation (co-current and countercurrent) and various operational parameters (reactor length, feed rates, pressure differential across membrane, feed temperature, catalyst activity, Vycor glass support permeability and membrane thickness) has been studied.



#### Legend

- A - Radius of inner tube (Lumen) ( $19 \times 10^{-3} m$ )
- B - Radius of outer tube (Shell) ( $12.5 \times 10^{-3} m$ )



### 3.2.2 Environmental studies

#### Monitoring of carbon disulphide and hydrogen sulphide from Rayon industry

Rayon industry emits carbon disulphide and hydrogen sulphide in substantial quantity, which poses health hazard. Central Pollution Control Board assigned this project for actual monitoring of carbon disulphide and hydrogen sulphide up to parts per billion level. Three Rayon industries were visited for measurement of these gases and for ascertaining the present level of these gases in industry and surrounding areas. We have identified the pollution abatement methods for bringing down the levels of carbon disulphide and hydrogen sulphide. This will help the industry to control the same.

#### Review of effluent standards and development of emission standards for dyes and dye intermediates industry

The effluent standards for liquid effluent of dyes and dye intermediates industry are due for revision and there are no standards for gaseous emissions for this sector. Central Pollution Control Board (CPCB) has assigned the work of reviewing the present quality of liquid effluent and gaseous emission of dyes and dye intermediates industry vis-à-vis standards in developed countries. Twelve dyes and dye intermediate industries were visited for in-depth study of effluents, emissions and processes. The possibilities of minimizing the waste and achieving better standards are being studied. This will help CPCB in revising the present standards of liquid effluent and develop standards for gaseous emissions.

#### Identification of hazardous waste streams their characterization, waste minimization and recovery/recycling options in pesticides sector

Central Pollution Control Board has assigned for work of identification and characterization of solid hazardous waste of ten pesticides manufacturing units. Ten pesticides manufacturing units were visited for in-depth study of the hazardous waste and the processes. Based on this study, NCL will recommend the measures for waste minimization and identify recovery and recycling options for the pesticides sector.

#### Control of offensive odour substances with specific reference to selected process industries

There is no legislation in India which directly specifies limit for the odour level of emissions. A number of chemical industries emit odorous substances. Odorous sulphur compounds such as hydrogen sulphide, methyl mercaptan, ethyl mercaptan, dimethyl sulphide are obnoxious as they have disagreeable odour which can be sensed by human nose even when they are present in parts per billion (ppb) concentration. The present instruments used in industry are not capable to measure these gases at ppb level. Central Pollution Control Board has assigned this work to develop and standardize analytical method to measure these gases at ppb level in specific industries namely ethion, phorate (pesticides) and ranitidine (pharmaceutical). NCL developed the method, standardized and used it in industries to assess the efficiency of present abatement methods. Based on this study, NCL has suggested suitable control methods,



achievable odour level and analytical method for maintaining the same. study, NCL has suggested suitable control methods, achievable odour level and analytical method for maintaining the same.

#### Innovative process for the treatment of toxics from air emissions Deodourisation processes

Odour is a key environmental issue and the presence of malodour in and around chemical industries is an unpleasant but seemingly ubiquitous fact all around the world. The prominent odorous emissions from chemical industries are sulphur compounds such as hydrogen sulphide, mercaptans and dimethyl sulphide. All these gases are highly odorous and can be sensed by human nose, even at a fraction of a ppb level. Gases such as hydrogen sulphide are toxic and are more dangerous as it cannot be sensed by human nose as its concentration increases. Therefore, it becomes essential to measure these gases at ppb level and develop control methods to reduce their emissions.

Under this project suitable method for measurement of gases such as hydrogen sulphide, methyl mercaptan, ethyl mercaptan and dimethyl sulphide was identified. Detectors such as flame photometric detector, flame ionization detector, chemiluminescence detector, photo ionization detector can detect these sulphur compounds. These detectors need to be used in combination with gas chromatograph to separate these compounds when present simultaneously. Portable gas chromatograph with photo ionization detector was chosen as it is economical, measures these odorous gases below parts per billion concentration and can be taken to industrial sites also. The instrument was standardized using authentic gas samples. Level of these gases in and around industries such as pesticides (Phorate), pharmaceuticals (Ranitidine), and man made fiber (rayon) was measured to assess the efficiency of control methods used in industries. Concentration of odorous compound after alkali scrubbers used in industries to abate hydrogen sulphide emission was found to be in the range of 1 to 60 ppm. Concentration of mercaptans after incineration was found to be in the range of 1 to 20 ppm. Ambient air in the industry showed 0.5 to 1 ppm of  $H_2S$  and up to 4 ppm of mercaptans. It was identified that biological methods can further reduce the emissions to ppb level. Biofilters provide a bed with microorganisms

which can bind and degenerate the odorous sulphur compounds. Bioscrubbers have microorganisms in scrubber solution which absorbs and decomposes odorous sulphur compounds. ppb level. Biofilters provide a bed with microorganisms which can bind and degenerate the odorous sulphur compounds. Bioscrubbers have microorganisms in scrubber solution which absorbs and decomposes odorous sulphur compounds.

### 3.3 REACTION AND REACTOR ENGINEERING

#### Predicting rates of dissolution of polydisperse solids in reactive media

Instantaneous rates of dissolution of poly-disperse solids in a batch dissolver depend on the aggregate surface area for mass transfer and the concentration driving force both of which can change with time. By generalizing the fluid-solid reaction framework to include the particle size distribution, a model was put in place for evaluation of the integral dissolution rates under widely applicable process and operating conditions without questionable assumptions made in mono-size particles based analysis.

Experimental dissolution rate data published by various researchers in a number of problems involving mass transfer controlled solid dissolution in reactive media could be successfully interpreted by the model in a consistent manner irrespective of the polydispersity of the charge, complex composition of the solutes and the underlying chemistry. While in most cases the estimated mass transfer coefficient was found to be in the range of those computed by the available correlations in the literature, both the value and the trend of its dependence on key variables like particle size and agitation speed was somewhat different in some cases. The discrepancy may be partly due to imperfect design and conduct of the dissolution experiments. But this may also be an indication of the inadequacy of the empirical correlations under reactive and/or high mass flux conditions. The model proved useful in estimating and correlating the transport coefficient.



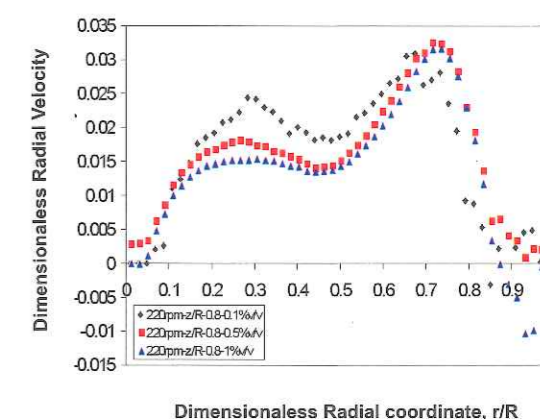
#### Re-tooling Benson's group additivity method for estimation of the enthalpy of formation of free radicals

Enthalpy of formation of free radicals is often required for the discrimination of reaction mechanisms (for complex processes such as combustion, hydrocarbon oxidation, or decomposition of peroxides and hydroperoxides) involving both molecular species and free radicals. Despite the expanding availability of the experimental measurements, the database for the enthalpy of formation of radicals is still not comprehensive. One of the simplest, efficient, and reliable methods for estimating the quantity for organic radicals from their molecular structure is the group additivity method due to Benson and co-workers. Perusal of the literature shows that the group-additivity values (GAV) for many radical groups have remained either undetermined or obtained by assignment to the corresponding molecular groups without justification. Simple methodologies were devised to evaluate GAVs for a number of new oxygen-containing radical groups and re-estimate several alkyl and oxygen-containing radical groups using experimental data on the radical enthalpy of formation. The validity of these GAVs has been established by comparing the predicted enthalpies with experimental data. Finally, some of these updated GAVs were used in estimating the enthalpy change associated with the typical elementary steps in a peroxide decomposition reaction. More recently the GAV data base has been extended to include about 100 groups covering unsaturated alkyl, cyclic and aromatic radicals, halogen-, nitrogen- and sulfur-containing radicals. These GAVs are being tested against more exhaustive and recent compilations of data on radical enthalpy of formation.

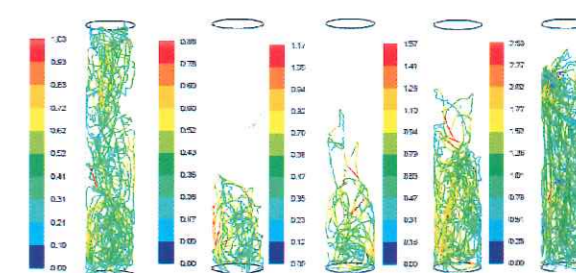
#### Flow mapping in stirred tank reactors using ultrasound velocity profiles

A non-intrusive measurement technique Ultrasound Velocity Profiler (UVP) is recently added to the existing measurement capabilities of iFMg. The technique works on the Doppler effect and uses the seeding particles in the system to measure the local instantaneous velocities along a line. This yields a linear one dimensional space-time data for a system. The technique is being used for the analysis of flow inside a stirred tank reactor for

suspension of glass particles. Typical velocity profiles obtained from the stirred tank reactor for different solid loadings are shown in the figure 1. The technique will be used for other applications viz. measurement of bubble rise velocity, measurement of liquid velocity in the vicinity of bubbles, analysis of three phase bubble column reactor, etc.



Dimensionless Radial velocity profiles at 220rpm,  $z/R = 0.8$



Simulated particle trajectories. From left (i)  $r_s = r_L$ ; (ii)  $r_s = 2.5r_L$ ,  $r_L = 1000 \text{ kg/m}^3$ ,  $U_0 = 0.05 \text{ m/s}$ , (iii)  $0.10 \text{ m/s}$ , (iv)  $0.20 \text{ m/s}$  and (v)  $0.40 \text{ m/s}$

#### CFD Simulation of two and three phase bubble column reactors

Liquid mixing in bubble columns is controlled by convective flows. The motion of identified liquid particles in the column can be tracked in the Lagrangian framework. When particles being tracked are neutrally buoyant and are very small, the particle tracking could also be used to estimate liquid phase mixing time. As the particle size and the particle density start increasing, the particles start to lag behind the motion of liquid phase. The models developed in this work can be used for





further understanding of interaction of solid particles with the flow generated in bubble columns. As an example, trajectories of neutrally buoyant particles of 500  $\mu\text{m}$  in a bubble column operated with superficial gas velocity of 0.05 m/s are shown in previous figure. Influence of particle density on simulated particle trajectories can be seen in figures (i)-(v). The simulation strategy will be extended for simulating the flow in a three phase bubble column reactor.

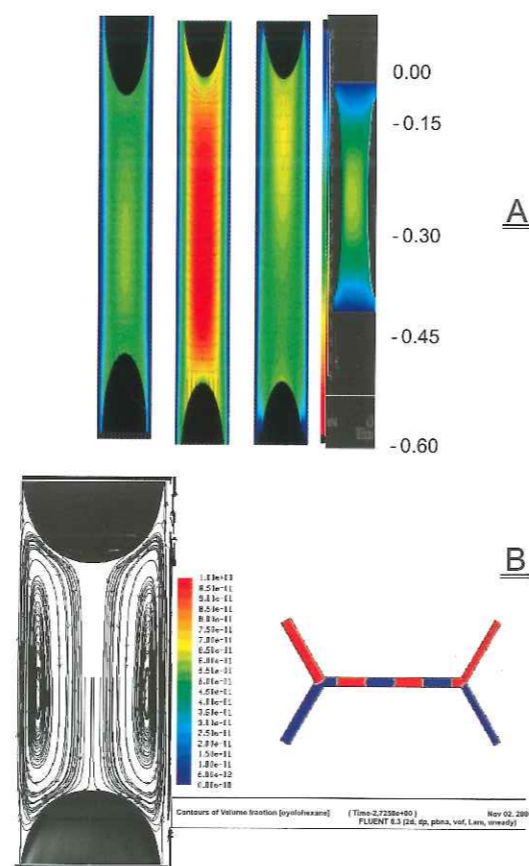
#### Modeling of bubble column slurry reactor for reductive alkylation of p-phenylenediamine

A Bubble Column Slurry-reactor model has been developed for the reductive alkylation of p-phenylenediamine (PPDA) with methyl ethyl ketone (MEK) to N, N'-di-secondary-alkyl-p-phenylenediamine (Di-amine). This particular reaction system has recent commercial relevance and involves a combination of parallel and consecutive reactions involving equilibrium non-catalytic (homogeneous) and catalytic (heterogeneous) steps. The developed model is based on the mixing cell approach and incorporates the contributions of gas-liquid and liquid-solid mass transfer, intraparticle diffusion effect, heat effects, and complex multistep reaction kinetics. Liquid phase back mixing is accounted for by including a backflow stream from all but the bottom most mixing cell. The effect of gas and liquid velocities, catalyst loading, inlet p-phenylenediamine concentration, and temperature on the conversion, selectivity, temperature rise and the productivity of the desired product is discussed. Influence of operating conditions on hydrodynamics and liquid phase mixing was quantified using a computational fluid dynamics (CFD) model. The bubble column slurry reactor models proposed could be useful to improve the overall performance of the process and design of reactors. It also may be utilized for guiding the design and scale up of such systems from lab scale to pilot scale data.

#### CFD Modelling of flow in microchannels

A CFD model has been developed to simulate slug flow in a capillary. The major objective of this work was to study the influences of various hydrodynamic and system parameters such as channel shape (circular/square), bubble velocity  $V_b$ , gas holdup  $e_G$ , and the equivalent channel diameter  $d_c$  on flow field in the

liquid slug and in the film surrounding the bubble. Typical simulation results are shown in the upper part of the figure. The model shall further be developed to gain insights into the mass transfer mechanism occurring in microchannels. Another interesting application of microchannel systems in the two phase extraction is being studied through experiments and simulations. Here, a flow splitting element ("Y" splitter) which separates the liquids based on preferential wettability of liquids to the solid materials has been introduced. Experimental data for the above concept was obtained from the collaborative research between Dortmund University, Germany and NCL. A CFD model based on free surface methodology, volume of fluid (VOF), was developed to generate and subsequently to separate the slug flow. Typical simulation results indicating the selective passage of fluid conditional to the surface properties of the flow channel can be seen in the lower part of the figure.



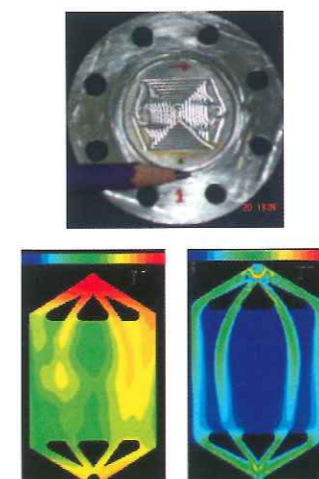
(A): Velocity vector and contour plot, (B) Typical simulated result for slug formation and separation in "Y" splitter



#### Microreactors

Recently the advantages of miniaturization are seen to realize efficient process development and process intensification. Smaller dimensions help in achieving higher effective transport area, practically isothermal conditions in the reaction system and also suitability towards extreme conditions. Being smaller in size, these devices handle very small volumes of reacting liquids. As a result, they offer a relatively smaller time scale and hence are more suitable for the fast reactions. New microdevices like a micro heat exchanger, micro fixed bed reactor, mesh microreactor were designed, developed and tested. The group is also focusing on understanding the microfluidic aspects of two phase flows in capillaries, heat transfer in microchannels, pressure drop variation and residence time distribution in microreactors, etc.

The group is also working on using the microreaction technology for various industrially important reactions viz. nitration, chlorination, hydrogenation, etc. Apart from the above areas, the industrial flow modelling group (iFMg) is also involved in development of a new ejector system for gas-liquid reactions, understanding the bubble motion in shear flows, flow in riser down-comer configuration for gas-solid flows, design of new boiler configurations and understanding the role of nanoparticles in improving the heat transfer in microchannels.

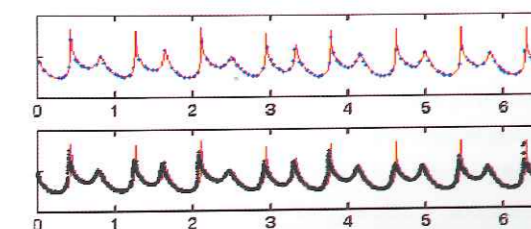


(i) Typical  $\mu\text{Hex}$  plate, (ii) assembled  $\mu\text{Hex}$  with 10 heat transfer plates (designed by NCL and fabricated by L&T, Mumbai), simulated (iii) temperature and (iii) velocity field on a plate

Apart from the above areas, the industrial flow modelling group (iFMg) is also involved in development of a new ejector system for gas-liquid reactions, understanding the bubble motion in shear flows, flow in riser down-comer configuration for gas-solid flows, design of new boiler configurations and understanding the role of nanoparticles in improving the heat transfer in microchannels.

#### Wavelet transforms for analysis of data obtained at unequal time intervals

The spectral analysis of data in the frequency domain requires that data from instruments/sensors be obtained at equally spaced intervals. This is not often the case because even sophisticated instruments like Laser Doppler Anemometry (LDA) that measure turbulent velocities in liquids do not satisfy this requirement. In which case there exists a need to develop new algorithms that interpolate highly non-stationary and noisy data. We have developed an efficient algorithm employing Wavelet Transform (WT) that produces accurate interpolations of difficult to treat unequally spaced data. The methodology is generic and can be applied to data obtained from interdisciplinary systems. The Interpolation methodology when applied in conjunction with the efficient noise reduction algorithms that has been developed earlier at NCL (again using WT) has been found to be very effective for pattern recognition amongst sets of complex data not amenable to conventional spectral analysis. Work is underway on applying the algorithm for analysis of data obtained from turbulent systems.



The red trace in the figure on the top shows the desired trace of points in time after interpolation from the unequally spaced blue data points. The bottom figure with the black trace is seen to follow the red and shows the accuracy in interpolation by the present WT methodology. The red trace was obtained by a synthetic simulation of the chaotic and non-stationary reaction dynamics observed in a non-isothermal CSTR.



### Improved times series prediction with a new method for selection of model parameters

Prediction and characterization of time series have always been of significant importance in process engineering. We have employed the wavelet transform modulus maxima (WTMM)-based method for characterizing and quantifying the singularities in a chaotic time series. The method provides the density estimates of the local Hölder exponents that characterize the regular/irregular local behaviour of time series. Higher the value of the local Hölder exponent, the more regular is the local behaviour of time series and vice versa. The density estimates of the local Hölder exponents represent the most informative features regarding the singularities in the time series. Thus, an estimate of the error in the density spectrum of the predicted validation set, which we will henceforth denote as HRSME, can be very useful for tuning the model parameters. For certain time series data it may be possible that both RMSE and HRMSE information would be useful for obtaining optimal performance. In this work, errors in the density estimates (HRMSE) (along with regular RMSE) of the validation set have been employed as an additional criterion for the selection of optimal model parameters. Thus the problem of model selection is formulated in terms of a multiobjective optimization i.e. the selection of model parameters has been done by minimizing both criteria, namely, RMS errors based on the original time series as well as on the error in the singularity distribution. In this problem, we have to find the decision vector (parameters of model used for time series prediction), which will minimize RMSE as well as HRMSE. Multiobjective optimization, however, gives rise to a set of optimal solutions, instead of a single one. These optimal solutions are called as Pareto-optimal solutions. We have used this concept of non-dominated Pareto-optimal solutions for finding the optimal parameters of the KPCR model to improve the generalization capability of the model. Kernel PCA, a nonlinear version of PCA, has recently been extensively used because of its computational simplicity and nonlinear feature extraction and denoising capabilities. We have chosen KPCR because of its excellent performance on time series prediction problems. The problem of model selection is solved by simultaneously

minimizing both criteria, namely, RMS error based on the original time series as well as on the error in the singularity distribution. The method was tested on three time series: two simulated and one based on real observations. Predictions of these time series have been done using KPCR and model parameters of KPCR have been selected employing the proposed as well as the conventional methods. The problem now being a multiobjective optimization problem, we get a set of Pareto-optimal solutions. Results obtained demonstrate that the proposed method helps in better prediction of the unseen test data and improved the generalization capability of the KPCR model. Model selection has produced results, which are better than those yielded by the conventional method in all the cases of the simulated and real time series. Thus, the new method can be very useful in the prediction of time series data having sharp singularities.

### DATA Driven dynamic modelling and control of surface aeration systems

Data-driven modelling (DDM) employing artificial intelligence and machine learning methods is finding increasing relevance and importance in chemically reacting systems. Surface aerator is one such industrially important system that mainly finds application in wastewater treatment and in many chemical reactions such as hydrogenation, alkylation, and so forth. In this study we have developed a support vector regression (SVR) based data-driven model for predicting two important design parameters of surface aerators, namely, the volumetric mass transfer coefficient ( $k_L a$ ) and fractional gas hold-up ( $\epsilon_G$ ). The dynamical state of the surface aerator system was captured by acquiring pressure fluctuation signals (PFSs) at various designs and operating conditions.

H=Liquid height, D=Impeller diameter,  
T= Tank diameter,  
C=Impeller clearance, a= Surface aerator, b=transmitter,  
c= battery,  
d=channel box, e= personal computer



In order to avoid intensive computational work, the most informative features from PFS were extracted using the chaos analysis technique, which includes estimation of Lyapunov exponent, correlation dimensions, and Kolmogorov entropy. At similar conditions the values of  $k_L a$  and  $\epsilon_G$  were also measured. Thus attempt was made to generate a data-driven model by establishing a nonlinear relationship between chaotic invariants, design parameters, operating parameters, and  $k_L a$  and  $\epsilon_G$ . Two different SVR models for predicting the volumetric mass transfer coefficient ( $k_L a$ ) and overall gas hold-up ( $\epsilon_G$ ) as a function of chaotic invariants, design parameters, and operating parameters were developed. Also in order to check for the nonlinearity associated with the data set, a simple multiple linear regression (MLR) technique was employed to generate the linear regression models for the surface aerator. The performance of the method was found to be excellent and much superior to classical multilinear regression methods.

### 3.4 ARTIFICIAL INTELLIGENCE SYSTEMS

#### Density measurements of coal samples by different probe gases and their interrelation

Density is useful in deducing the spatial structure of coals. In this study, nitrogen has been used instead of the commonly employed helium, for the gas displacement pycnometer based density determination of a number of coals of Indian origin. The results showed that the nitrogen-based densities are always higher than the helium-based ones. Also, empirical relationships between the helium-based and nitrogen-based coal densities have been developed by two modeling methods, namely, multi-variable regression and artificial neural networks. Although the two models have fared well, the neural network model exhibited a relatively better prediction accuracy and generalization performance than the regression model. The study, thus, demonstrated that nitrogen, which is cheaper and easily available, can be used gainfully as the probe gas for estimating the true density of coals densities have been developed by two modeling methods, namely, multi-variable regression and artificial neural networks. Although the two models have fared well, the neural network model exhibited a relatively better prediction

accuracy and generalization performance than the regression model. The study, thus, demonstrated that nitrogen, which is cheaper and easily available, can be used gainfully as the probe gas for estimating the true density of coals.

### Improve polyethylene process control and product quality

The difficulties associated with regression-based empirical modelling can be overcome by using an artificial intelligence (AI)-based modelling formalism-artificial neural networks (ANNs). Software-based sophisticated monitoring systems can relate less accessible and infrequently measured process variables with those measured easily and frequently. Once developed, a soft-sensor model can be readily used for predicting, in real time, the value of less accessible and difficult-to-measure process variables. Soft-sensors are useful in controlling and monitoring chemical processes where appropriate hardware sensors are unavailable and important QC values are not continuously obtainable. A soft-sensor's ability to accurately predict QC variable magnitude depends upon the availability of reliable hardware sensors and the mathematical and statistical techniques used in correlating and interpreting process data. Meanwhile, in any set of real-world process data, instrumental noise and measurements errors is unavoidable. Thus, the data in its raw noisy form must be used to build the soft-sensor models. Noise and errors present in the data create a threshold limit to accurately predict and generalize the ANN-based soft-sensor model performance. An improvement in the generalization performance of an ANN model is therefore needed. One method generates an enlarged noise-superimposed data set. Multiple patterns are synthesized by adding an optimal amount of noise to variables for each example set input-output pattern.

### Estimation of gross calorific value of coals using artificial neural networks

The gross calorific value (GCV) is an important property defining the energy content and thereby efficiency of fuels, such as coals. There exist a number of correlations



for estimating the GCV of a coal sample based upon its proximate and/or ultimate analyses. These correlations are mainly linear in character although there are indications that the relationship between the GCV and a few constituents of the proximate and ultimate analyses could be nonlinear. Accordingly, a total of seven nonlinear models have been developed using the artificial neural networks (ANN) methodology for the estimation of GCV with a special focus on Indian coals. The comprehensive ANN model developed here uses all the major constituents of the proximate and ultimate analyses as inputs while the remaining six sub-models use different combinations of the constituents of the stated analyses. The comprehensive model developed here was found to be the most accurate GCV predictor. Also, the performance of the ANN models has been found to be consistently better than that of their linear counterparts. Additionally, a sensitivity analysis of the comprehensive ANN model has been performed to identify the important model inputs, which significantly affect the GCV. The ANN-based modelling approach illustrated in this paper is sufficiently general and thus can be gainfully extended for estimating the GCV of a wide spectrum of solid, liquid and gaseous fuels.

#### Improved performance of artificial neural network models in the presence of instrumental noise and measurement errors

A method is described for improving the prediction accuracy and generalization performance of artificial neural network models in presence of input-output example data containing instrumental noise and/or measurement errors. The presence of noise and/or errors in the input-output example data used for training the network models create difficulties in learning accurately the nonlinear relationships existing between the inputs and the outputs, to effectively learn the noisy relationships. The methodology envisages creation of a large-sized noise-superimposed sample input-output data-set using computer simulation. Here, a specific amount of Gaussian noise is added to each input/output variable in the example set and the enlarged sample data set created thereby is used as the training set for constructing the artificial neural network model. The amount of noise to be added is specific to an input/output

variable and its optimal value is determined using a stochastic search and optimization technique, namely, genetic algorithms. The network trained on the noise-superimposed enlarged training set showed significant improvements in its prediction accuracy and generalization performance, the invented methodology is illustrated by its successful application to the example data comprising instrumental errors and/or measurement noise from an industrial polymerization reactor and a continuous stirred tank reactor (CSTR).

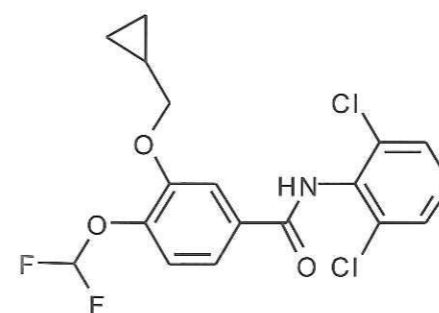
## 4 ORGANIC CHEMISTRY

Advances in the central disciplines of chemistry are essential in amalgamating chemistry, biology, material science and medicine to contribute to human progress. Organic synthesis is definitely an indispensable tool to develop the molecules of natural origin and the designer molecules with properties desired. In this regard, synthesis of complex natural products with inherent stereochemical specificity is a critical exercise that needs integration of knowledge with intuition. Discovery of newer methodologies and new catalysts is a prerequisite where generating molecular complexity from readily available starting materials is desired and for developing innovative cost effective processes for the drugs of today and tomorrow. The research program in Organic Chemistry integrates various aspects mentioned above in addressing key aspects like:

- Process chemistry
- Total synthesis
- New methods
- Organic biomolecular chemistry
- Supramolecular crystal engineering.
- Near IR colorants

### 4.1 PROCESS CHEMISTRY

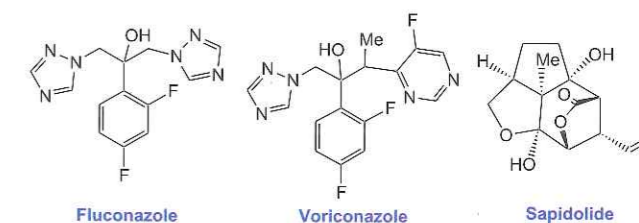
Process for Roflumilast : Roflumilast 3 (cyclopropylmethoxy)-N-(3,5-dichloropyridine-4-yl)-4 difluoromethoxy benzamide is categorised as antiallergic/antiasthmatic. It is used in the treatment of chronic obstructive lung diseases (COPD) and is also a phosphodiesterase 4 (PDE4) inhibitor. A laboratory scale process was developed for Roflumilast.



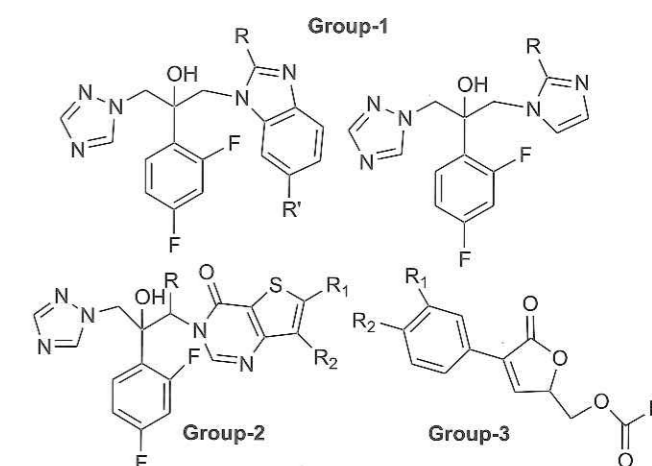
Roflumilast

### 1,2,4-Triazole based anti-fungal compounds

Various novel anti-fungal molecules based on the structural features of fluconazole, voriconazole and sapidolide were synthesized and scaled up in effort to identify active compounds.



The compounds synthesized at NCL were screened for anti-fungal activity at FDC. Most of the compounds exhibited significant antifungal activity against *Candida albicans*. Secondary screening was carried out in case of compounds which exhibited good activity in primary screening.

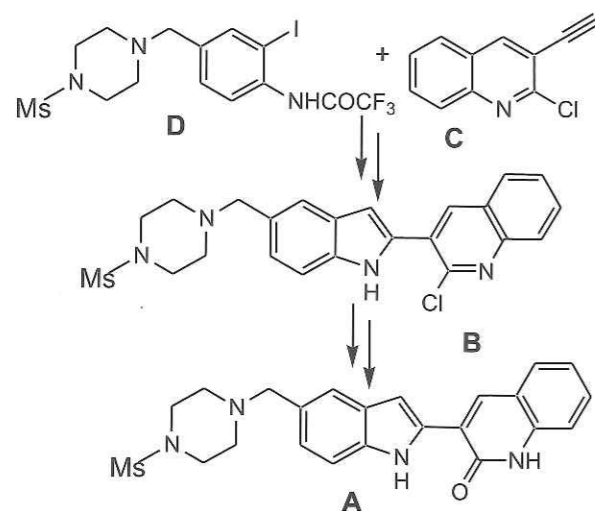


### Merck KDR inhibitor

We have developed a new alternative route to the synthesis of the potent and selective KDR kinase inhibitor **A** which has potential use in cancer therapy by using Sonogashira coupling-5-endo-dig-cyclization strategy. Recently Merck reported a class of potent KDR kinase inhibitors containing the indol-2-yl quinoline-2-one as the key pharmacophore. KDR (kinase insert domain-containing receptor) is one of the human tyrosine kinases that has a high affinity for vascular endothelial growth factor (VEGF) and is believed to be a primary mediator of tumor-induced angiogenesis. Compound **A** was found to be of use in the treatment of cancer. The important intermediate of this process is indole-chloroquinoline **B** was synthesized by a key palladium catalyzed tandem Sonogashira coupling -5-endo-dig-cyclization of o-iodoaniline derivative **D** with

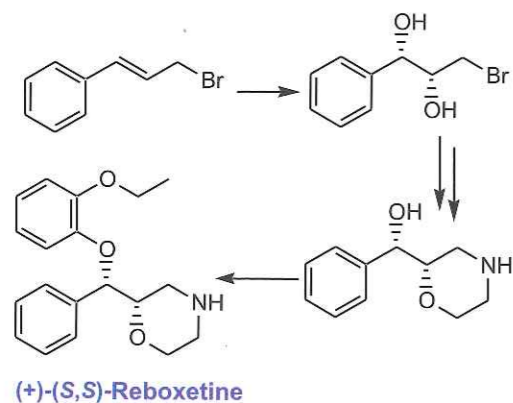


terminal alkyne **C** using  $\text{Pd}(\text{OAc})_2$  as the catalyst,  $\text{Bu}_4\text{NOAc}$  as the base was optimized under ligand-, copper- and amine- free condition.

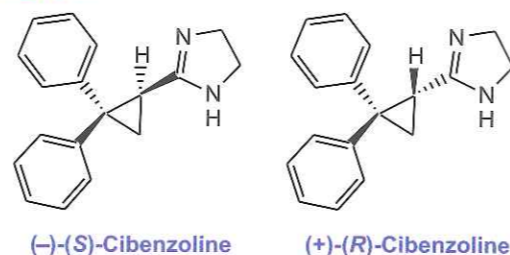


#### Asymmetric process for (+)-(S,S)-Reboxetine

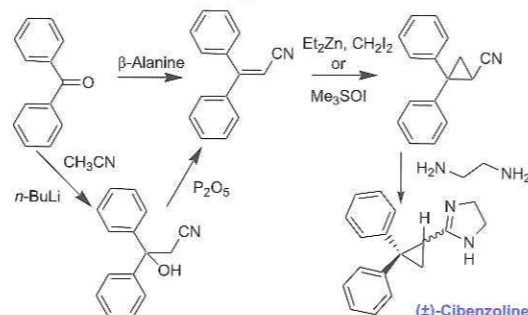
Reboxetine has been marketed as a mixture of two enantiomers (*S,S* and *R,R*) for the treatment of depressive illness in several European countries. It has comparable efficacy to that of imipramine, desipramine and fluoxetine, and has an improved side-effect profile. However, (*S,S*)-reboxetine is approximately 24 times more potent than the (*R,R*)-reboxetine and presents the best affinity and selectivity for norepinephrine transporter (NET). By employing Sharpless asymmetric dihydroxylation a process for enantioselective synthesis of (+)-(*S,S*)-reboxetine from commercially available *trans*-cinnamyl bromide was developed.



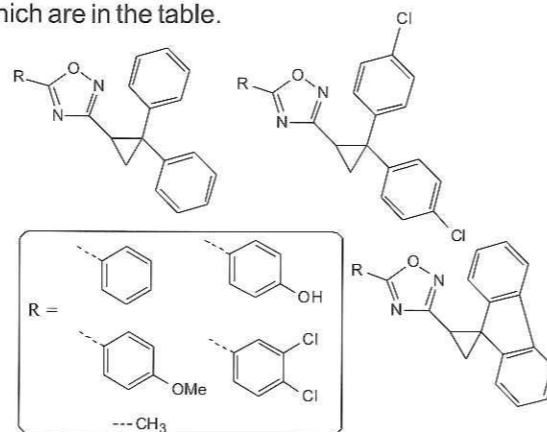
#### Process for racemic Cibenzoline and their analogues.



Cibenzoline was an anti-arrhythmic agent. All the reported and patented procedures have several disadvantages like reactions at high temperature, use of toxic reagents like  $\text{HgO}$ . The process developed at NCL addresses several these issues by employing some of modern reactions and reagents.



**Part B:** We have synthesized various analogues which are in the table.



#### Oral penem anti-bacterial agents for community acquired infections

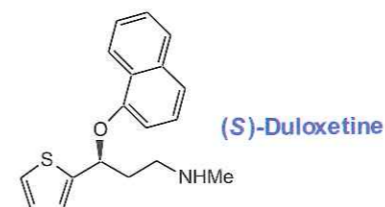
Beta lactam antimicrobials are widely recognized for their efficacy and low toxicity for the treatment of infections caused by gram positive and gram negative bacteria.



However, extensive use of beta lactams during the past 50 years has resulted in the development of microbial resistance to these agents amongst clinically important bacteria. The issue of resistance continues to drive the search for new compounds with increased stability and efficiency against resistant pathogens. The excellent broad spectrum activity achieved with the penem derivatives against both gram positive and gram negative bacteria coupled with their extreme stability towards the hydrolysis by beta lactamases has given a great impetus to synthesize and study a huge number of new penem derivatives. Synthesis of New Chemical Entities (NCEs) under this project was undertaken to find a new active oral penem. 28 NCEs have been synthesized and evaluated for their anti-bacterial activity, along with their potential as beta lactamase inhibitor. Four NCEs showed promising anti-bacterial activity. NCLP-024 is active and almost similar to ferropenem against *S.pneumoniae* only. It is inactive against *H.influenzae* and *S.aureus*. NCLP-026, 035 and 036 have moderate activity against penicillin sensitive *S.pneumoniae* and *S.pyogenes* only.

#### 2. (S)-Duloxetine

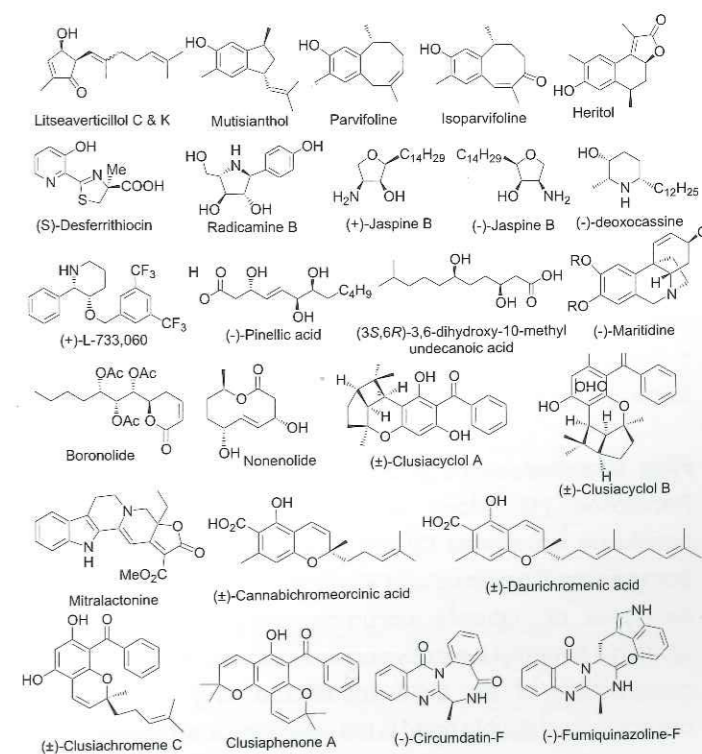
Duloxetine is a dual inhibitor of serotonin and norepinephrine reuptake and has a better pharmacological profile for an antidepressant drug. Serotonin and norepinephrine neurotransmitters are intimately involved in a number of physiological and behavioural processes, suggesting that duloxetine is not only a high efficient anti-depressant agent for treating psychiatric disorders, but also can be used for treating symptoms such as urinary incontinence, obsessive compulsive disorder etc. Improved efficacy, tolerability, safety, faster recovery, fewer side effects, low affinity for neural receptors and dual inhibiting nature gives duloxetine an edge over other existing antidepressants such as fluoxetine. It is anticipated that, duloxetine may reach its peak sales of over US \$1 billion.



A convenient process for (*S*)-duloxetine was developed under sponsorship from M/s FDC Ltd., Mumbai. The process involves seven steps and key steps of the process are the resolution of the alcohol and N-demethylation. All the steps have standardised on a laboratory scale. The process know-how along with the analytical and physical data has been transferred to M/s FDC Ltd., Mumbai for commercialisation. M/s FDC has scaled this process at their end.

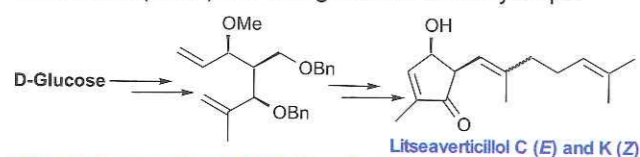
#### 4.2 TOTAL SYNTHESIS

The field of discovery and synthesis of biological active natural products represents a dynamic and largely growing research area. By the use of new strategies to discover natural products of interest, many molecules with novel structural features have been isolated and their structures have been elucidated. The development of new strategies for total synthesis combines in ideal platform for different areas in organic synthesis. Total synthesis is one of the major activities of this group. This year, total synthesis of several natural products with varying complexity has been accomplished. Structures of some representative natural product were given below.



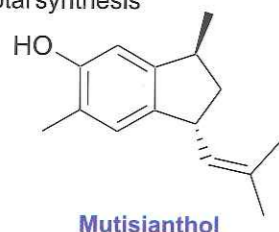


**litseaverticillol C and K:** The first enantioselective synthesis towards the litseaverticillols C and K has been achieved, from D-Glucose, using the ring closing metathesis (RCM) and Wittig reactions as key steps.



#### Total synthesis of Mutisianthol

Mutisianthol, a phenolic sesquiterpene isolated from the root of *Mutisia homoeantha*, in 1979 belongs to structurally diverse indans (other examples are fredericamycin, a potent anti-tumour compound as well as the architecturally complex alkaloid (+)-ribasine). It is plausibly derived in nature from a  $\alpha$ -curcumene type precursor by cyclisation to form the indane nucleus. The most intriguing aspect of mutisianthol is the *trans*-relationship assigned to the two side chains of the five membered ring and this has attracted many groups to undertake a total synthesis



Mutisianthol

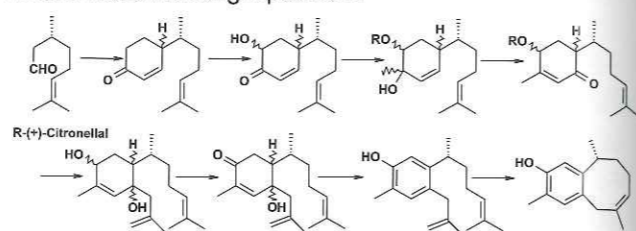
Till now two synthesis are reported for mutisianthol; a stereoselective synthesis (reported in 1997) and diastereoselective total synthesis of ( $\pm$ )-mutisianthol (reported in 2003). Last year, we undertook a new total synthesis of ( $\pm$ )-mutisianthol and also of the chiral mutisianthol where BINAP type ligands are being used for asymmetric induction. The route involves 2,4-dihydroxy benzaldehyde as the readily available starting material. Synthesis of ( $\pm$ )-mutisianthol involve about 16 steps and the chiral synthesis is currently in progress.

#### First enantiospecific synthesis of (-)-Parvifoline

Parvifoline (1), along with isoparvifoline (2) and parvifoline isovalerate (3) are sesquiterpenes; isolated from genera '*Coreopsis*' and '*Perezia*'. These are the only examples of naturally occurring compounds, which contain a trimethyl benzocyclooctane structural unit. The construction of an eight membered ring with a deconjugated double bond is the main structural feature

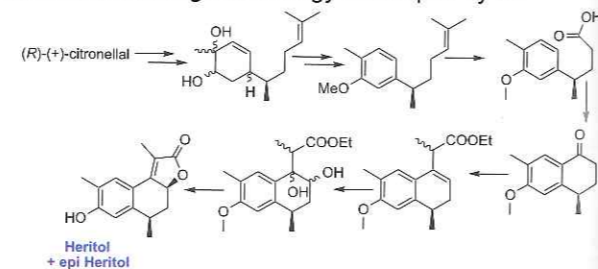
that challenges the synthesis of parvifoline. We have been interested in employing the renewable resources of the nature for the synthesis of natural products. We have identified citronellal as the key synthon, which is abundantly available both from plants and of synthetic origin and have accomplished syntheses of laevigatin and herbertenol.

The first enantiospecific synthesis of (-)-parvifoline starting from naturally occurring *R*-(+)-citronellal in 12% yield using ring-closing metathesis as the key step for the formation of cyclooctene ring, which efficiently places the double bond in the right position.



#### First Enantiospecific synthesis of Heritol

Miles et al. isolated an active toxin, called heritol (1) and heritonin (2), a naturally occurring sesquiterpene, from the sap of the mangrove plant *Heritiera littoralis*, which was shown to possess ichthyotoxicity in ppm quantities to *Tilapia nilotica* fingerlings. Both these compounds have a novel structure of the cadinane sesquiterpene class containing an  $\alpha,\beta$ -unsaturated  $\gamma$ -lactone moiety with an unusual oxygenation pattern. The relative stereochemistry in heritol was established by single crystal X-ray analysis, but its absolute stereochemistry was only tentatively proposed to be *R* at C10 by comparison with other cadinanes. As outlined in the below our main target was to construct the tetralone unit enantiospecifically followed by butenolide ring construction using the strategy developed by us.



(-)-Heritol (1) has been synthesised enantiospecifically for the first time from naturally occurring (*R*)-(+)-citronellal and the absolute configuration of natural

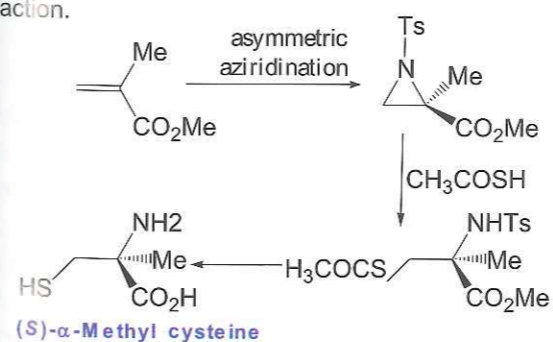
heritol proposed to be (*S,R*) at C10, C8 by comparison of the specific rotation with that of synthetic Heritol.

#### Synthesis of chiral $\alpha$ -methyl cysteine

$\alpha$ -Methyl cysteine is an unusual amino acid and an important building block for a new family of natural products, thiagazoles, tantazoles and mirabazoles which exhibit antitumour and anti HIV activities. It is also a potent enzyme inhibitor. (*S*)-Desferrithiocin is a unique and unusual naturally occurring ferric iron chelator (siderophore) which also has  $\alpha$ -methyl cysteine moiety.



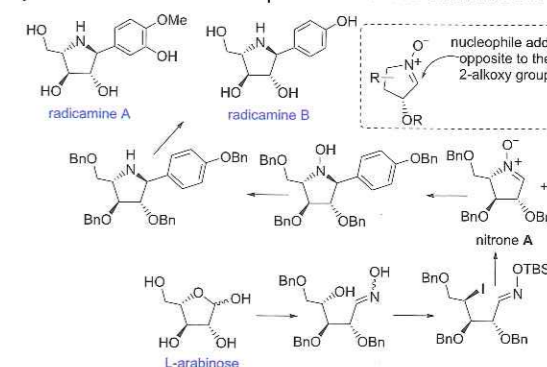
Last year, we reported a concise synthesis of ( $\pm$ )- $\alpha$ -Methyl cysteine. The route essentially involved aziridination of methyl methacrylate, ring opening of the aziridine formed with thioacetic acid / thiobenzoic acid followed by hydrolysis to yield ( $\pm$ )- $\alpha$ -methyl cysteine similar route applies to the chiral  $\alpha$ -methyl cysteines. Currently, synthesis of chiral  $\alpha$ -methyl cysteines have been undertaken. The key reaction is the asymmetric aziridination of methyl methacrylate using different ligands / catalysts. Several new ligands/ catalysts have been prepared and characterized and applied in the key reaction.



#### Radicamine B

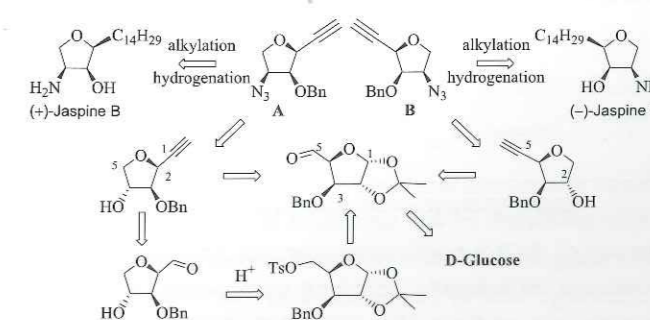
Radicamines A and B, two new pyrrolidine alkaloids were isolated as inhibitors of  $\alpha$ -glucosidase from the plant *Lobelia chinensis* Lour., a herb that is used as a diuretic, an antidote, a hemostat and as a carcinostatic agent for stomach cancer in Chinese folk medicine. The structures and relative stereochemistry of both these compounds were determined on the basis of extensive NMR studies.

However, the absolute configuration of these compounds was assigned by comparing the specific rotation with the natural codonopsinine and with its antipode. Due to its remarkable biological properties we have undertaken the synthesis of radcamine B. The total synthesis of radcamine B with the proposed absolute configuration was accomplished. The facial selective addition of a suitable aryl Grignard to the *L-arabino* configured cyclic nitronone **A** forms the key approach of our intended synthesis of Radcamine B. Synthesis of the key nitronone **A** was accomplished from *L-arabino*.



#### Jaspine B and its enantiomer

Pachastrissamine, isolated and characterized by Higa and co-workers in 2002 from the Okinawa marine sponge *Pachastrissa* sp. is a novel anhydro-phytosphingosine with important bioactivity. It was later (in 2003) isolated from another marine sponge, genus *Jaspis* by Debitus and co-workers and named as Jaspine B. As shown in figure, our strategy exploited the pseudo-symmetry present in the pentodialdo-1,4-furanose **C** to derive the enantiomeric azidoalkynes **A** and **B** which upon alkylation and hydrogenation resulted in the synthesis of (+)-Jaspine B and its enantiomer respectively.



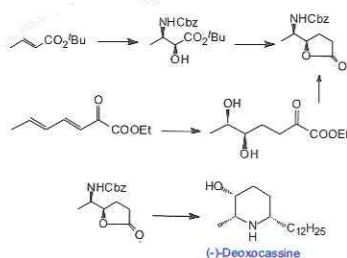
The key pseudodesymmetrisation strategy adopted for (+)- and (-)-pachastrissamine





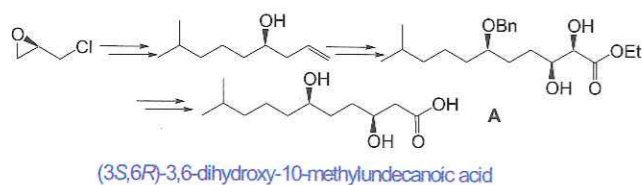
### An asymmetric aminohydroxylation route to *cis*-2,6-disubstituted-3-ol: (-)-Deoxocassine

Functionalized piperidines are among the most ubiquitous heterocyclic building blocks in natural products and synthetic compounds with important activities. Hydroxylated piperidine alkaloids are frequently found in living systems and display a wide range of biological activities due to their ability to mimic carbohydrates in a variety of enzymatic processes. 2,6-disubstituted 3-piperidinols are abundantly found in nature and have received much attention from the synthetic community. Besides the interesting structural features, these compounds are also of pharmaceutical interest as they exhibit a wide range of biological activities. NCL has developed a highly efficient, flexible and convergent route to *cis*-2,3,6-trisubstituted piperidines employing the Sharpless asymmetric aminohydroxylation and stereoselective reductive amination by catalytic hydrogenation as the key steps. Its usage is illustrated by the short synthesis of the piperidine-3-ol alkaloid, (-)-deoxocassine.



### (-)-(3*S*,6*R*)-3,6-dihydroxy-10-methylundecanoic acid

(-)-(3*S*,6*R*)-3,6-Dihydroxy-10-methylundecanoic acid (**A**) was isolated from the aerial parts of *Lafuentea rotundifolia* Lag. It has been a synthetic target of considerable interest due to its  $\beta$ -hydroxyl acid skeleton and unique structure with an array of functionalities.

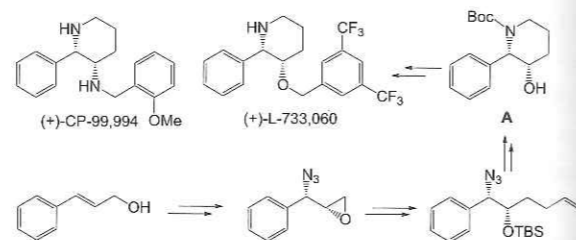


As part of NCL's ongoing program towards asymmetric synthesis of naturally occurring compounds, the total synthesis of (-)-(3*S*,6*R*)-3,6-dihydroxy-10-methylundecanoic acid was accomplished from commercially available (*R*)-epichlorohydrin using

Sharpless asymmetric dihydroxylation and regioselective opening of epoxide and cyclic sulfate as the key steps.

### (+)-L-733,060

The peptide neurotransmitter, Substance P (SP) involves a variety of biological actions such as pain transmission, vasodilation, smooth muscle contraction and neurogenic inflammation. This tachykinin family peptide member binds preferentially to the NK1 receptor. The search for non-peptide antagonists of the NK1 receptor led to the discovery of 2,3-disubstituted piperidine derivatives L-733,060 and CP-99,994. They have excellent affinity and selectivity with human NK1 receptors and possess potent antiemetic activity. They are expected to act as remedy for a wide range of diseases, including arthritis, asthma and migraines.

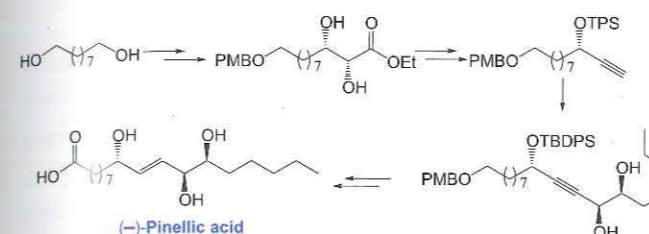


An efficient enantioselective synthesis of (+)-L-733,060 from cinnamyl alcohol was developed using the key steps such as a Sharpless asymmetric epoxidation, a regioselective allyl opening of epoxide and piperidine ring formation by one pot Staudinger/aza-Wittig reaction.

### Enantioselective synthesis of (-)-pinellic acid

Pinellic acid (9*S*,12*S*,13*S*-trihydroxy-10*E*-octadecenoic acid) was isolated from the tuber of *P. ternata*, one of the eight component herbs of the Kampo formula, Sho-seiryu-to (SST). Pinellic acid is a novel and potentially useful oral adjuvant when used in conjunction with intranasal inoculation of influenza HA vaccines. Pinellic acid showed no hemolytic activity. Among the series of pinellic acid isomers, the (9*S*,12*S*,13*S*)-compound, which is a natural product, exhibited the most potent adjuvant activity.

An enantioselective convergent approach towards the total synthesis of pinellic acid from 1,9-nonanediol was developed. The synthetic strategy features the iterative Sharpless asymmetric dihydroxylation, Sonogashira coupling and Birch reduction.

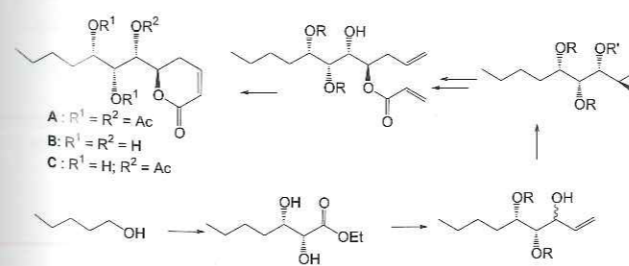


### (+)-Boronolide

Many natural products with different biological activities such as insect growth inhibition, antitumor, antibacterial, antifungal or immunosuppressive properties, possess  $\alpha,\beta$ -unsaturated  $\delta$ -lactone moiety as an important structural feature.  $\alpha,\beta$ -Unsaturated  $\delta$ -lactone functionality is presumed to be responsible for biological activities. The pyrone units are widely distributed in all parts of plants (Lamiaceae, Piperaceae, Lauraceae, and Annonaceae families) including leaves, stems, flowers and fruits.  $\alpha$ -Pyrone possessing polyhydroxy or polyacetoxy side chains have attracted much attention from synthetic and medicinal chemists due to their broad range of biological activities. Examples of such compounds include (+)-boronolide **A** and its deacetylated **B** and dideacetylated derivative **C**.

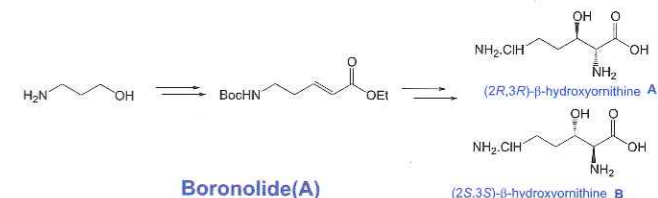
Boronolide is an  $\alpha,\beta$ -unsaturated C-12 lactone isolated from the leaves and branches of *Tetradenia fruticosa* and from the leaves of *Tetradenia barberae*, which have been used as a local folk medicine in Madagascar and South Africa. Deacetylated **1a** and dideacetylated boronolide **1b** have been obtained from *Tetradenia riparia*, a Central African species typically employed by the Zulu as an emetic, which is an infusion of the leaf has also been reported to be effective against malaria.

An efficient stereoselective total synthesis of (+)-boronolide from valeraldehyde was developed. The key steps include a Sharpless asymmetric hydroxylation, a chelation controlled vinyl Grignard reaction followed by Sharpless asymmetric epoxidation, hydrolytic kinetic resolution and a ring closing metathesis.



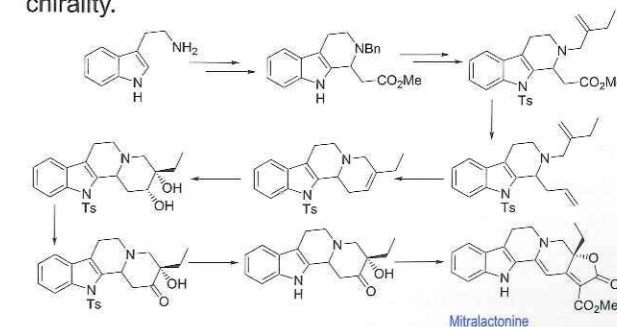
### (2*R*,3*R*)- & (2*S*,3*S*)- $\beta$ -Hydroxyornithine

$\beta$ -Hydroxyornithines **A** and **B**, serve as intermediates in the synthesis of important natural products like  $\beta$ -lactams and amino polyols and as biosynthetic precursors to both the-lactamase inhibitor clavulanic acid and the anticancer agent acivicin. Proclavaminic acid has been recognized as the biosynthetic precursor of clavulanic acid, a potent inhibitor of bacterial  $\beta$ -lactamase. An efficient and short synthesis of (2*R*,3*R*)- and (2*S*,3*S*)- $\beta$ -hydroxyornithine was developed using Sharpless asymmetric dihydroxylation and regioselective nucleophilic opening of a cyclic sulfite as the key steps.



### Mitralactonine

(-)-Mitralactonine, along with nine corynanthe-type indole alkaloids, namely, was isolated from tropical plant *Mitragyna speciosa* which is endemic to southeast asia and whose leaves have been traditionally used for their biological profile similar to that of opioids. The synthesis of this indole alkaloid has been accomplished employing RCM strategy as the key step to construct the D ring. In an another approach this molecule was synthesized in optically pure form in a convergent manner employing Sharpless asymmetric dihydroxylation as the source of chirality.

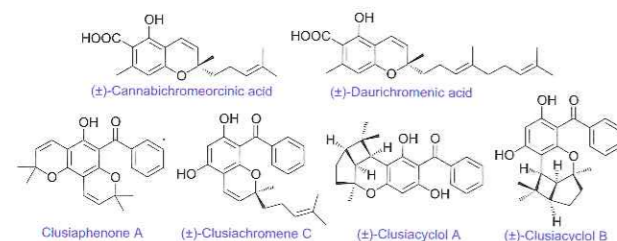


Total synthesis of bioactive natural products with flexible strategies pose real challenge lies in delivering highly efficient and practical routes for related analogues. Past several years, we have been busy in total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors,

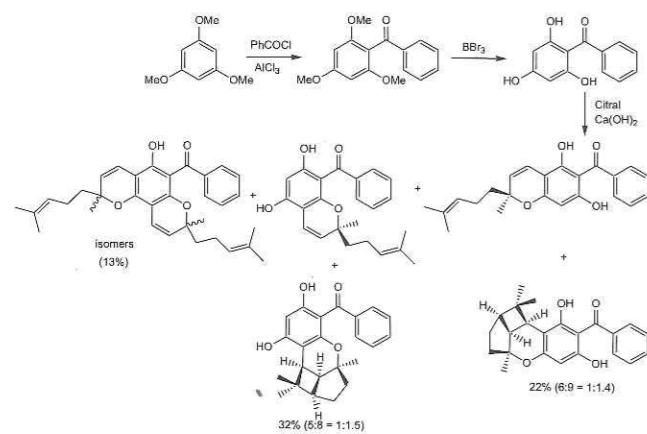


employing variety of new synthetic strategies. The list of natural products synthesized during the past year includes fimbrolides, sclerotigenin, (-)-circumdatin-F, (-)-fumiquinazoline-F, cannabichromeoric acid, daurichromenic acid, clusiaphenone A, clusiachromene C, clusiacyclol A and clusiacyclol B.

### Benzopyran Natural Products

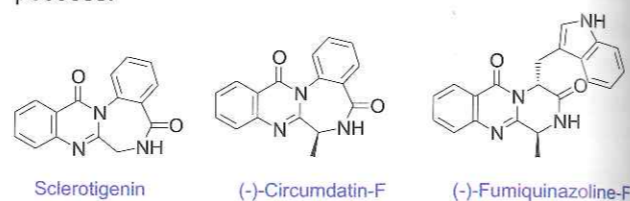


The complex bioactive natural and unnatural benzopyran congeners have been synthesized using one- / two-step approaches in very good yields from the reactions of two different dihydroxyphthalides, natural resorcylic acid derivative, and trihydroxybenzophenone with citral and/or farnesal, via the phenol-driven intramolecular diastereoselective thermal/base-catalyzed dipolar [2 + 2] cycloaddition reactions and three different thermal intramolecular cyclization reactions. The effects of the nature and the position of phenolic groups in the starting materials on the course of these cycloaddition reactions have also been described. Depending upon the absence or presence of intramolecular hydrogen bonding of the phenolic group with the carbonyl moiety in the starting materials, these phenol-driven intramolecular thermal/base-catalyzed dipolar [2 + 2] cycloaddition reactions either furnished the kinetically controlled products or directly formed the thermodynamically controlled rearranged products, respectively.

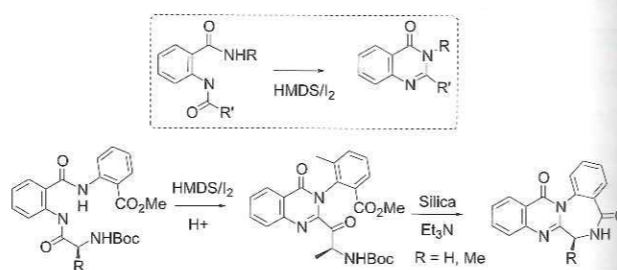


### Quinazolinone Alkaloids

Quinazolinones are an important class of compounds and a large number of natural and unnatural quinazolinone skeletons with a variety of substituents have been prepared via several synthetic strategies, owing to the wide range of biological activities that they possess.

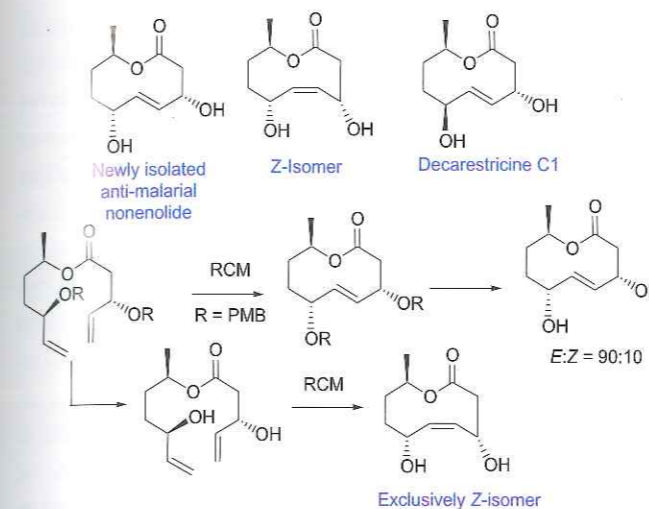


A simple and efficient general approach to various quinazolinone scaffolds, including peptidomimetic examples, has been demonstrated by employing HMDS/I<sub>2</sub> for the intramolecular dehydrative cyclization of diamides. The protecting groups Boc, Fmoc and Cbz tolerated the present reaction conditions and we did not observe any racemization. This protocol has also been used as a key step for the efficient four-step syntheses of the naturally occurring quinazolinones, sclerotigenin, (-)-circumdatin-F and (-)-fumiquinazoline-F.



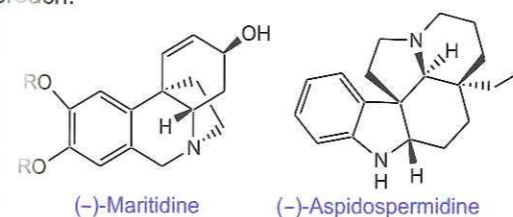
### Protecting group directed ring-closing metathesis (RCM): the first total synthesis of anti-malarial nonenolide

The first synthesis of a newly found naturally occurring anti-malarial nonenolide is described. A pivotal step in the synthesis is the ring-closing metathesis of a dienolic ester prepared by coupling an acid and alcohol that were stereoselectively synthesized from (*S*)- $\alpha$ -hydroxy- $\beta$ -butyrolactone and 1,2-*O*-isopropylidene-D-glycer-aldehyde, respectively.

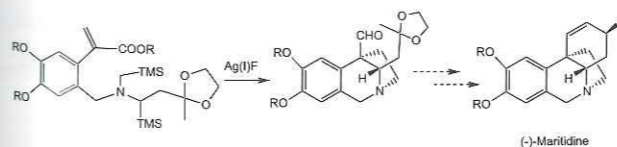


### A novel [3+2] cycloadditions of nonstabilized AMY strategy for the synthesis of architecturally complex alkaloids

The Crinine class of alkaloids like Maritidine, Oxomaritidine and Vittatine possessing immunostimulatory, cytotoxic and anti-cancer activities are being synthesized employing an intramolecular 1,3-dipolar cycloaddition of nonstabilized azomethine ylide (AMY) generated in situ by sequential double desilylation approach.

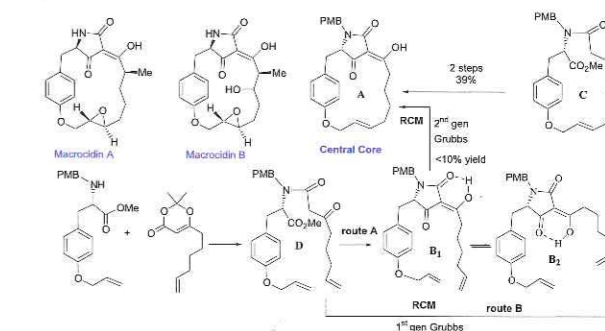


A new route for the synthesis of optically active indole alkaloid Aspidospermidine, having pentacyclic framework with quaternary and tertiary stereo centers from cheaply available starting material 2-bromopyridine developed, utilizing asymmetric birch reduction and intramolecular 1,3-dipolar [3+2] cycloaddition of nonstabilized AMY. An advanced intermediate of Aspidospermidine is under progress.



### Towards the total synthesis of macrocidines

Macrocidins A and B, the first representatives of a new family of cyclic tetramic acids, were recently isolated from the liquid cultures of *Phoma macrostoma* obtained from diseased Canada thistle growing in several geographically diverse regions. The novel macrocyclic skeleton and the relative configuration of macrocidines were determined by extensive 2D NMR and by a single crystal X-ray structure. Biological testing of purified samples against different types of herbs revealed that these compounds have significant herbicidal activity on broadleaf weeds but apparently not on grass weeds. The observed bleaching and stunting, primarily in the new growth of susceptible weeds led to conclude that the macrocidines were phloem mobile. The combination of interesting herbicidal activity and novel chemical structures makes the macrocidines attractive targets for synthesis.



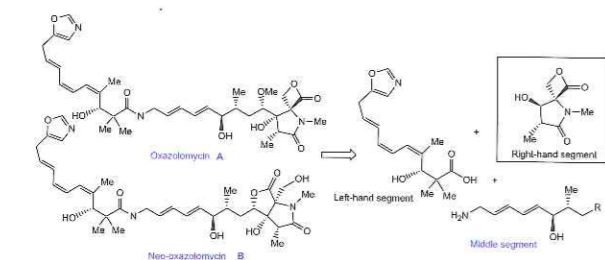
To this end we were able to construct the central carbon framework of macrocidines by employing RCM as the key reaction (route-B). Two different strategies viz route-A and route-B, which differ in order in which the critical structural elements the tetramic acid or the 18-membered macrocycle are formed, were executed. The major issue in case of route-A would be the effect of the tautomeric structures B<sub>1</sub> and B<sub>2</sub>. The tautomeric structure represented by B<sub>2</sub> could prevent the RCM reaction takes place. The surrogate of the epoxide present at C16-C17 of would be the *E*-double bond. A condensation of a tyrosine derivative and a substituted [1,3]dioxin-4-one to produce the key intermediate D. Lacey-Dieckmann cyclization was utilized to construct acyltetramic acid unit.

### Towards the total synthesis of oxazolomycin

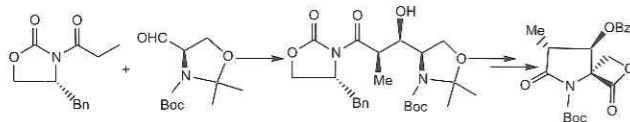
Oxazolomycin (A) and neooxazolomycin (B) which were isolated from the strain of *streptomyces* sp. KBFP-2025.



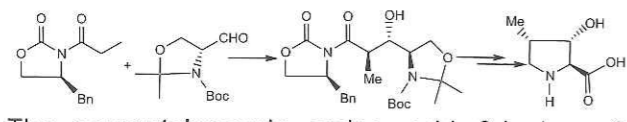
These drew initial attention for their strong antibacterial and anticancer activities. Later studies revealed their exceptional ability to suppress replication of vaccinia, herpes simplex virus type-1 and influenza A virus in both human and chicken cells. Unique structural features of oxazolomycin are a triene moiety (*Z,Z,E*) attached to an oxazole ring, a diene system (*E,E*) and a spiro-bicyclic  $\beta$ -lactone- $\delta$ -lactam subunit. Their fascinating biology allied with their structural complexity and novelty of the backbone has resulted in several groups dedicating efforts towards the synthesis of these molecules.



An effective synthetic strategy for construction of the novel spiro-bicyclic  $\beta$ -lactone- $\delta$ -lactam system present in oxazolomycin has been demonstrated. The 3,4-disubstituted pyrrolidine ring system was constructed via an Evans aldol reaction. The spiro  $\beta$ -lactone ring was elaborated from a *gem*-hydroxymethyl moiety that was successfully installed by an aldol followed by a crossed Cannizzaro reaction.



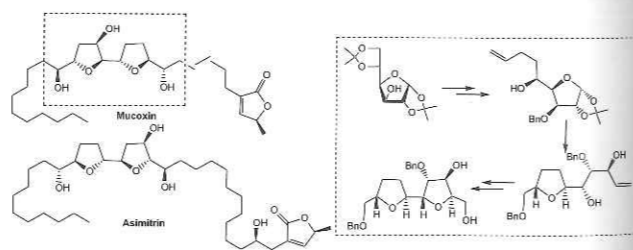
We have extended this approach with other isomeric Garner aldehyde and Evans auxiliary to provide general strategy for a short and efficient synthesis of 3-hydroxy-4-methylprolines (HMP) and its isomers.



The nonproteinogenic amino acid 3-hydroxy-4-methylproline (HMP) is an active constituent of some potent antimicrobials, echinocandins, nostopeptins, pneumocandins, spirofungin, and mulundocandins. A synthesis has been achieved in ten steps with 29% overall yield. The Evans' aldol reaction under Crimmins' modified method was pivotal to the success of the strategy.

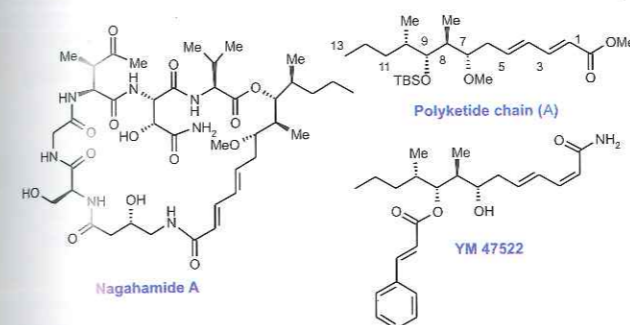
### Towards the total synthesis of annonaceous acetogenins

In recent years, the annonaceous acetogenins have been the focus of extensive synthetic efforts as a result of their remarkable range of biological properties such as antitumor, antiprotozoal, antifeedant, immunosuppressive, pesticidal, anthelmintic, and microbial. In particular, the 2,5-disubstituted bistetrahydrofuran (classical acetogenins) subgroup of this family has been found to inhibit the growth of human tumor cells at sub-micromolar levels. A large proportion of such compounds are also cytotoxic to tumor cells that are resistant to typical chemotherapeutic agents. Mucoxin A, a nonclassical acetogenin, is the first of its kind found to contain a trisubstituted hydroxylated tetrahydrofuran ring. Recently, asimitrin B a ring-hydroxylated unsymmetrical bis-tetrahydrofuran acetogenin was isolated from the seeds of *Asimina triloba*. This class of compound showed cytotoxic selectivity with 100-10,000 times the potency compared to the classical acetogenins. Because of their diverse array of biological activities and by virtue of their extremely limited availability in nature, these compounds have attracted the attention of synthetic organic chemists worldwide.

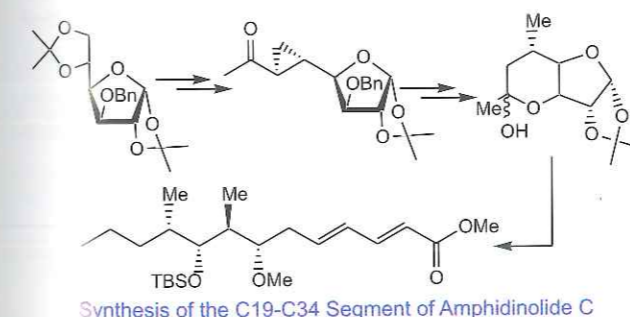


Stereocontrolled construction of the tetrahydrofuran unit plays a pivotal role in the total synthesis of Annonaceous acetogenins. Stereoselective intramolecular oxymercuration has been demonstrated as the key reaction for the efficient preparation of mono- and dihydroxylated unsymmetrical bis-tetrahydrofuran skeletons present in naturally occurring biologically active acetogenins using carbohydrates. These *trans*- and *syn*-selective intramolecular oxymercurations were explored in an enantioselective synthesis of the bis-tetrahydrofuran skeleton of mucoxin.

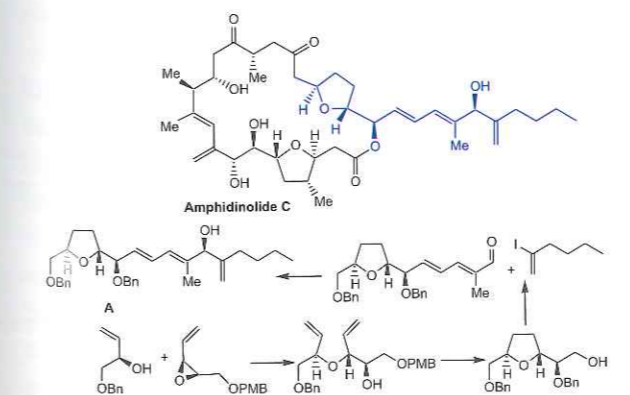
### Stereoselective synthesis of the polyketide chain of nagahamide A



A carbohydrate based approach for the enantioselective synthesis of the polyketide acid unit present in nagahamide A has been reported. Reductive ring opening of a chiral cyclopropane ketone group to enantioselectively install the methyl and propyl groups, is a salient feature of this synthesis.



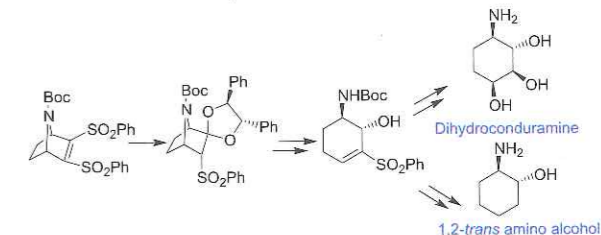
The synthesis of the C19-C34 segment of amphidinolide C is described. The key steps include the Mioskowski's Lewis acid catalyzed epoxide opening with the alcohol, ring closing metathesis, Wittig reaction, and Nozaki-Hiyama-Kishi coupling reaction.



### 4.3 NEW METHODS

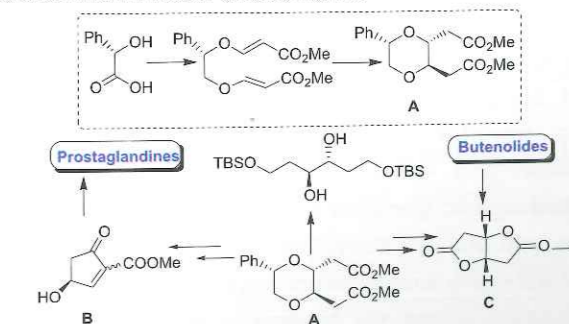
#### Asymmetric desymmetrization: An efficient way of making enantiopure scaffolds

Conduramines are purely synthetic aminocyclohexanetriol which shows significant glycosidase inhibitory activity and constitutes aglycon portions of the therapeutically useful aminoglycoside antibiotic. The development of an efficient methodology for the asymmetric synthesis of aminocyclitols is highly demanding and challenging. The asymmetric desymmetrization protocol leads the formation of enantiopure azabicyclo [2.2.1] heptane skeleton which undergoes base triggered anionic fragmentation to generate cyclohexenoid moiety which on further synthetic manipulation gives the asymmetric 1,2-aminoalcohol and dihydroconduramine.



#### Synthesis of multitailed designer substrate for biologically active natural products.

A multitailed synthon with unique structural features is synthesized from chiral 6-phenyl-2,3-bis(methoxymethyl)carbonyl-[1,4]-dioxane. Simple functional group manipulations to synthesize a variety of biologically active natural product intermediates such as prostaglandin, butenolide and  $C_2$ -symmetric *trans*-1,2-diol as shown below are achieved.

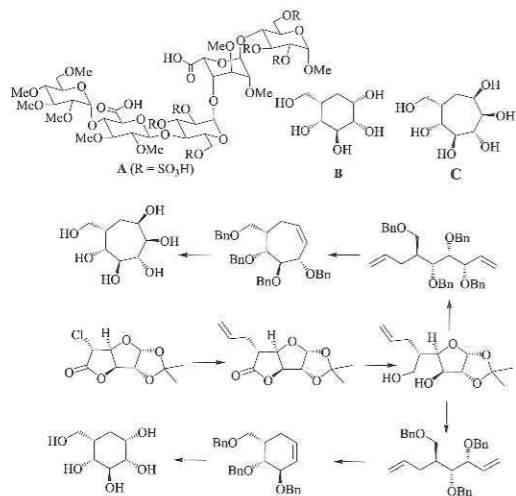


L-Iduronic acid, one of the L-sugar available naturally, is the major component of three glycosaminoglycans heparin, heparan sulfate, and dermatan sulfate. It has been already well established that low molecular weight heparin analogues (A) are better



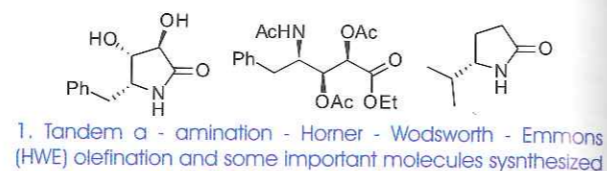
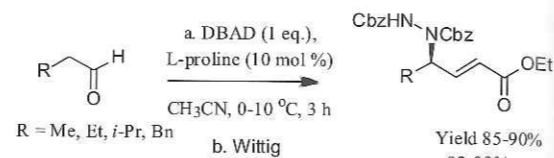


anti-coagulants when compared to the heparin polymer that is in market for several decades. The flexibility of the pyranose ring of L-iduronic acid to adopt either a chair  ${}^4C_1$  or a  ${}^2S_0$  skew boat conformation has been accentuated as a critical factor in the biology of heparin. This established importance of conformationally flexible L-iduronic acid analogues, taken together with the fact that carba-analogues of the sugars (carba- or pseudo-sugars) are metabolically more stable and conformationally more flexible compared to their corresponding oxygen analogues, we have designed a project dealing with the synthesis of carba-L-iduronic acid (with varying ring size) containing methylated anti-factor Xa pentasaccharide analogues. In this context, we recently described a flexible method for the synthesis of L-ido-configured carbacycles **B** and **C** using ring closing metathesis (RCM) as the key reaction.

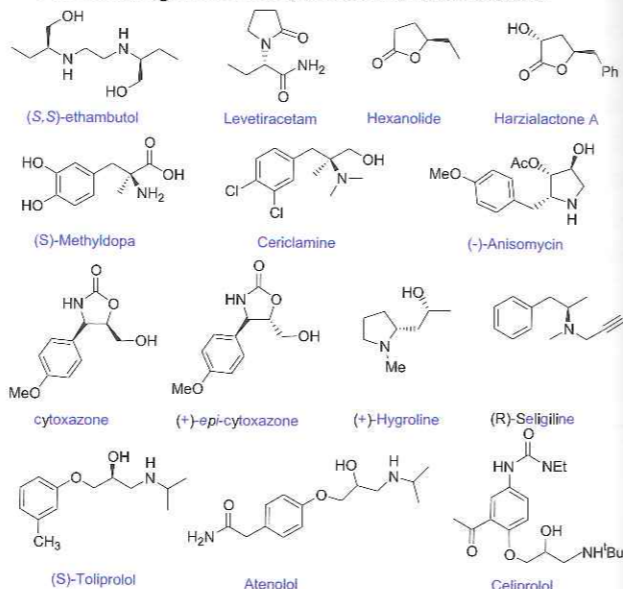


### Organo Catalysis

Asymmetric synthesis of bioactive molecules using organo catalysts and development of novel water soluble metal complexes as catalysts for organic functional group transformations. Proline-catalyzed direct amination and  $\alpha$ -aminoxylation of  $\alpha$  aldehydes is a valuable organic transformation for the synthesis of  $\alpha$ -amino acid and diol derivatives. We have developed a novel and highly enantio selective synthesis of  $\delta$ -amino  $\alpha$  unsaturated esters *via* tandem  $\alpha$ -amination-Horner-Wodsworth-Emmons (HWE) olefination of aldehydes. This novel methodology was successfully applied to the synthesis of biologically important intermediates pyrrolidone, triacetoxo aminodiols and (S)-5-isopropylpyrrolidin-2-one.



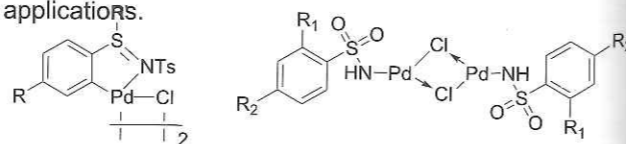
We have also used proline-catalyzed direct  $\alpha$ -amination and  $\alpha$ -aminoxylation of aldehydes for the synthesis of several drug molecules, which are listed below.



Drug molecules synthesized using proline catalyzed  $\alpha$ -functionalization

### Synthesis of DAB using palladium catalyzed homocoupling

We have synthesized a variety of novel palladacycles and palladium complexes for C-C bond formation reaction like Heck, Suzuki and Sonogashira coupling. These palladium complexes are used for the synthesis of PBI monomer which is used as monomer in the Fuel Cell applications.



R = H; R' = Me; 66%  
R = H; R' = CH(CH<sub>3</sub>)<sub>2</sub>; 70%  
R = Me; R' = Me; 60%  
R = Me; R' = Bn; 55%

Palladacycles

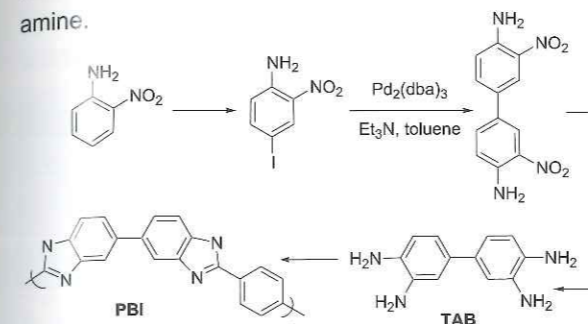
R<sub>1</sub> = H; R<sub>2</sub> = CH<sub>3</sub>; 82%  
R<sub>1</sub> = H; R<sub>2</sub> = OCH<sub>3</sub>; 78%  
R<sub>1</sub> = H; R<sub>2</sub> = NH<sub>2</sub>; 76%  
R<sub>1</sub> = CH<sub>3</sub>; R<sub>2</sub> = CH<sub>3</sub>; 72%

Palladium complex

Structure of palladacycles and palladium complex

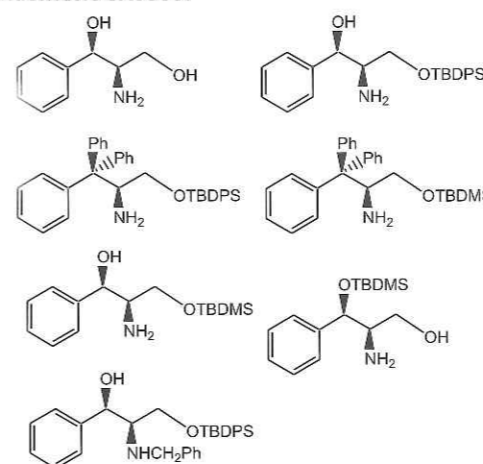


In connection with our ongoing program to prepare diamino benzidine (TAB) we envisioned the simple route i.e. Iodination of 2-nitroaniline and palladium catalyzed homocoupling followed by reduction of nitro group to amine.



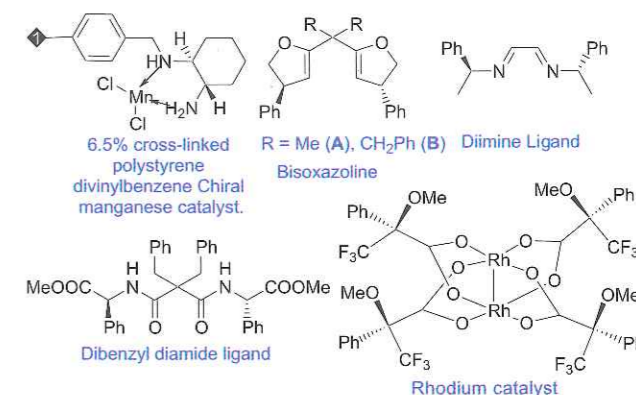
### Ligands for asymmetric catalysis

Six new chiral 1,2-amino alcohol derivatives have been synthesized starting from (1R,2R)-2-amino-1-phenylpropane-1,3-diol. Asymmetric reduction of aryl ketones with in-situ generated oxazaborolidine from these amino alcohol derivatives and BH<sub>3</sub>·Me<sub>2</sub>S afforded secondary alcohols with good yield and moderate to high enantiomeric excess.



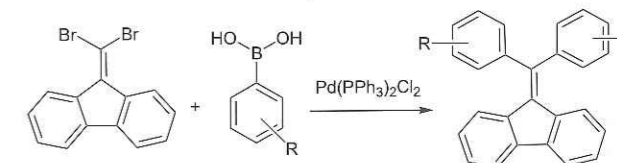
### Ligands/catalysts for the asymmetric aziridination of methyl methacrylate

Naturally occurring alkaloids like cinchonine, quinine, ephedrine etc have been applied as homogeneous / heterogeneous ligands/catalysts. Upto 40% ee has been achieved with cinchonine (homogenized *insitu*). Evans bisoxazoline (A) gave 20% ee in the asymmetric aziridination. Further work with the new bisoxazoline (B) and other ligands/catalyst is in progress to achieve a target of > 75% ee in the asymmetric aziridination of methyl methacrylate.



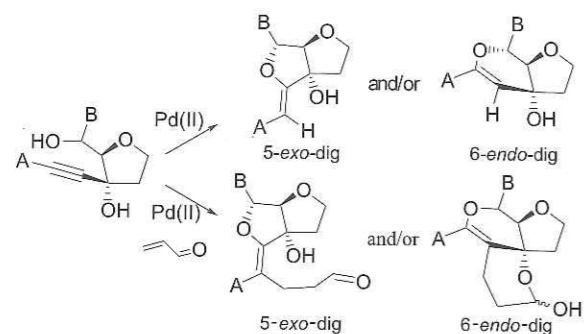
### A double-suzuki approach for synthesis of diarylmethylidene fluorene derivatives

There is a great current interest in the chemistry of fluorenes and its polymers as electroluminescent compositions, and the alkylidene fluorine liquid crystalline semiconducting polymers as organic field effect transistor devices. Diarylmethylidene fluorenes in general and the dications<sup>3</sup> or radical anions derived from them in particular are subject of extensive physical studies related to antiaromaticity or electron spin distribution-conformation evaluated by means of either *magnetic* criteria focusing on the consequences of the existence of a ring current or ESR and ENDOR spectra. While there appears to be a great deal of discussion about the derived transient intermediates by theoretical and experimental calculations, however a little has been focused on the synthesis of these diarylmethylidene fluorene derivatives.



### Palladium mediated cycloisomerization of sugar alkynols: synthesis of cyclic enol-ethers and spiroketals

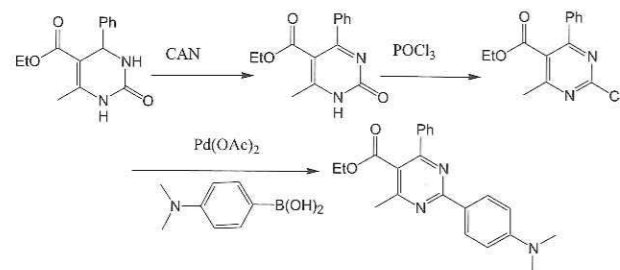
Functionalized bicyclic enol-ethers and spiroketals are prepared by Pd catalyzed cycloisomerization of 3-C-alkynylfuranosyl derivatives. Cycloisomerization of differently substituted alkyne derivatives revealed a preference for 6-*endo*-dig cyclization over 5-*exo*-dig, if the substituent is not sufficiently electron withdrawing.



Pd mediated cycloisomerization and subsequent conjugate addition

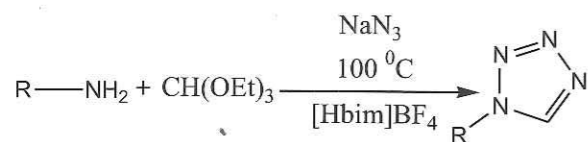
### Efficient synthesis of tetrasubstituted pyrimidines

The combination of a multicomponent reaction followed by an intermolecular carbon-carbon bond formation reaction generates heterocycles of significant molecular complexity in just a minimum number of steps, which by other routes are difficult to synthesize. In the same vein, an efficient regioselective approach to the synthesis of tetrasubstituted pyrimidines was developed by sequential functionalization of the easily available Biginelli 3,4-dihydropyrimidine-2(H)-one via dehydrogenation, chlorination followed by palladium catalyzed Suzuki cross-coupling reaction.



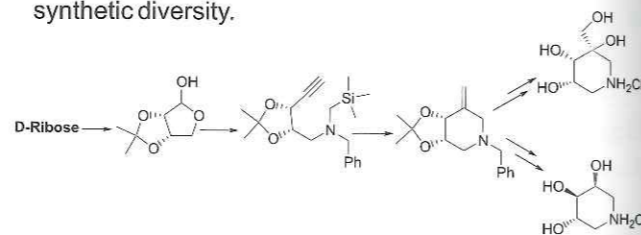
Efficient and rapid synthesis of 1-substituted-1H-1,2,3,4-tetrazoles in the liquid 1-n butylimidazolium tetrafluoroborate

A mild, convenient, and efficient protocol for the synthesis of 1-substituted-1H-1,2,3,4-tetrazoles was developed via the condensation of amines, triethyl orthoformate, and sodium azide using a RTIL as a recyclable medium as well as a promoter. The process gave rise to excellent isolated yields of 1-substituted-1H-1,2,3,4-tetrazoles in short reaction times (15-35 min).

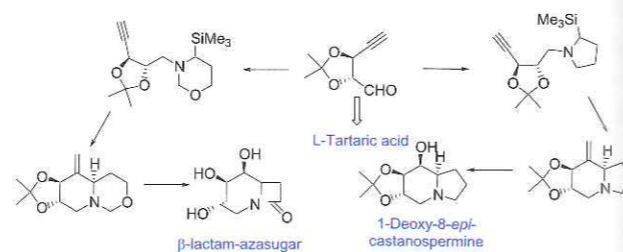


### 4.4 ORGANIC BIOMOLECULAR CHEMISTRY Design and synthesis of Glycosidase inhibitors

Polyhydroxyazasugars are potent drugs for HIV, cancer, influenza and other diseases because of their glycosidase inhibitory activity. Development of synthetic strategy for these inhibitors is an important challenge and needful. These inhibitors and their analogues have been synthesized by employing a novel and innovative method by the generation of amine radical cation, followed cyclization to electronrich multiple bond. The olefin functionality generated was utilized to create synthetic diversity.

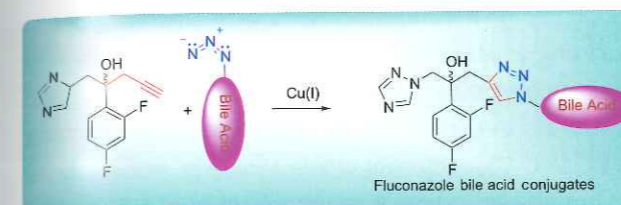


$\beta$ -lactam-azasugar hybrid molecules as referred polyhydroxylated carbacephem, function as a potent glycosidase inhibitor due to its conformationally constrained structural features,  $\beta$ -lactam ring compelling the polyhydroxylated piperidine ring to adopt a nearly half-chair conformation mimicking the shape of the glycosidase inhibition transition state, and carbonyl group in the  $\beta$ -lactam ring may provide an additional hydrogen bonding site for specific enzyme-substrate interactions. The 1-Deoxy-8-*epi*-castanospermine exhibited a non-specific competitive inhibition against galactosidase, and glucosidase. In these context, the diverse array of polyhydroxyazasugars and  $\beta$ -lactam-azasugars have been synthesized by employing the amine radical cation cyclization to alkyne, followed by olefin functionalization as shown below.

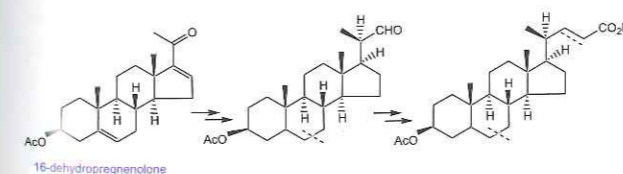


### Fluconazole bile acid conjugates

Novel fluconazole/bile acid conjugates were designed and their regioselective synthesis was achieved in very high yield via Cu(I) catalyzed intermolecular 1,3-dipolar cycloaddition. These new molecules showed good antifungal activity against *Candida* species.



A stereoselective total synthesis of naturally occurring 20-*epi* cholanolic acid derivatives has been realized, starting from readily available 16-dehydropregnenolone acetate. The key step of these syntheses involves an ionic hydrogenation of a C-20,22-ketene dithioacetal and deoxygenation of steroidal C-20 tert-alcohols, to set up the unnatural C(20R) configuration with 100% stereoselectivity. The unnatural C-22 aldehydes with C(20R) stereocenters thus obtained were elaborated to 20-*epi* cholanolic acid derivatives. Two derivatives of 20-*epi* cholanolic acid were synthesized and their structures have been confirmed by single crystal X-ray analysis. Catalytic hydrogenation of 16-dehydropregnenolone acetate and 16-dehydropregnenolone in ethanol affords C-5, C-16 tetrahydro products. Crystal structure analysis of one of these products revealed C-5 $\alpha$  and C-17 $\alpha$  configurations of the hydrogen atoms.



### Peptide nucleic acids

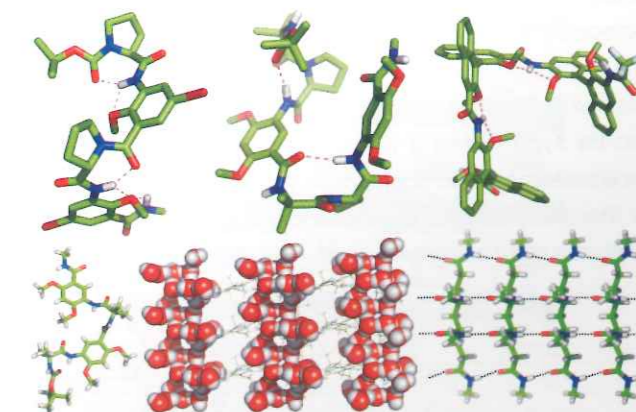
Our efforts to synthesize and evaluate nucleic acid mimics for biological applications resulted in a thioacetamido nucleic acid (TANA) backbone. The sugar-phosphate backbone in the nucleic acids was replaced by uncharged, 5-atom PNA like thioacetamido-sugar backbone. The backbone retains the 3'-5' directionality of natural nucleic acids. The pyrimidine-TANA oligomers were found to sequence specifically recognize and bind complementary RNA sequences. The binding was as strong as PNA:RNA oligomers. The

TANA was not found to be useful in mixed PNA-TANA backbone and destabilized the complexes. This is an important step forward in finding the ideal combination of backbone and nucleobases to afford antisense molecules that bind strongly and sequence specifically to complementary RNA.

The TANA backbone was further exploited in mixed DNA-TANA backbone sequences and it was found that the propensity to discriminate the DNA versus RNA backbone for binding selectivity. This new backbone confirms a postulation that analogs with longer internucleoside linkage, compared to DNA/RNA, can pair stably with them and the mixed backbone phosphate-/thioacetamido-linked oligonucleotides have ability to discriminate between DNA and RNA.

### Secondary structure mimicking through conformationally defined foldamers

The mystery of how a protein sequence specifies a unique structure and function has intrigued chemists leading to the design and development of foldamers, which are synthetic oligomers with a definite conformational backbone structure. The foldamer approach is being extensively utilized in generating diverse sets of structures which are able to mimic various protein secondary structure elements like  $\beta$ -turns, helices, and  $\beta$ -pleated sheets. The driving force for the enormous efforts and investigations expended in this area has been largely due to the possibility of achieving suitable templates for the design of biologically active molecules that would compete for a variety of protein-protein and protein-membrane interactions.



Foldamers with diverse structural architectures

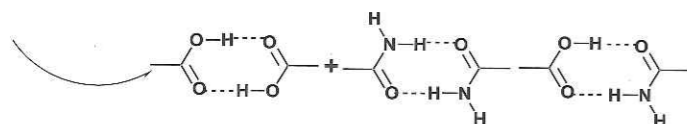


To extend the repertoire of foldamer design, we have recently suggested foldamers containing different residues of independent conformational preferences and backbones. For instance, we were able to design and develop foldamers that specifically stabilize various turn structures, in particular  $\beta$ - and  $\delta$ -turns, helices and pleated sheets. Further, we have also been able to develop new families of aromatic oligoamide foldamers based on binaphthol (BINOL) building blocks. It is demonstrated that the combination of inherently chiral aromatic building blocks provides a novel access to a wide variety of conformationally ordered synthetic oligomers with diverse and dazzling structural architectures, distinct from those classically observed. Such oligomers are expected to enormously extend the conformational space available for foldamer design which may provide considerable insights into the improved understanding of biopolymer structure, and function.

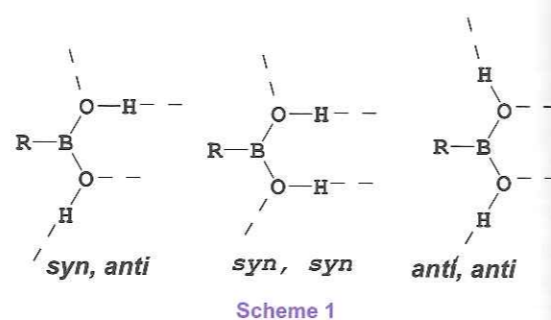
#### 4.5 SUPRAMOLECULAR CRYSTAL ENGINEERING

##### Crystals and/to co-crystals through noncovalent interactions

Crystallization, one of the popular strategies in organic synthesis to obtain compounds in pure form has become popular in recent times as a new methodology to prepare the molecular complexes with targeted structural features and tailor-made properties, due to the facile nature of noncovalent interactions such as hydrogen bonds that binds the molecules together in the complexes. In general, when a crystal is obtained, it would be considered as an assembly of millions of molecules that are being held together by interactions within the confined boundaries. As these interactions often exist in definite patterns, in principles, new patterns can be synthesized if the functional groups that yield such patterns are in conjunction to each other, favoured by thermodynamic and/or kinetic means. For example, synthesis of an acid-amide pattern is shown in scheme.

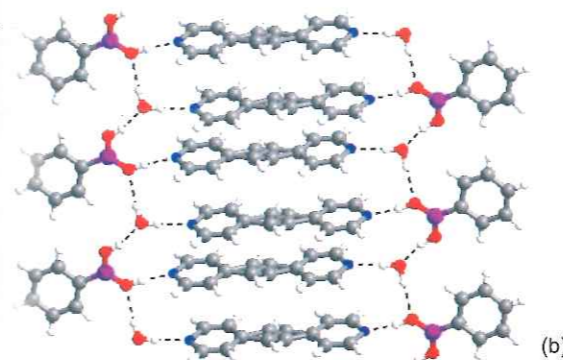
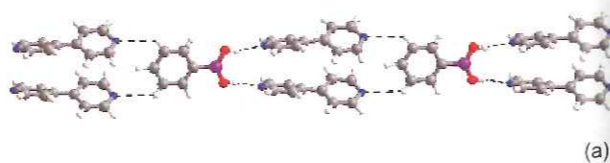


While the interplay of intermolecular interactions and patterns is a continuum exercise in the areas of supramolecular chemistry, thrust for new interactions and functional groups are at forefront to establish new patterns. In this connection, we have identified a new functionality, boronic acid, generally represented as  $B(OH)_2$  to be a flexible moiety to yield different types of patterns as shown in Scheme 1. Taking advantage of the importance of boronic acids in general organic synthesis through such as Suzuki coupling reactions and also the potential applications in the areas of pharmaceutical and material industry in the form of drugs, fire-retardants etc., we have focused to utilize this functionality in the preparation of numerous co-crystals and the salient features of these structures are described below.



##### Boronic Acids

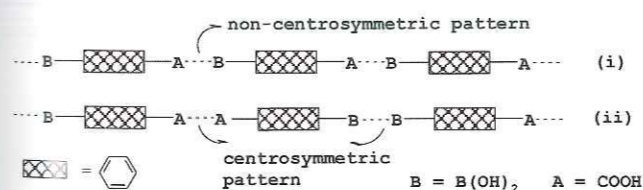
We have reported some molecular complexes of boronic acids, with aza donor compounds such as 4,4'-bipyridine, 1,2-bis(4-pyridyl)ethane, 1,2-bis(4-pyridyl)ethene etc. formed exclusively due to the  $O-H \cdots N$  hydrogen bonds, exemplifying the ability of the  $B(OH)_2$  moiety to form those bonds like  $COOH$  and  $OH$  groups. For example, formation of different type of networks with change of aza-donor compounds is shown in figure.



Supramolecular assembly formed by phenylboronic with (a) 4,4'-bipyridine and (b) 1,2-bis(4-pyridyl)ethene.

From these experiments and also from the crystal structure determination of various boronic acids done by others, it is clearly understood that  $B(OH)_2$  moiety adopts mainly three different types of conformations, as shown in Scheme 1, which yield different hydrogen bonding networks. Among these arrangements, while *syn-anti* conformation is observed in a majority of structures, the *syn-syn* and *anti-anti* are relatively uncommon.

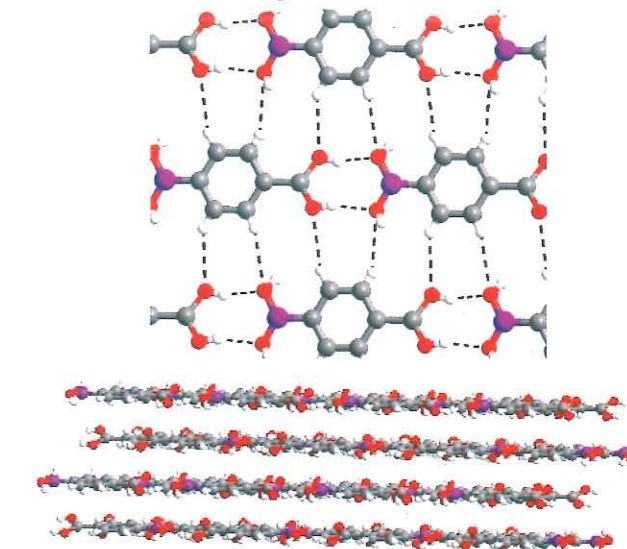
##### Non-centrosymmetric structure(s) through boronic acids



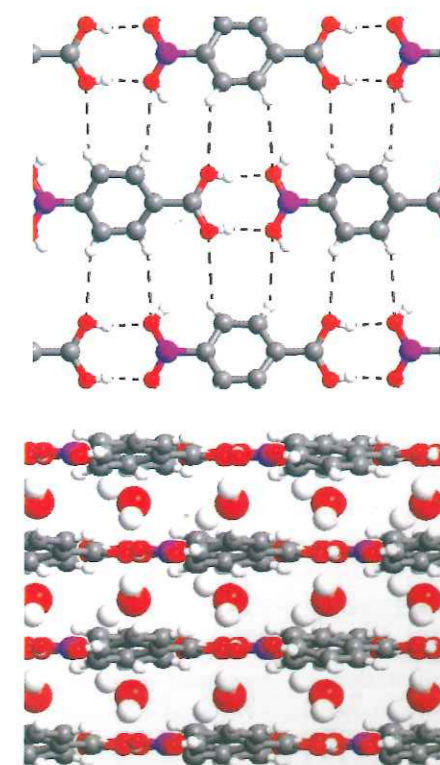
Scheme 2

Following the sequence depicted in above Scheme, 4-carboxyphenylboronic acid has been crystallized to obtain the desired non-centrosymmetric structure, but we realized such structure only in hydrate form obtained by crystallization from methanol. Otherwise, anhydrous form or another hydrate obtained from 2-propanol gave only centrosymmetric structures. In the anhydrous and monohydrate structures, the H-atoms on the  $B(OH)_2$  functional group exists in *syn-syn* conformation, but *syn-anti* conformation was found in the quarter-hydrate structure. In addition, while the two former structures establish interaction between  $B(OH)_2$  and  $COOH$  groups (*heteromeric*), *homomeric* interaction of the functional groups ( $COOH \cdots COOH$  and

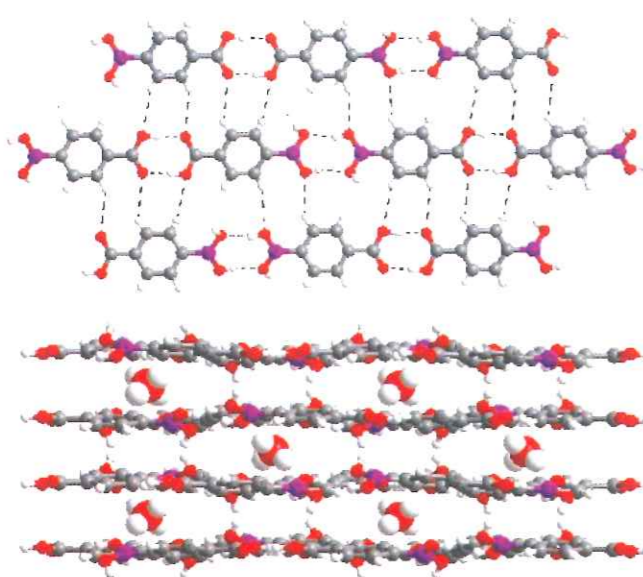
$B(OH)_2 \cdots B(OH)_2$ ) was observed in the latter structure (quarter-hydrate). The packing diagrams for all these structures are shown figures below.



(top) Molecular arrangement of a typical layer in the crystal structure of anhydrous 4-carboxyphenylboronic acid. (bottom) Stacking of layers in the three-dimensional crystal lattice.



(top) Two-dimensional arrangement of boronic acid molecules in the crystal lattice of monohydrate of 4-carboxyphenylboronic acid. (bottom) Three-dimensional arrangement of the molecular sheets with water molecules inserted between the sheets.

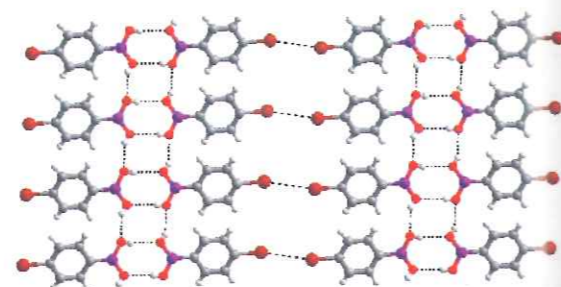
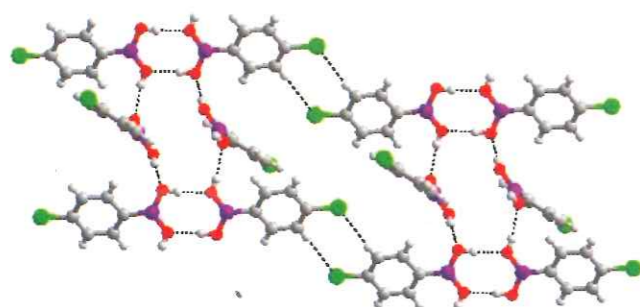


Packing of molecules in quarter-hydrate structure of 4-carboxyphenylboronic acid.

#### Supramolecular architecture in some 4-halophenylboronic acids

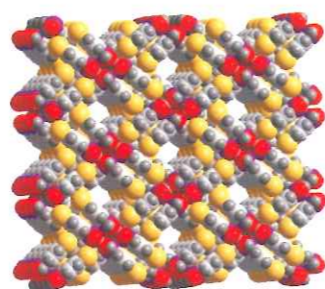
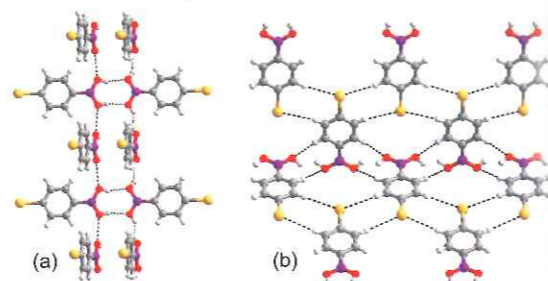
In continuation of further exploration of structural features of boronic acids, crystal structures of 4-chloro, 4-bromophenylboronic acids and hydrates of latter and 4-iodophenylboronic acid in two different forms that were characterized by single crystal X-ray diffraction methods have been reported.

In the anhydrous structures 4-chloro and 4-bromo derivatives, while the  $B(OH)_2$  forms *syn-anti* conformation, it exists in *syn-syn* as well as *anti-anti* conformations in the hydrated structures of 4-bromo and 4-iodo derivatives. In all the structures, the molecules are held together by  $O-H\cdots O$  interactions formed by  $B(OH)_2$  groups. The  $C-H\cdots X$  ( $X = Cl, Br$  and  $I$ ) interactions play an important role in crystal packing. In addition, in bromo derivative,  $Br\cdots Br$  interactions are also observed. These features are shown in figure.



Arrangement of molecules in the crystal structures of 4-chlorophenylboronic acid (left) and 4-bromophenylboronic acid (right) showing the interactions formed by  $B(OH)_2$  groups and also halogens.

Interestingly, all the hydrates, form similar types of three-dimensional structures with the formation of channels, being occupied by water molecules. The two hydrates of 4-iodophenylboronic acid are distinguishable on the basis of  $O\cdots O$  short contacts, with an identical host lattice of the boronic acid. The arrangement of molecules in a and b are shown in figures c.

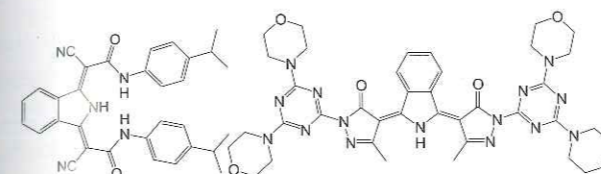


Arrangement of molecules in the water adducts. Typical intermolecular interactions are shown for the structure of 4-iodophenylboronic acid in its two hydrate forms (a) and (b). In (c), the channels observed in both the structures is shown.

#### 4.6 NEARIR COLORANTS

##### Novel weatherable colorants for polycarbonates

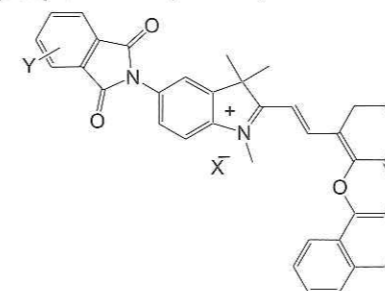
The following novel weatherable colorants for polycarbonates based on 1,3-bisindolines were synthesized.



After ascertaining their thermal stability by thermo gravimetric analysis, the colorants are being tested in-polymer.

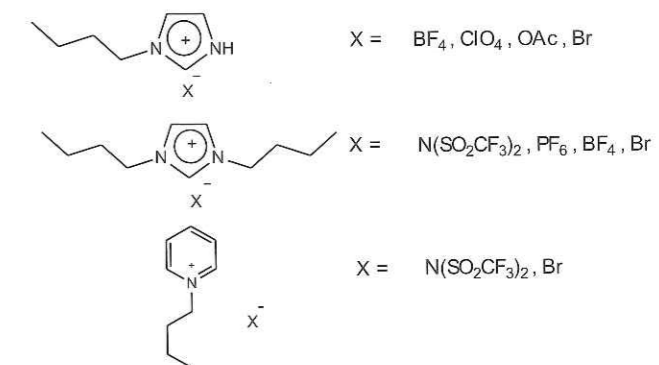
##### Near IR colorants for polycarbonates

Near IR colorants are those chromophores which show significant absorption in the near infrared region ranging from 650-900 nm. The near IR is a region in which sun light poses around 50% of its radiation intensity. Broad band infrared absorbers function as efficient hat ray blocking agents e.g. in car wind screens, architectural glasses and agricultural films. These chromophores also convert IR radiation in to heat for thermal imaging and optical data storage. For these two applications there is a need for commercial NIR dyes with improved photo stability. At NCL, we have synthesized some novel NIR colorants as shown below with good stability for application to plastics. They are based on trimethine cyanine group of chromophoric systems.



Design of ionic liquids as neoteric solvents for selective sorption of  $CO_2$  from gaseous streams

Anthropogenic emission of  $CO_2$  may cause significant climate change. To mitigate this,  $CO_2$  sequestration approach is being widely pursued. Efficient separation of  $CO_2$  is a key to the economically viable sequestration efforts. Ionic liquids (ILs) are neoteric solvents which have high  $CO_2$  sorption capacity in comparison to other gases. The properties of the ILs have been tuned for improving  $CO_2$  sorption capacity while designing the structure of cations followed by metathesis with appropriate anions. A variety of ILs with varying anions and cations have been synthesized for  $CO_2$  for sorption/desorption studies. Some examples are shown below.



##### Development and commercialization of bioactive substances from plant sources

Under this CSIR Co-ordinated Programme extracts and formulations prepared from plant species, which are used in the Traditional Systems of Medicines have been evaluated for the development of new drugs, pest control agents, Herbal Drugs and Botanical pesticides. Some of the promising leads obtained are being followed for the identification of active principle(s).

##### Development of microbicides for protection against human immuno-deficiency virus (HIV) infection

Under this collaborative programme work towards the development of microbicides from indigenous biomaterials for protection against Human Immuno-deficiency virus (HIV) infection has been initiated. The developed products will be taken up for pre-clinical studies which will be followed by clinical studied.

##### Identification of lead molecules for the development anti-viral, tuberculostatic, anti-malarial and immuno-modulatory drugs

This collaborative programme is being initiated for the development anti-viral, tuberculostatic, anti-malarial and immuno-modulatory drugs. Under this programme the secondary metabolites isolated from medicinal plants with Ethnopharmacological background. These molecules will be assayed for different enzyme and whole cell assays and the leads obtained will be taken up for further drug development studies.



## 5 PHYSICAL AND MATERIALS CHEMISTRY

## 5.1 THEORETICAL CHEMISTRY

## 5.1.1 Multi-reference coupled-cluster response properties

Fock space response theory developed at NCL has now been coded to evaluate electric dipole moments, polarizability of open shell radicals and excited states. These are the first results of such properties of the radicals and excited states using completely extensive and state-of-the-art multi-reference coupled-cluster theory. For the open shell radicals, one valence model space was used and for low-lying excited states, one valence hole-particle model space was used in the Fock space framework. Molecules used as test examples are: CO, HF, OH, OOH, HCOO, NO etc. In addition, codes for magnetic properties, like susceptibilities have been undertaken in this period using gauge-independent atomic orbital (GIAO) basis. This activity is still currently on-going.

## 5.1.2 Density functional response method for molecular properties

A computationally viable alternative to fully analytic response for Kohn-Sham density functional theory is getting developed. This will be used to calculate properties based on quadrupole moment. The change of properties with the cluster size of sodium atoms and the substituents in *p*-nitro aniline derivatives has been studied.

## 5.1.3 Study of reactivity descriptors using normalized Fukui functions and Bond-deformation kernel

A study based development on bond-deformation kernel using the concept of normalized Fukui functions is appropriate to take care of systems with differing size. Thus these descriptors are being tested which were introduced at NCL last year for inter-molecular reactivity and were introduced for study of interaction-induced OH shift.

## 5.1.4. Application of reactivity descriptors

Local reactivity descriptors, such as the condensed local softness and Fukui function, have been employed to investigate the inter-cluster reactivity of the metalloaromatic ( $\text{Al}_4\text{Li}$  and  $\text{Al}_4\text{Na}$ ) and anti-aromatic

( $\text{Al}_4\text{Li}_4$  and  $\text{Al}_4\text{Na}_4$ ) compounds and characterize the strength of the nucleophilicity of the  $\text{Al}_4$  unit in these compounds. Analysis shows that the  $\text{Al}_4$  unit of the  $\text{Al}_4\text{Li}$  cluster has the highest nucleophilicity compared to the other clusters. Hence, it is believed that the formation of the  $\text{Al}_4\text{Li}(-)$  type of metalloaromatic clusters would be responsible for the increase in the efficiency of the electron injection of the Al-Li cathode.

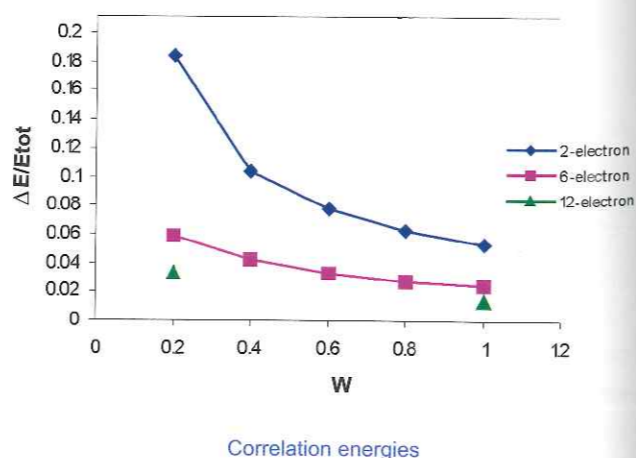
The effect of electric field on local reactivity descriptors, e.g. Fukui functions as well as global descriptors, such as softness, hardness etc. of diatomic molecules has been systematically studied. The analysis of the results has been based on the relative electro-negativities of atoms.

## 5.1.5 Development of principle of minimum magnetizability

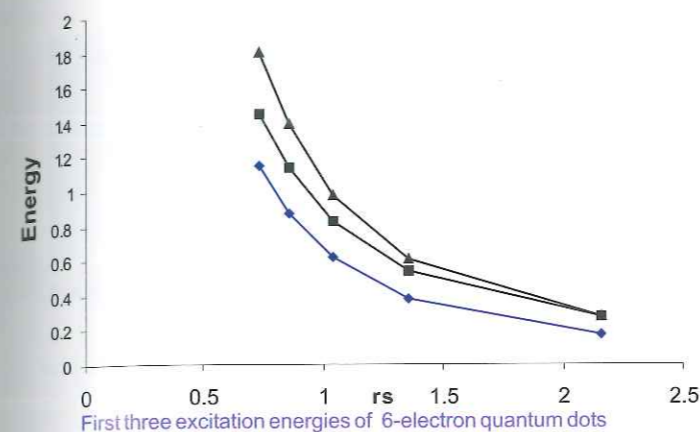
In line with the principle of electric polarizability, a principle of minimum magnetizability has been shown. This relates to stability of systems based on the minimum magnetizability for cases, like asymmetric stretch. It has been shown using water as an example, that mainly paramagnetic contribution plays a major role in this principle.

## 5.1.6. Quantum dots in spherical potential

Quantum dots have been of recent interest. Correlation energies, charge densities and first three low-lying excitation energies have been studied for 2, 6 and 12 electron quantum dots in spherical potential as a function of confining strengths using highly correlated coupled-cluster based theories.



Correlation energies

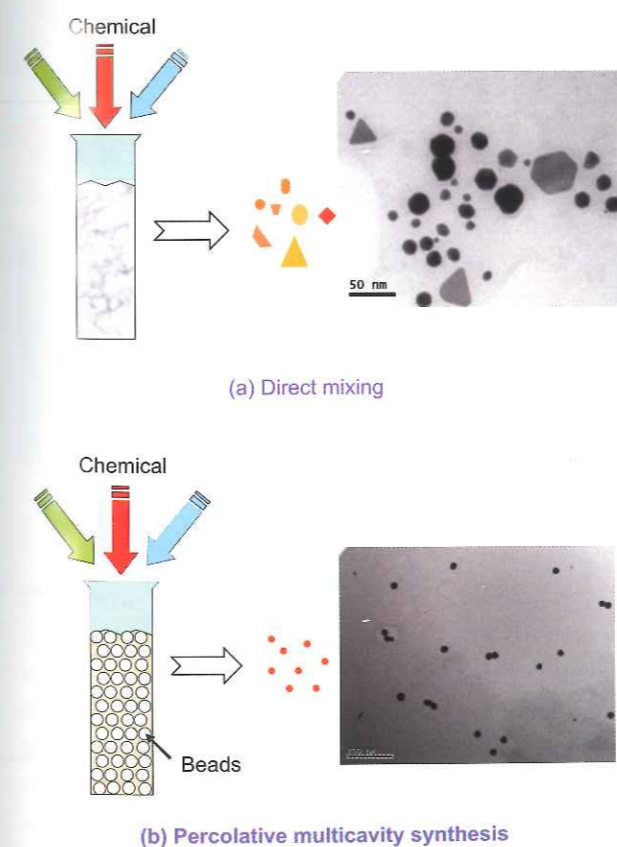


First three excitation energies of 6-electron quantum dots

## 5.2 NANOSCIENCE AND TECHNOLOGY

## 5.2.1 Percolative microcavity synthesis: A new way to control of nanosynthesis

By performing chemical or biological synthesis of gold nanoparticles (NPs) in granular medium instead of a free solution, result shows that monodispersed gold NPs can be realized and the size of NPs can also be controlled by controlling the granularity.

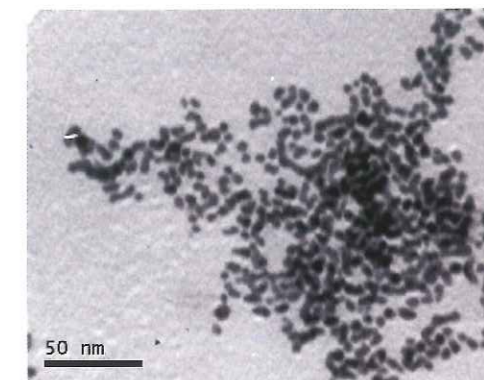


(a) Direct mixing

(b) Percolative multicavity synthesis

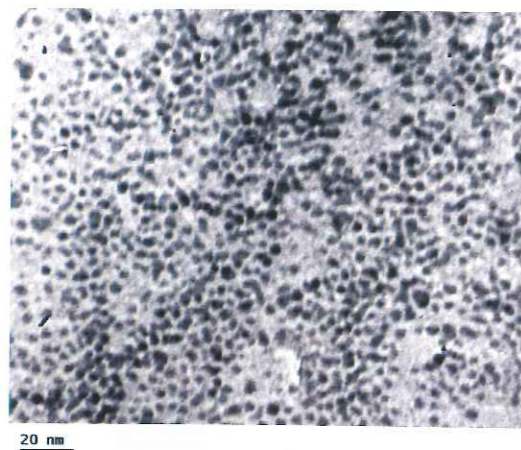
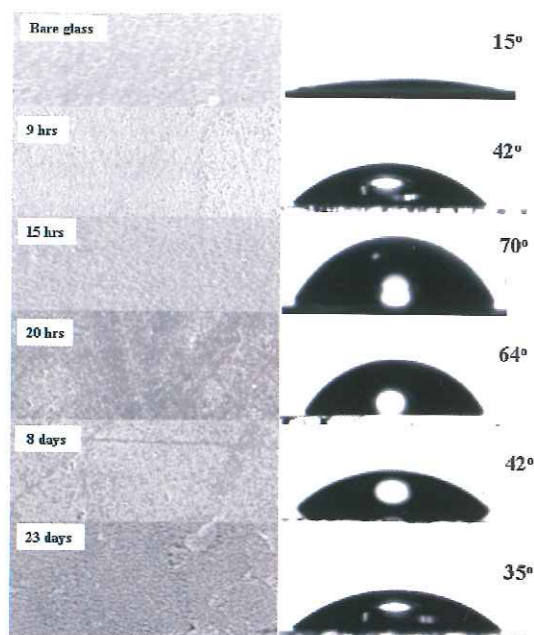
5.2.2 Fungal synthesis of chemically hard-to-synthesize ternary  $\text{CuAlO}_2$ 

The p-type transparent conducting oxide  $\text{CuAlO}_2$ , which is useful in many applications, is difficult to synthesize chemically without a direct or indirect use of high temperature due to the relative peculiar chemistry of Cu and Al. It is shown that a fungal process enables synthesis of ~4-5 nm nearly monodispersed nanoparticles of  $\beta\text{-CuAlO}_2$  just at 50 °C. The particles show blue luminescence.



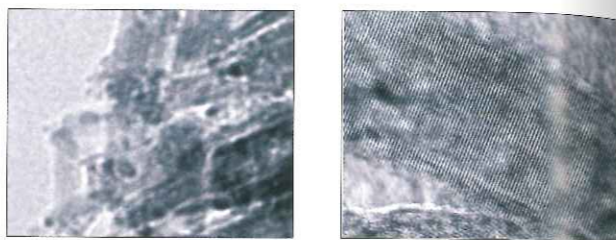
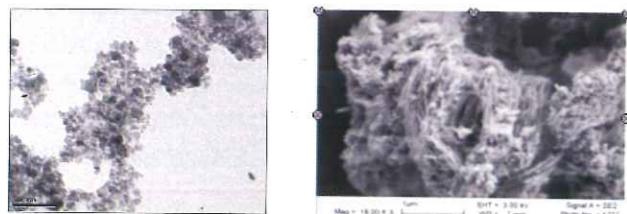
## 5.2.3 Silicate nanoparticles by fungal bioleaching of glass and surface bioactivation

Fungal processing of borosilicate glass is shown to lead to monodispersed silicate nanoparticles with boron inclusion. Interesting hierarchical morpho-chemical surface modification is also observed with implications for hydrophobicity and bio-activity. Fungal micellia grow easily on the processed surface.



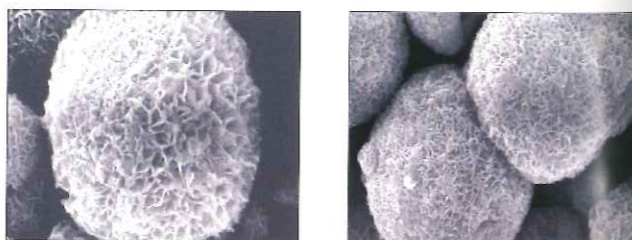
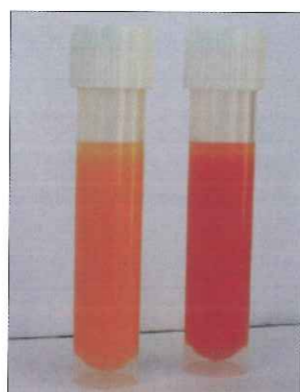
#### 5.2.4 Nanoparticles, nanowires and nanotubes of magnetite and maghemite

Nanoparticles, nanowires and nanotubes of different phases of iron oxide are synthesized by controlled low temperature hydrothermal synthesis using specific directing molecules. (This work was done in collaboration with Dr. Athavale of Pune University and Prof. Beatrice Hannoyer from Rouen, France).



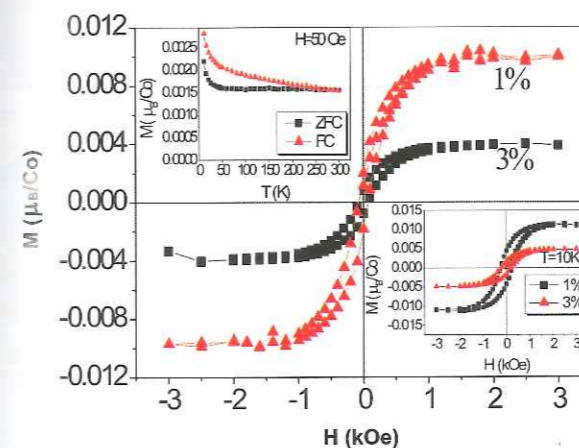
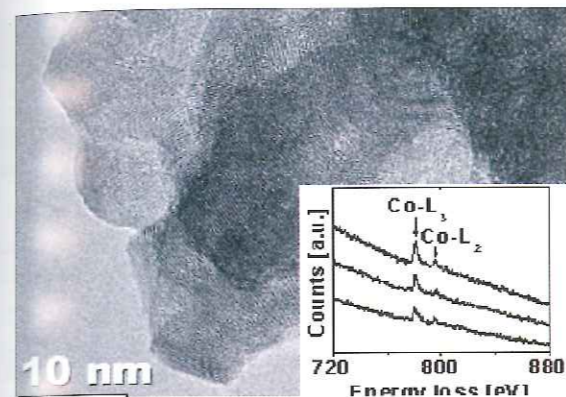
#### 5.2.5 Phase controlled synthesis of $\beta$ - $\text{In}_2\text{S}_3$ Dandelion flowers

Dandelion flower type morphology of  $\beta$ - $\text{In}_2\text{S}_3$  optical semiconductor in phase pure tetragonal or cubic forms is realized via microwave solvothermal synthesis using different reaction media. These phases exhibit interesting luminescence properties. (This work was done in collaboration with Dr. B. B. Kale, C-MET, Pune).



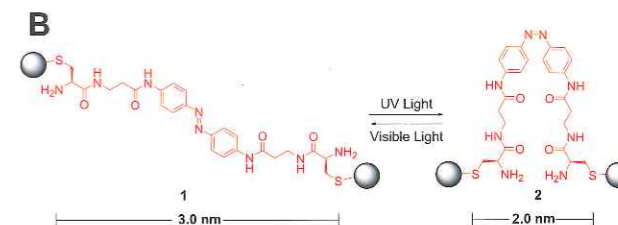
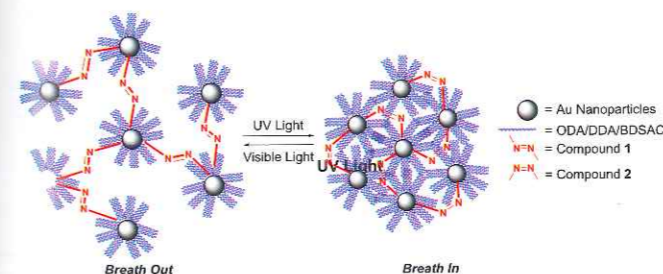
#### 5.2.6

Diluted magnetic semiconductor quantum dots of Co doped CdS are synthesized by high energy electron irradiation method. The structural, magnetic and optical properties of the quantum dots reveal that it is possible to dope nanoparticles with dopants with concurrent doping of defects without surface functionalization. (This work was done in collaboration with Prof. V. N. Boraskar, Pune University and Prof. G. P. Das, IACS, Kolkata).



A photo-responsive gold nanoparticle network was prepared earlier and was linked with ligands bearing azobenzene moieties. As a novel extension of this past work, ligands have been devised that can sense and phase transfer alkali metal ions in aqueous media to organic media. These approaches can find applications in sensors and drug delivery systems

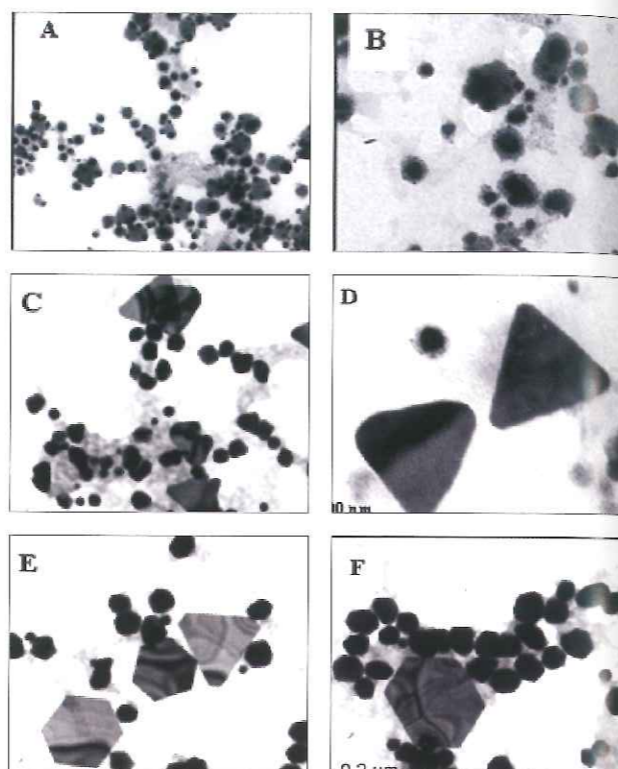
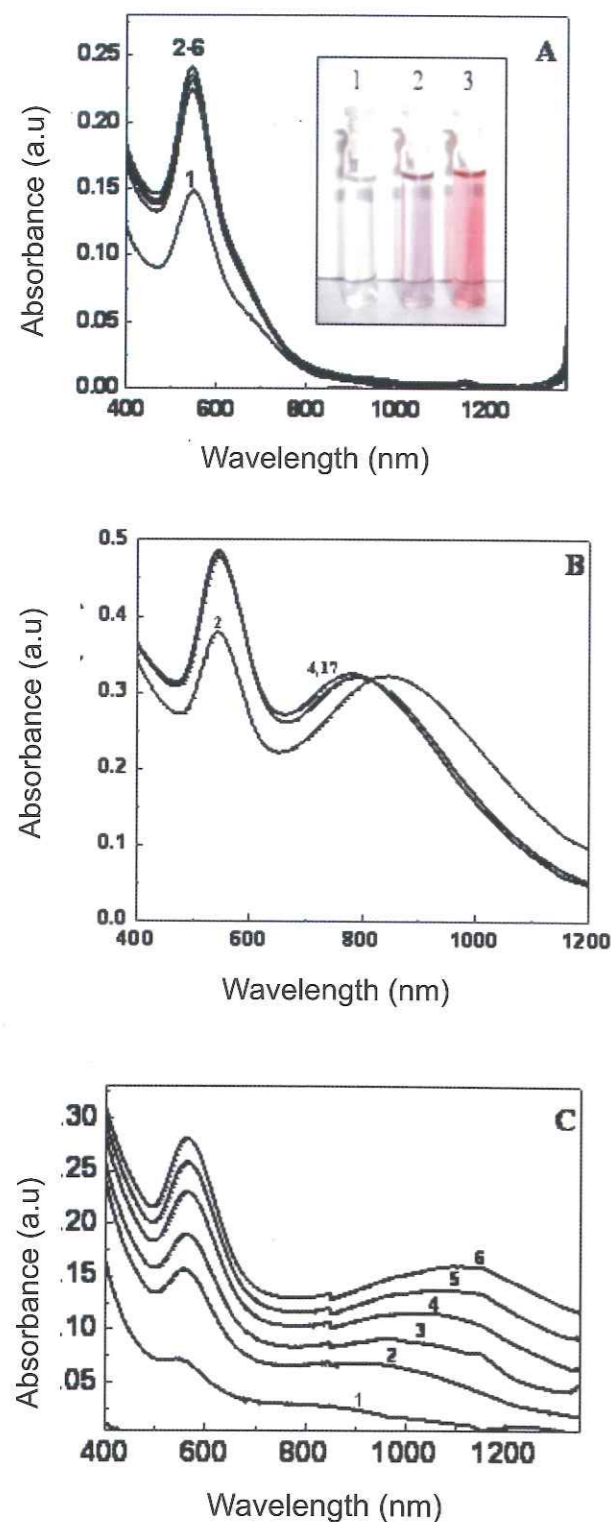
#### A



Photoresponsive and ion sensing gold nanoparticle networks

#### 5.2.8 Surface functionalization of metal nanoparticles using antibiotics for the biomedical applications

Binding gold nanoparticle surfaces with drug molecules is attractive for several biomedical applications which comes with full of challenges and opportunities of exploring new methods to bind the nanoparticle surfaces with small molecules such as drugs, proteins, genes, etc and to deliver them. So far, the processes of conjugating drug molecules, especially antibiotics, on metal nanoparticles remain a complex chemical synthesis involving multiple steps such as formation of metal nanoparticles, their surface modification and finally the capping of drug molecules. These challenges are overcome by demonstrating a single-pot synthesis route as well as conjugation of the antibiotics at the nanoparticle surfaces without the use of unwanted chemicals. Among several drug molecules, conjugation of a vast variety of antibiotics opens up a new field. This is especially interesting, as at present, this field is full of several challenges such as increasing the shelf-life of these drugs, enhancing the chemical stability (especially at room temperature), and enhancing bio-activity against different microorganisms. Usually, the amount in which the antibiotics are administered into the body is very high and efforts are undertaken to control their release (dose) and interaction with bacterial cells. Hence gold nanostructures in aqueous medium were synthesized by reducing gold ions using cephalaxin, a potent broad-spectrum antibiotic, where the morphology of the gold nanoparticles is found to be dependent on the concentration of chloroauric acid. The characterization techniques indicated that particle surfaces are coated with the robust layer of the antibiotic making them stable for a long time. Thus, cephalaxin acts as both reducing and capping agent. NMR and XPS analysis indicated that sulfur moiety is responsible for the reduction and binding process.



TEM of Au-nano particles with Au-ion concentration of  $10^{-4}$  M (top),  $2 \times 10^{-4}$  M (middle), and  $2 \times 10^{-4}$  M (bottom panel)

### 5.3 MATERIALS CHEMISTRY

#### 5.3.1 Mimicking superhydrophobic surfaces

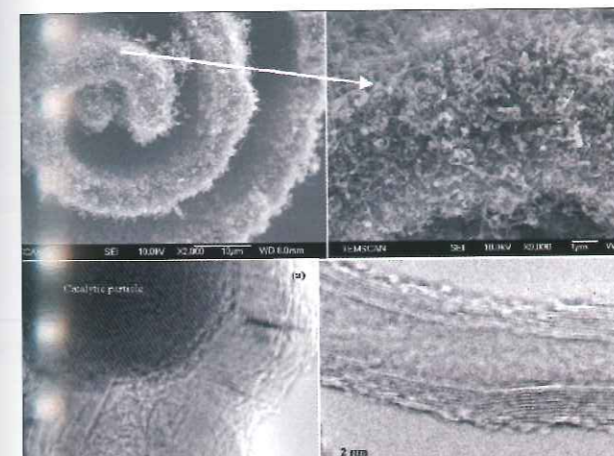
Various strategies to develop artificial superhydrophobic surfaces (analogous to lotus leaf) have attracted significant attention in recent time due to its fundamental relevance of molecular level manipulation of surface energy and consequent implications in commercial applications ranging from self-cleaning window glasses, paints, and fabrics to low-friction surfaces. Several recent studies of lotus leaf reveal that its waxy surface is made up of many micron-sized bumps that, in turn, are covered with nanoscale hair-like tubules responsible for the 'roll-off' action of water. Since SAMs can act like these nanoscale hair like structure both structurally and functionally, the utility of this approach was explored to design an artificial superhydrophobic surface. More specifically, the hydrophobicity of the silica nanoparticle (~100 nm) was tuned by surface functionalization using different self-assembled mono/multilayers of alkyltrichlorosilanes (silanization process). Silanization change both the surface chemical composition and the geometrical microstructure to generate hierarchical



structures, where the contact angle can be anywhere between  $60^\circ$  to  $168^\circ$ . These results indicate that superhydrophobic surfaces obtained by forming mixed mono/multilayer on the silica surface could be useful for many potential applications due to the low surface energy with enhanced thermal stability and tunable contact angle.

#### 5.3.2 Synthesis of high purity scrolled mats of MWNTs

Felt-like mats (6-7 mm thick) of highly pure (>98%) multiwalled carbon nanotubes (MWCNTs) wrapped into scrolls were synthesized by chemical vapor deposition from a toluene-ferrocene mixture using a temperature ramp from  $680^\circ\text{C}$  to  $550^\circ\text{C}$  in  $\text{H}_2$ -Ar atmosphere.

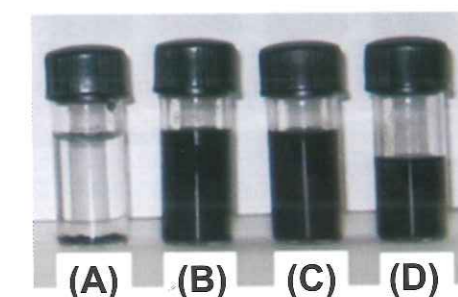
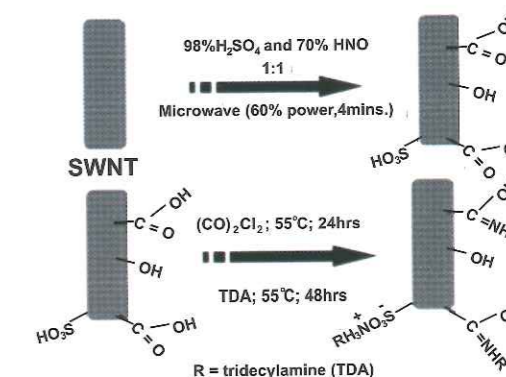


Scrolled mats of MWNTs with herringbone texture rather than concentric graphine structure of nanotubes

#### 5.3.3 Solubilization of SWNTs: near-complete phase transfer of single-wall carbon nanotubes by covalent functionalization using oxalyl chloride

A novel method for the near-complete phase transfer of SWNTs from aqueous to organic medium facilitated the way for a new generation of CNT composites capable of controlling their unique properties in a determinable manner. A simple strategy is reported for an efficient phase transfer of Single-wall carbon nanotubes (SWNTs) from an aqueous to non-aqueous medium using a unique amide functionalization route, where the water soluble SWNTs (2.6 mg/mL) were transferred to solvents like chloroform, toluene and  $\text{CS}_2$ .

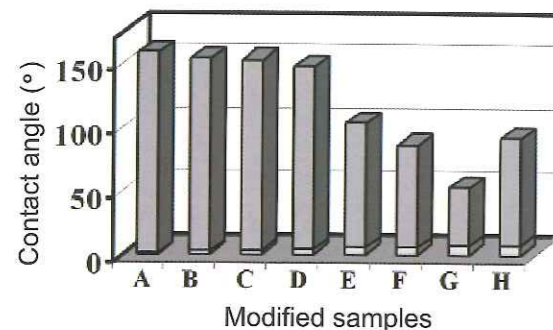
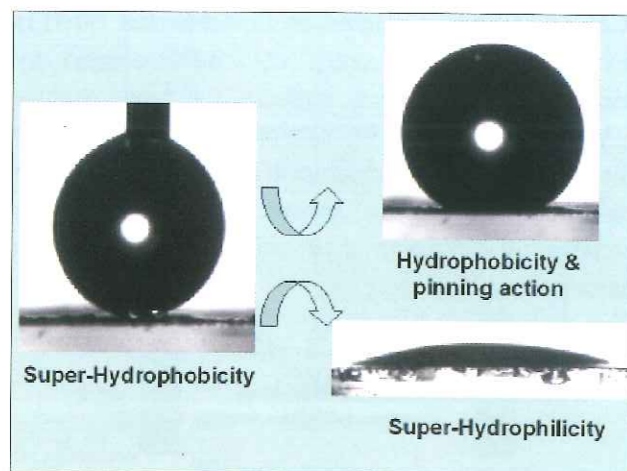
A clean and higher degree of amidation (ca. 50%) is achieved by using oxalyl chloride preceded by microwave treatment in acid media. This fundamentally new technique for the complete phase transformation of SWNTs/MWNTs from aqueous to organic medium could pave the way for a new generation of CNT composites capable of controlling their unique properties in a determinable manner.



Near-complete phase transfer of single-wall carbon nanotubes By covalent functionalization using oxalyl chloride

#### 5.3.4 Tuning the wetting properties of multiwalled carbon nanotubes by surface functionalization

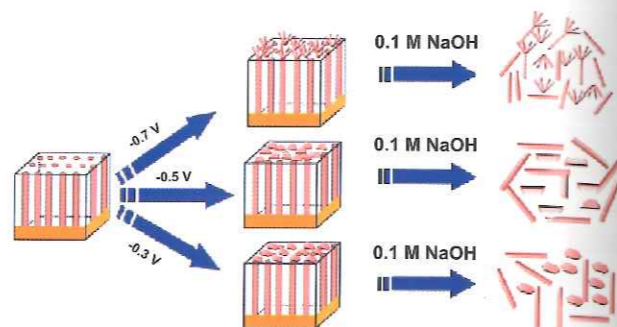
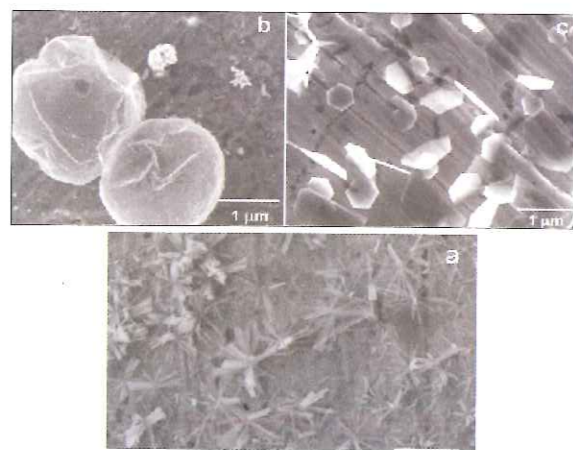
The achievement of tuning the wetting characteristics of multiwall carbon nanotube surfaces implies that the fabrication of CNT composites with an amazing range of superhydrophobic to superhydrophilic properties could be realized by improving the surface functionalization strategies. The practical utilization of such tunable CNT surfaces to make high performance polymer composites (e.g., controlling the interfacial adhesion between CNT surface and polymer) would significantly open up new perspectives in the preparation of various polymer composites extending the range of their possible applications.



Wetting behavior. Histogram exhibition the variation in the contact angle ( $\theta$ ) of pristine MWNTs sample (A) and modified bucky paper sample (B-H), indicating the effect of surface functionalization on wetting behavior of MWNTs papers

### 5.3.5 Template-assisted formation of platinum mesostructures

A potential-dependent morphological evolution of platinum mesostructures in the form of multipods, discs and hexagons using porous anodic alumina membranes (PAAM) was observed. These remarkable structures prepared by templated electrodeposition at potentials of -



Scanning electron micrographs of platinum multipods at -0.7 V (a), disc at -0.5 V (b) and hexagonal structure at -0.3 V (c), after etching the alumina membrane in 0.1 M NaOH. Various steps involved in the formation of these structures are shown.

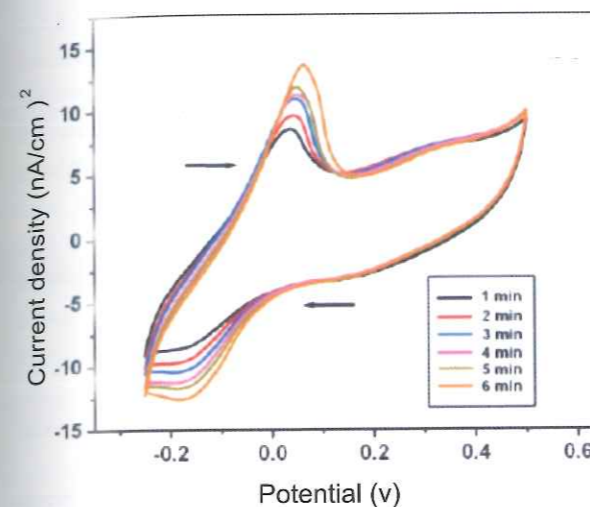
0.7, -0.5 and 0.3 V, respectively, revealed unique shape-dependant electrocatalytic activity towards both oxygen reduction and methanol oxidation reactions.

### 5.3.6 Autoreduction of cyanoferrate(III) ions in a polymer electrolyte membrane (Nafion)

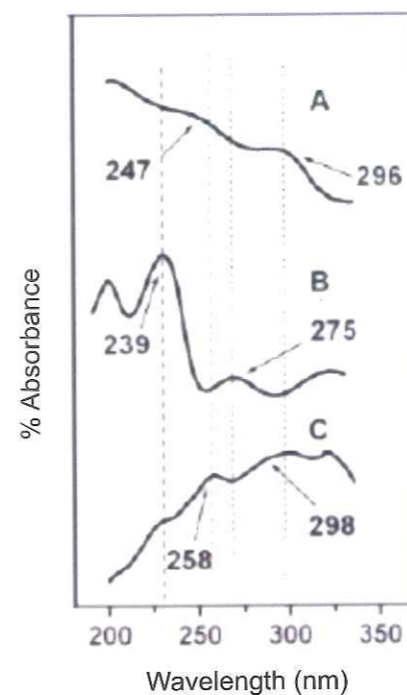
A new approach for probing the molecular level interactions between an ionically conducting polymer and its environment, by incorporation of redox active species, having charges similar to that of the pendant ionic groups present in the polymeric backbone has been developed. Using this protocol, the thermodynamic stability and proton coupled electron transfer behavior of potassium hexacyanoferrate(II) ( $K_4[Fe(CN)_6]$ ) and potassium hexacyanoferrate(III) ( $K_3[Fe(CN)_6]$ ) complexes, incorporated in a proton exchange membrane have been investigated in an "all solid state" cell configuration, using electrochemical techniques. More significantly, the coupling of proton transfer with the outer sphere electron transfer ability of the redox couple has direct significance for optimizing the design of catalyst coated membranes for applications like fuel cells, supercapacitors, solid state hydrogen sensors and analytical techniques based on ion-exchange membranes.

### 5.3.7 Magnetostrictive smart materials

The research work on developing ceramic oxide magnetic materials for use as magnetostrictive smart materials for various technological applications is an ongoing programme. The objective is to develop suitable sintered polycrystalline materials. Spinel type ferrites are being evaluated for identifying suitable materials with high magnetostriction at low magnetic fields. From the studies

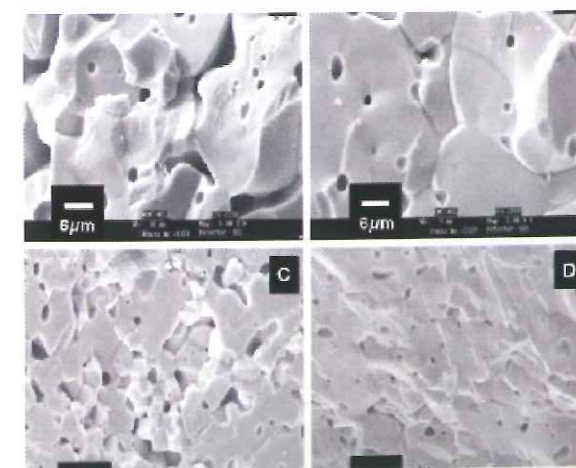
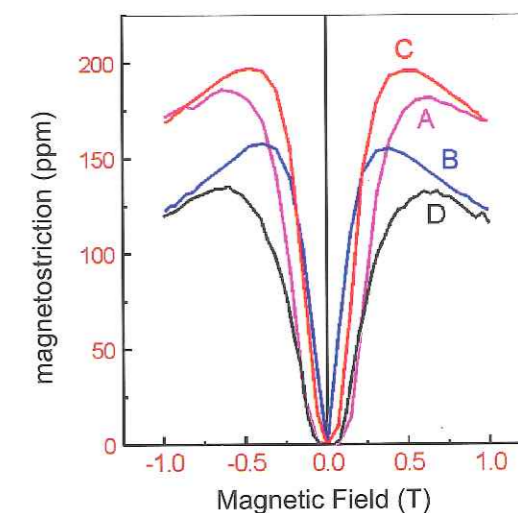


Hydrogen oxidation signal of the  $K_4[Fe(CN)_6]$  membrane at 100 mV/s and scaling of the peak current with the partial pressure of  $H_2$



UV-visible spectra of (A)  $K_3[Fe(CN)_6]/Nafion$ , (B)  $K_4[Fe(CN)_6]$ , and (C)  $K_3[Fe(CN)_6]$  recorded in the solid state.

ongoing programme. The objective is to develop suitable sintered polycrystalline materials. Spinel type ferrites are being evaluated for identifying suitable materials with high magnetostriction at low magnetic fields. From the studies on cobalt ferrite, it has been found that controlling the processing parameters, microstructure and composition of the sintered products are essential to enhance the magnetostriction at low magnetic fields. Figure below compares the dependence of the magnetostriction of sintered cobalt ferrite on the microstructure.



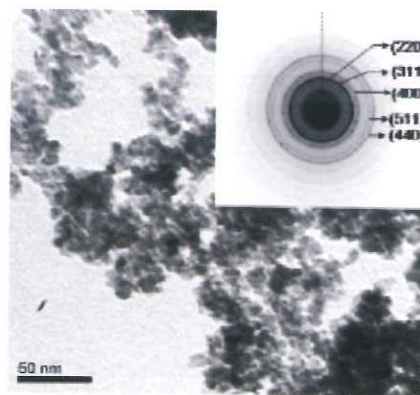
Magnetostriction curves and the corresponding microstructures for sintered cobalt ferrite



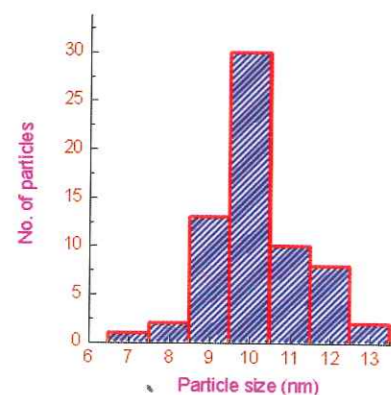


### 5.3.8 Nanomagnetic materials

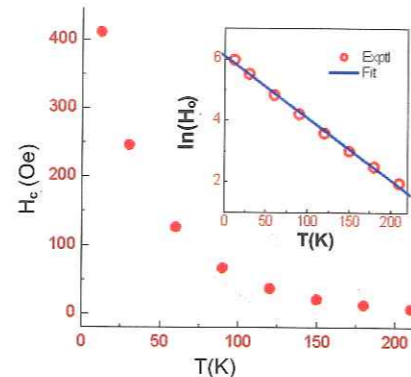
Understanding the magnetic behaviour of magnetic nanoparticles is very essential for various applications such as in biomedical applications, information storage, ferrofluids, etc. The magnetic properties of the nanoparticles can be fine tuned by controlling the particle size and morphology during the synthesis. Various synthetic strategies such as co-precipitation, hydrothermal, combustion, etc, have been adopted for obtaining magnetic nanoparticles. Maghemite is used for various applications including magnetic recording and superparamagnetic iron oxide nanoparticles are highly desirable for various biomedical applications. Figures below show the transition electron micrograph of  $\delta$ - $\text{Fe}_2\text{O}_3$  (maghemite) nanoparticles of almost uniform particle size of 10 nm, synthesized by a microwave hydrothermal method. The nanoparticles showed superparamagnetic behavior at room temperature, with a blocking temperature of 200 K and the variation of the coercivity of the nanoparticles as a function of temperature follows an exponential behaviour indicating strong interparticle interactions.



TEM of maghemite nanoparticles

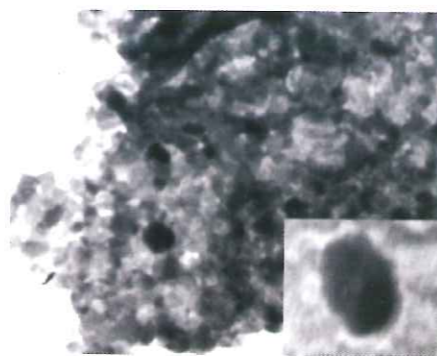


Particle size distribution

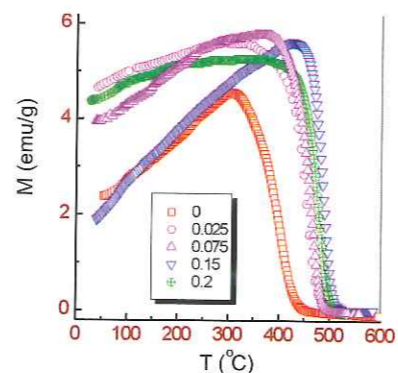


Variation of coercivity with temperature

Maghemite undergoes an irreversible structural phase transition at 400 °C. Increasing the phase transformation temperature without affecting the magnetic properties is desired for various applications. Figures below show the transmission electron microscopic image of Zn doped maghemite nanoparticles synthesized by a combustion method and the enhancement of the phase transformation temperature on doping with Zn. The phase transformation temperature of the maghemite nanoparticles could be increased up to 500 °C by Zn doping.



TEM photograph of Zn doped  $\delta$ - $\text{Fe}_2\text{O}_3$  nanoparticles

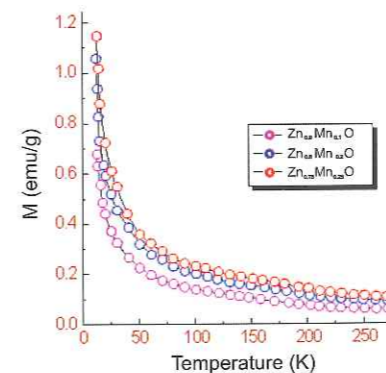
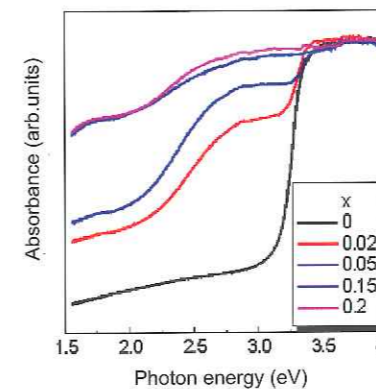
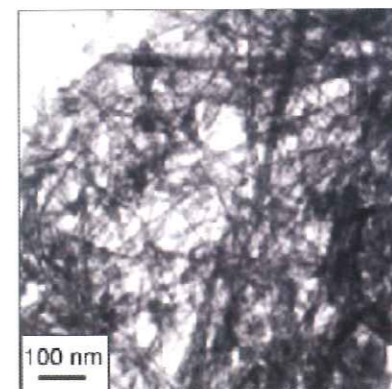


Increment of the phase transformation temperature of maghemite on Zn doping



### 5.3.9 Diluted magnetic semiconductors

Diluted magnetic semiconductors based on simple semiconducting oxides such as ZnO, doped with transition metal ions, are emerging new materials for spintronics applications. Our aim is to synthesize these new materials and study their structural, magnetic, electronic and optical properties in detail, which is essential for different applications. Figures below show optical and magnetic properties of Mn doped ZnO nanorods synthesized by a combustion method. The material is paramagnetic at room temperature and shows ferrimagnetic behavior below 50 K.



TEM, optical and magnetic properties of Mn doped ZnO nanorods

### 5.3.10 Low temperature synthesis and processing

Low temperature synthesis is an efficient route for the synthesis of nanosized materials. Wet-chemical synthetic routes such as co-precipitation, reflux-digestion, hydrothermal and microwave hydrothermal, citrategel, urea gel and combustion techniques have been applied to prepare a variety of polycrystalline functional ceramics at low temperatures. The advantages of these techniques are i) nanoparticles can be synthesized with controlled size, shape and distribution, the increased reactivity due to high surface area, low sintering temperatures, homogeneity in chemical composition, stabilization of new phases, cost reduction, etc.  $\delta$ - $\text{Fe}_2\text{O}_3$  is used for various applications including magnetic recording. However, it undergoes an irreversible phase transition at 400 °C. Figures below show the transmission electron microscopic image of Zn doped  $\delta$ - $\text{Fe}_2\text{O}_3$  nanoparticles synthesized by a combustion method and the enhancement of the phase transformation temperature on doping with Zn. The phase transformation temperature could be increased by 100 °C by Zn doping.

### 5.4 INSTRUMENTATION

A design and development of remote controlled high current power supply for energizing the electromagnet has been developed. The unit is capable of supplying DC current upto 45 Amperes. It is an intelligent unit with intelligence in the form of RISC microcontroller. The unit has features of RS232 communication, remote control operation beside LCD and key panel for housekeeping and control functions of the unit. The technology is not available in the Indian market and will be immensely useful to R & D institutes and universities. Commercialization can bring down the cost and make it affordable.

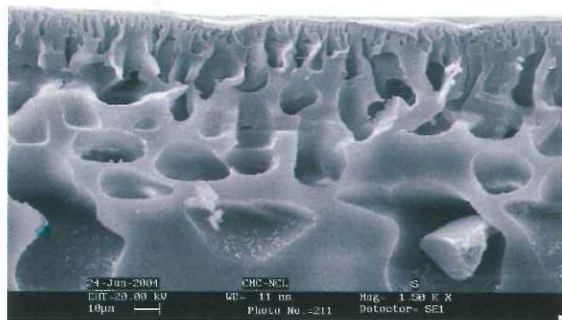


## 6 POLYMER SCIENCE AND ENGINEERING

## 6.1 MEMBRANE SCIENCE AND TECHNOLOGY

## 6.1.1 Gas permeation

Thin film composite (TFC) membrane is used for large scale separation it consist of a thin skin layer responsible for separation is supported onto a porous ultrafiltration (UF) membrane support. TFC membranes based on amine functionalized silicone rubber were prepared while optimizing parameters such as support type and porosity, coating characteristics, dip time, concentration of crosslinking agent and reaction time.

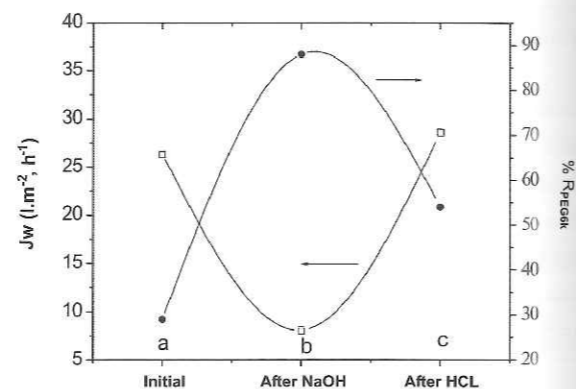


SEM of TFC membrane based on aminated silicone rubber

Permeance of ASR based TFC membrane decreased and selectivity of various gas pairs increased up to 20 minute crosslinking time and then remained constant at higher dip times. The permeance of TFC membranes based on different UF supports decreased in the order of decreasing porosity and increasing solution concentration. Selective TFC membranes could be easily obtained even with 1% ASR coating solution concentration when (PAN) based UF supports were used. On the other hand, when PSF based support was used, even with 2% ASR concentration, selective TFC membrane could not be obtained. ASR bearing-NH<sub>2</sub> groups thus had better compatibility with PAN, containing nitrile (-C≡N) functionality; than with hydrophobic PSF. When PAN<sub>20</sub> was used as the support, the reduction in effective layer thickness in case of 4% ASR coating than that of 2% coating indicated that pore penetration can be minimized while taking the advantage of increased coating solution viscosity and reduction in pore size. Thus the careful variation of porosity and coating solution characteristics could lead to optimum combination of permeance and selectivity.

## 6.1.2 Ultrafiltration

Polyacrylonitrile (PAN) based UF membranes with low porosity (molecular wt.6-10kD) were prepared by surface treatment of the higher porosity UF membranes. They can act as pH responsive membrane, as seen from following Figure, which shows (PEG) (MW 6000) rejection and water flux analysis of the same membrane after base or acid treatment. The porosity changes due to pH lead to variation in permeation performance.



Water flux (Jw) and PEG rejection analysis (R) of (a) unmodified membrane, (b) after NaOH treatment and (c) NaOH followed by HCl treatment

## 6.1.3 Proton exchange membrane for fuel cell application

Polybenzimidazole based membranes were prepared with active area of 5-150 cm<sup>2</sup>. The optimized process for membrane preparation was utilized for preparation of MEA following factorial optimization technique. Membranes with active area of 150 cm<sup>2</sup> are being used for development of 1 kW fuel cell stack. Investigations towards new polymer materials design and new strategies to make proton exchange membranes are being explored.

## 6.2 POLYMERISATION AND POLYMERIC MATERIALS

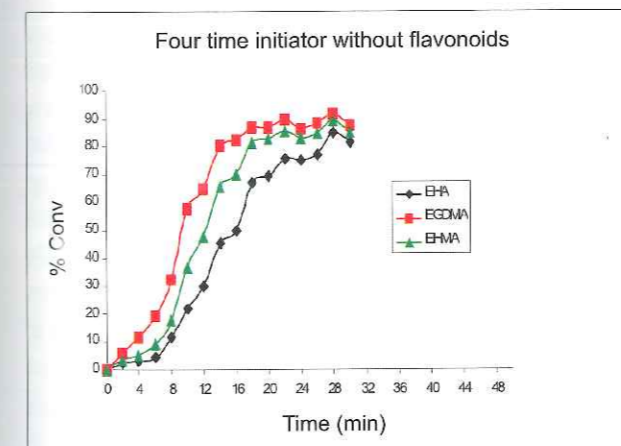
## 6.2.1 Poly(High internal phase emulsion) of EHA, EHMA and EGDMA with naturally occurring phenolic compounds

Flavonoids are the main components in green tea, wines and spices. Flavonoids such as catechin are phenol derivatives present in plants and are popular as antioxidants. Flavonoids and polyphenols act as efficient



antioxidants of alkyl peroxy and superoxide/hydroperoxy radicals, because of the favorable reduction potentials of the phenoxy radicals.

The aim was to study the inhibit ion effect on free radical high internal phase emulsion (HIPE) copolymerization of acrylic monomers with the cross linking ethylene dimethacrylate of flavonoids and/or phenolic compounds. The inhibition period of quercetin and vanillin were found to be higher than that with apigenin, (-) epicatechin, hesperidin and vitamin E. The inhibition period of HIPE depends preferably on solubility, steric hindrance, and resonance overlap between two aromatic rings. Cycloaliphatic ring reduces the resonance overlap thereby reducing the efficiency as inhibitor. Formation of flavonoid phenoxy radical is an essential step after initial scavenging of an oxidizing radical. The stability of the phenoxy radicals strongly depends on their bimolecular disproportionate reaction and electron delocalization.



Plot of percentage conversion with respect to time for without inhibitor

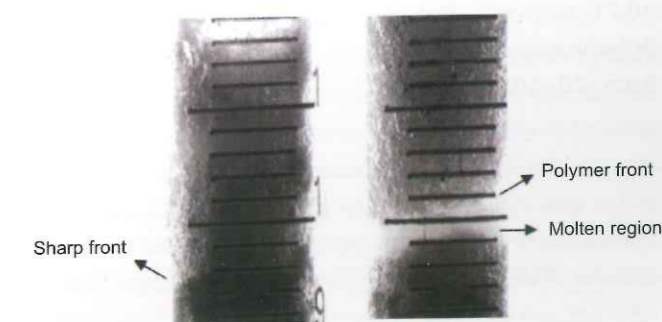
## 6.2.2 Water triggered frontal polymerization

Self-propagating high temperature frontal polymerization (FP) involves the transformation of monomer to polymer in a localized reaction zone. The propagation rate is determined by interplay of thermal conduction and temperature-dependent reaction rates. The localization of reaction and fast increase in temperature allow for rapid synthesis of a wealth of polymers with spatially controlled microstructures and morphologies.

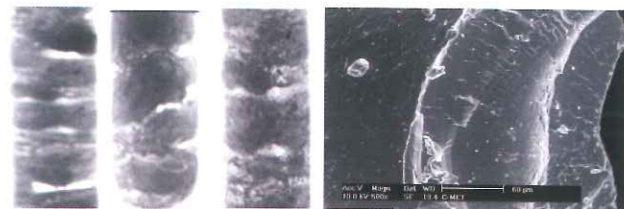
The simplest free radical frontal polymerization consists of a tube filled with monomer and initiator. Under appropriate conditions, when the reactions are initiated at one end of the tube, a thermal front develops and propagates with constant velocity. This apparent simplicity of frontal polymerization has led to this technique being steadily adopted for laboratory scale and possibly industrial polymer syntheses. FP has many advantages over traditional polymerization such as: (i) rapid reaction rates, (ii) reduced waste, (iii) reduced energy costs, (iv) unique and tunable microstructures and morphologies and (v) more "green" method as no solvents are used.

In the frame of free radical thermal frontal polymerization, a new sub branch; water triggered frontal polymerization, was investigated. In this method, polymerization is triggered by simple addition of minute and specific volume of water. Indeed, the required technology is as simple as running a reaction in a test tube or a custom built reactor at ambient temperature and pressure. There is also added benefit of minimum energy consumption, since zero heat input is needed to start the self-sustained propagation reaction. Acrylamide homopolymers and copolymers (like starch-acrylamide) were synthesized using different new and conventional redox pairs. semi-pilot scale and developed empirical relation between front velocity and reactor diameter and induction period and reactor diameter. The results were validated with experimental findings.

The rich nonlinear dynamics involved in the process was demonstrated. They helical as well as layered patterns on the formed specimen was observed for the first time. A complete mathematical model and the physico-chemical understanding of the pattern formation process were established.



Front propagation in two different types of redox systems

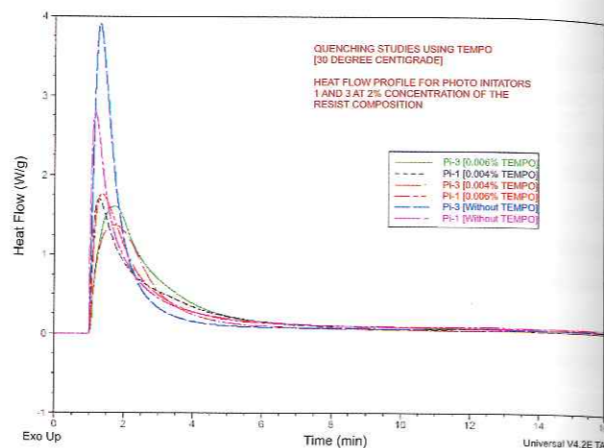


Helical and layered patterns observed on polyacrylamide sample

### 6.2.3 Photopolymerizable oligomers

The objective of the work involves synthesis and photochemical evaluation of a series of photopolymerizable oligomers with and without crosslinking agents and other additives. A series of photopolymerizable oligomers were synthesized and subjected to photochemical studies after addition of different amounts of photoinitiators and photosensitizers. The oligomers constitute a series of linear monomeric units, end capped with an acrylate or a methacrylates moiety. The backbone of the oligomer generally constitutes polyether, polyester or polyurethane linkages. Macromonomers, having multiple acrylate ends, based on hyper branched structures have been synthesized. Further, photoquenching studies have been done. The photopolymerization kinetics of these oligomers were studied and the kinetic constants were determined using differential photo calorimetry (DPC) method. Many formulations with excellent cure characteristics have been synthesized and analysed. Promising formulations can be used in surface coating applications.

Differential scanning calorimetry (DSC) plot gives the short listed heat flow profile of a photopolymerizable negative photoresist composition containing photo initiator and TEMPO [as free radical scavenger] at 30 °C using a 100 W medium pressure mercury vapor lamp at 18.71 mW/cm<sup>2</sup>. The system was analysed using a polychromatic band pass filter having wavelength range from 320 - 500 nm.



Heat flow profile of a photopolymerizable negative photoresist composition containing photo initiator and TEMPO at 30 °C using a 100 W medium pressure mercury vapor lamp at 18.71 mW/cm<sup>2</sup>

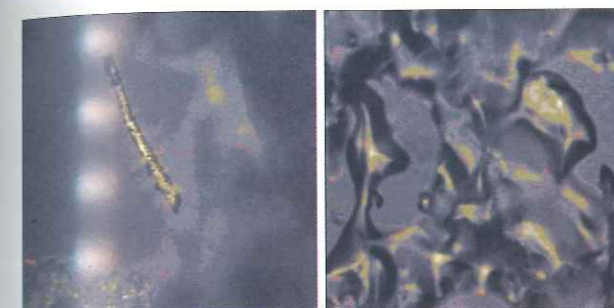
### 6.2.4 Cholesteric thermotropic liquid crystalline polyesters

Cholesteric thermotropic liquid crystalline polymers (ChLCPs) many form enantiotropic chiral melts, which show a selective transmission and reflection of circularly polarized light, if a macroscopic orientation of all domains (Grandjean texture) are feasible. Grandjean textures can be thermotropic, when the pitch of the helical order of the mesogen is sensitive to change in temperature. ChLCPs have ability to produce supermolecular structures characterized by a helical organization. The synthesis of cholesteric polyesters based on sugar diol, such as isosorbide as a chiral building block because it is easily accessible from renewable resources in the form of pure enantiomer. Isosorbide is known to possess a high twisting power, but it is more flexible and inexpensive.

The objective was to synthesize the cholesteric liquid crystalline polyesters from isosorbide, methyl hydroquinone and isophthaloyl chloride. Homopolyester of isosorbide and isophthaloyl chloride is thermally stable up to 380°C. Homo/copolyesters derived from isosorbide, methyl hydroquinone and isophthaloyl chloride exhibited thermal stability more than 300°C on the basis of 10 % weight loss. The copolyesters derived from isosorbide, methyl hydroquinone and isophthaloyl chloride are soluble in chloroform (when isosorbide percentage is more than 50 mol %). Optical microscopy study reveals that copolyester showed "yellow iridescent



strip" at 209°C on heating and it also showed formation of a "grandjean texture" at 270°C on heating. These are typical textures of cholesteric liquid crystalline phases.



Optical texture of copolymer at 209°C on heating

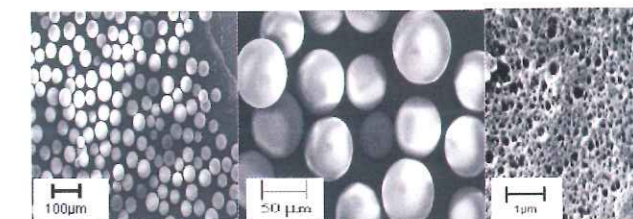
Optical texture of copolymer at 270°C on heating

### 6.2.5 Polymer supported catalysts

#### Removal of As (III) and As (V) from contaminated water sources by sorption onto novel PEI-attached poly(HIPE) beads

Contamination of water by heavy metal ions is becoming a serious issue due to their associated ecological and health effects even at very low concentrations. Arsenic is a carcinogen and its ingestion may deleteriously affect the gastrointestinal tract, cardiac, vascular and central nervous systems. Due to its high toxic effect on human health, recently the United States Environmental Protection Agency (USEPA) has lowered the maximum contaminant level for arsenic in drinking water from 50 to 10 µg/lit.

Removal of As (III) and As (V) from contaminated water sources was studied by sorption onto novel PEI-attached poly(HIPE) beads. Poly(ethyleneimine) (PEI) is a cationic polymer used for a wide variety of applications. PEI acts as a chelating agent for the removal of many metal ions, including cadmium. PEI was used for the metal binding, and this was followed by an ultra filtration operation to retain the PEI polymer. The sorption of both As (V) and As (III) is seen to be sharply influenced by pH, with the sorption of As (V) falling drastically both at low and high pH and that of As (III) at low pH. The sorption maximum for As (V) occurs under acidic conditions (pH, 2-4) and that of As (III) under alkaline conditions (pH, 7-10). Maximum adsorption capacity of PEI-attached poly(GMA-EGDMA) copolymer for As (III) in alkaline pH was found 262 mg/g and that for As (V) in acidic pH was found 225 mg/g, respectively.



Scanning electron micrographs of poly(GMA-EGDMA) copolymer beads synthesized by HIPE at different magnification; a) 100X, b) 500X, and c) 30000X

### 6.3 POLYMER SYNTHESIS

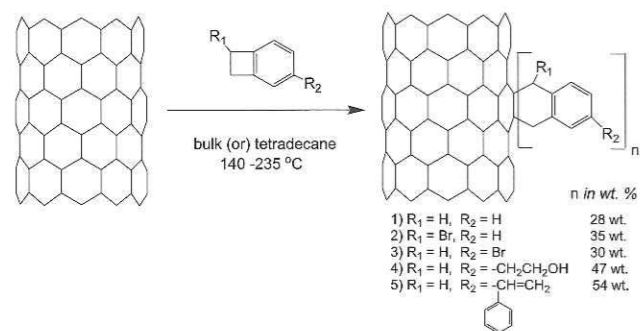
#### 6.3.1 Controlled covalent functionalization of multi-walled carbon nanotubes using [4+2] cycloaddition of benzocyclobutenes.

Surface modification of carbon nanotubes (CNTs) through covalent functionalization is vital for the development of high-performance composite materials, chemosensors, nanoelectronics, photovoltaic devices, as well as for a range of biomedical applications. The introduction of acid groups by acid-digestion disrupts the structural integrity of CNTs. Apart from shortening the tubes, oxidatively generated acid groups are inhomogeneously located at the tips of broken CNTs and hence, functionalization using acid groups as precursors does not give a statistical distribution of functional groups throughout the surface of the CNTs. Though, several methods are reported for the functionalization of the sp<sup>2</sup> network of the CNTs, the adequate control of the functionalization has not been achieved. An attempt is being carried out to develop a strategy for controlled functionalization of CNTs without affecting their structural integrity. We have explored the reaction of various benzocyclobutene in the Diels-Alder reaction with the sp<sup>2</sup> carbons of the CNTs.

Benzocyclobutene (BCB) is a class of diene and undergoes Diels-Alder reaction with aromatic system through an o-quinodimethane intermediate. The strained ring of the benzocyclobutene is susceptible to thermal ring opening to form o-quinodimethane which can undergo [4+2] Diels-Alder cycloaddition exclusively to 6-6 bonds of fused aromatic rings. Accordingly, in an attempt to add organic moieties on the surface of CNTs, several substituted benzocyclobutenes (1-5) were reacted with multi-walled carbon nanotubes (MWNTs). BCBs



containing a hydroxyl group (**4**, BCB-CH<sub>2</sub>CH<sub>2</sub>OH) and 1,1'-phenyl-benzocyclobutene ethylene (**5**, BCB-DPE) were synthesized from the reaction of Grignard reagent of 4 bromobenzocyclobutene with ethylene oxide and acetophenone, respectively. Experiments were performed in bulk as well as in tetradecane. In a typical experiment, 20 mg of pristine MWNTs were reacted in bulk with 150 mg of benzocyclobutene (BCB) at different temperatures ranging from 140 °C to 235 °C for 24 h. In case of a reaction in tetradecane, 100 mg of MWNTs were taken in 5 ml of tetradecane and 1 ml of BCB or substituted-BCB was added drop-wise via a syringe-pump with vigorous stirring under argon.



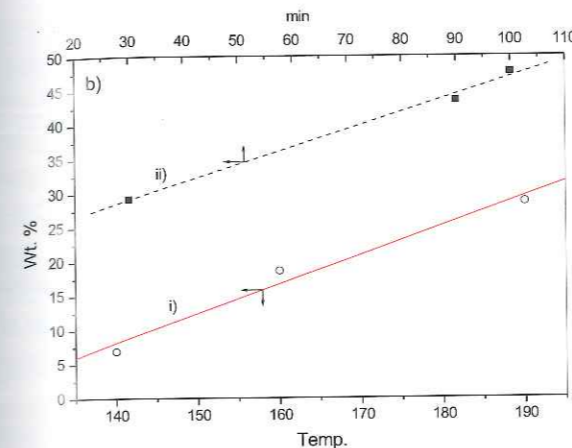
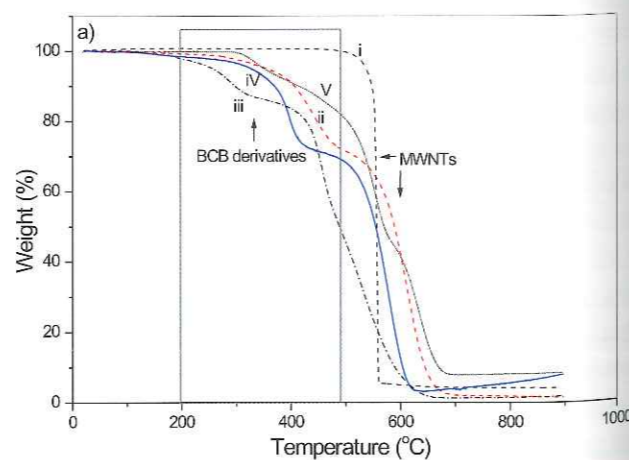
Diels-Alder adduct of various benzocyclobutenes with multi-walled carbon nanotubes

After the reaction, the MWNTs were collected by washing with copious amount of tetrahydrofuran (THF) and filtered using a teflon membrane (0.2 μm pore). The washing was repeated several times until the filtrate showed absence of BCB by thin-layer chromatography. Benzocyclobutenes containing hydroxyl (**4**) and 1,1'-phenyl-benzocyclobutene ethylene (**5**) were reacted in tetradecane using drop-wise addition. The side wall functionalized MWNTs (MWNTs-g-(BCB)<sub>n</sub>) each having different substitution in BCB, **1-5**, were dried at 60 °C for 5h under vacuum and characterized using FT-IR, UV-vis absorption spectroscopy, Raman spectroscopy, and thermogravimetric analysis (TGA).

The quantity of BCBs attached to the surface of MWNTs-g-(BCB)<sub>n</sub> was determined from TGA which showed two distinct weight losses, i) starting from 200 °C to 480 °C and ii) a major weight loss at 590 °C to 625 °C. The decompositions in the temperature ranges from 200-480 °C and 590-625 °C were assigned to the attached BCBs and the MWNTs, respectively (a). The amount of BCBs grafted to the tubes varies from 6-54 wt. %

depending on the reaction temperature as well as the mode of addition (b).

As the reaction proceeds through the formation of o-quinodimethane radicals, the rate of Diels-Alder adduct formation is dependent on the temperature of the reaction. The control of the process is evident as the wt. % of BCB on the surface of MWNTs increases with increasing reaction temperature in bulk (Figure 1b-i). At 140 °C, only 6.9 wt % BCB was grafted on the surface of the MWNTs. On the other hand, when the reaction was performed at 190 °C, the grafting of BCB increased up to 28.6 wt %. The reaction of 1-bromobenzocyclobutene with MWNTs in bulk gave MWNTs-g-(BCB-Br)<sub>n</sub> with 35 wt % functionalization. However, it was observed that a prolonged reaction time has no significant influence on the % of grafting which could be attributed to the dimerization of o-quinodimethane radical intermediate. In order to minimize the dimerization of BCBs, the substituted BCBs, **4** and **5** were kept at room temperature and added drop-wise into tetradecane containing MWNTs at 235 °C. The drop-wise addition method significantly improves the percentage of grafting depending on the duration of the reaction. The reaction performed with **4** was kept stirring for 30, 90 and 100 min and the TGA revealed that the wt % decomposition of the substituted BCB increased from 29.2, 43.5 and 47.6 wt %, respectively. This indicates that the Diels-Alder reaction using BCB is controllable and the extent of grafting on to the surface of the MWNTs can be tailored using a suitable reaction temperature and time (Figure 1b-ii).

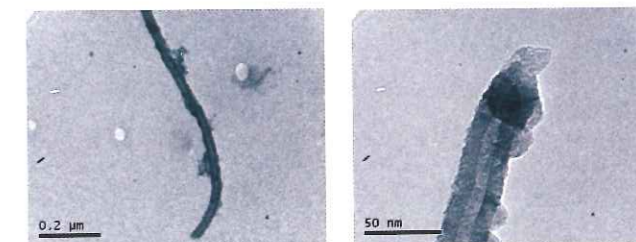


a) TGA of MWNTs grafted with various derivatives of BCB. i) pristine MWNTs, ii) MWNTs-g-(BCB)<sub>n</sub>, 28 wt % BCB, iii) MWNTs-g-(BCB-Br)<sub>n</sub>, 35 wt % BCB-Br, iv) MWNTs-g-(BCB-CH<sub>2</sub>CH<sub>2</sub>OH)<sub>n</sub>, 47 wt % BCB-CH<sub>2</sub>CH<sub>2</sub>OH, and v) MWNTs-g-(BCB-DPE)<sub>n</sub>, 54 wt % BCB-DEP b) the extent of functionalization depending on the reaction temperature and duration. i) bulk reaction of BCB with MWNTs at different temperature for 24 h, and ii) drop-wise addition of BCB-CH<sub>2</sub>CH<sub>2</sub>OH at 235 °C for different duration.

### 6.3.2 Organic nanoclusters on the surface of MWNTs

It was expected that a polymer containing benzocyclobutene (BCB) repeat units such as poly (4-vinylbenzocyclobutene) (PVBCB) would react at multiple sites on the surface of the MWNTs. If the proximity of the tubes permits, inter-linking of MWNTs can be realized. The PVBCB was synthesized using anionic polymerization of 4-vinylbenzocyclobutene and reacted with MWNTs. Accordingly, 20 mg of MWNTs were refluxed in 15 mL of diphenylether containing 20 mg of PVBCB ( $M_{n,SEC} = 30,000$  g/mol,  $M_w/M_n = 1.05$ ) at 240 °C for 2 h. After the reaction, the MWNTs-g-(PVBCB)<sub>n</sub> were washed with copious amount of tetrahydrofuran and recovered by filtration and dried at 90 °C for 4 h. The recovered MWNT-g-(PVBCB)<sub>n</sub> had a weight increase of 19 mg (~100 wt %) indicating total amount of PVBCB had under cross-linking either inter- or intramolecularly. It is known that PVBCB undergoes intramolecular cross-linking to form organic nanoparticles. The MWNTs-g-(PVBCB)<sub>n</sub> was found soluble in THF and CHCl<sub>3</sub> at low concentration. The TEM analysis of a drop coated solution of MWNTs-g-(PVBCB)<sub>n</sub> showed the presence of cross-linked organic nanoparticles on the surface of MWNTs.

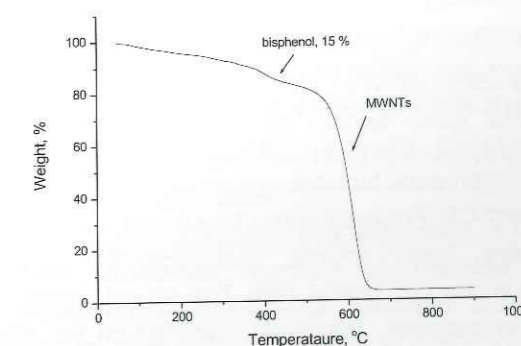
The nanoparticles on the surface of MWNTs are non-uniformly located as a result of random Diels-Alder reaction with *sp*<sup>2</sup> carbons of the MWNTs. It appears that once the chemical anchoring occurs at one site, the remaining tangling-polymer chain undergo intramolecular cross-linking reaction to form a collapsed nanocluster on the surface of the MWNTs.



Organic nanoclusters of intramolecular cross-linked poly(4-vinylbenzocyclobutene) on the surface of MWNTs (a and b).

### 6.3.3 Functionalization of MWNTs with bisphenol-A to use in exchange reaction with commercial polycarbonate.

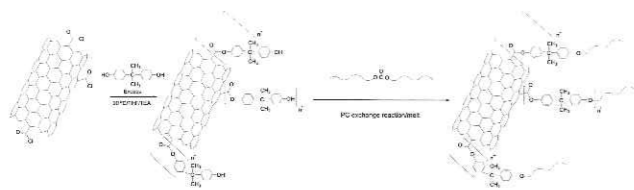
In our continuing effort to functionalize carbon nanotubes using polymeric chains, grafting of polycarbonate was attempted using exchange reaction as shown in scheme 2. Reaction of bisphenol-A with the acid groups of MWNTs was performed at various conditions in the presence of a small amount of acid in bulk or in solvent. The esterification reaction proceeded up to 20 wt % addition of bisphenol-A on the surface of the MWNTs depending on the reaction condition. The TGA of MWNT-g-(bisphenol)<sub>n</sub> exhibited two distinct decompositions at  $T_{max} = 325$  °C and at  $T_{max} = 590$  °C corresponding to the decomposition of attached bisphenol and MWNTs, respectively. Further experiments are underway to increase the amount of bisphenol on the surface.



TGA of MWNTs-g-(bisphenol)<sub>n</sub>, in air.



Currently, MWNT-*g*-(bisphenol)<sub>n</sub> is being used in post-carbonate exchange reactions with commercial polycarbonate to produce nanocomposite. (A part of the report given here is done in collaboration with Prof. Jimmy Mays, University of Tennessee, USA).



Exchange reactions of polycarbonate with biphenol functionalized MWNTs

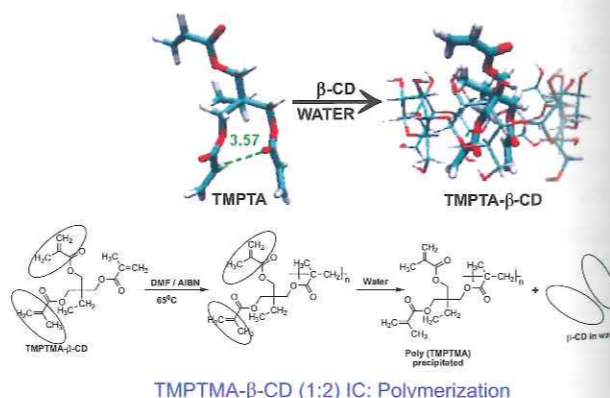
### 6.3.4 Latent cross-linkable polymers from trivinyl monomers via cyclodextrin host guest chemistry

The latent cross-linkable, soluble polymers are increasingly being explored in view of their applications in electronics, optoelectronics, molecular imprinting, microlithography, and nanotechnology. The approaches explored to develop latent cross-linkable polymers include a) synthesis of linear polymers with pendant hydroxyl functionality and its subsequent conjugation with vinyl monomers and b) polymerization of cross-linkers containing the multiple unsaturated groups of different reactivity. These approaches have their own limitations. The first approach is limited by the choice of monomers for the synthesis of precursor polymers bearing hydroxyl functionality. The second approach is limited by the number of cross-linkers available which have unsaturated groups differing in reactivity. Clearly there is a need to have a single step methodology to obtain latent cross-linkable polymers.

A methodology to control the reactivity of multivinyl monomers using cyclodextrin (CD) host guest chemistry, was reported earlier. This approach is extended to polymerization of cross linkers containing three unsaturated groups. The trivinyl monomer, trimethylolpropane trimethacrylate (TMPTMA) formed a 1:2 IC with CD. Polymerization of the complex resulted in a soluble, linear polymer containing two pendant unsaturations per repeat unit. The trivinyl monomer, trimethylolpropane triacrylate (TMPTA) on the other hand formed a 1:1 complex with CD. Surprisingly

polymerization of the complex yielded a soluble polymer containing two pendant unsaturations per repeat unit. Computational analysis showed that in TMPTA the two acryloyl groups are included in the same CD cavity. The analysis was corroborated by the fact that the hydrogen bonding interactions between two acryloyl groups (C-H...O=C) which brought them in close vicinity of one another so that both acryloyl groups were included in the same CD cavity. The FTIR and NMR characterization of the TMPTA-CD IC as well as the poly (TMPTA) support the presence of these hydrogen bonding interactions. This was further confirmed by the synthesis of new trivinyl monomer trimethylolpropane diacrylate 4-vinyl benzoate (TMPDAVB) yielded soluble polymers containing two pendant double bonds. Thus the hydrogen bonding in trivinyl monomers governs the stoichiometry of the IC and yields latent cross-linkable polymers containing higher cross link density as compared to EGDMA.

The single step methodology described herein to control the reactivity of trivinyl monomers can be extended their copolymerization with a wide range of functional monomers to obtain the functional, latent cross-linkable polymers containing high cross link density. These polymers have potential in the form of photolithography, optical sensors, molecular imprinting and for the functional nanoparticles synthesis. Work on development of some of these applications is in progress.

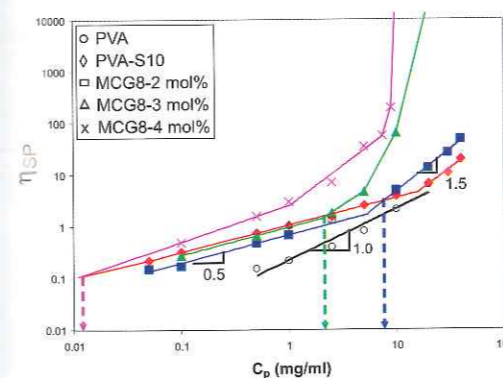


TMPTMA-β-CD (1:2) IC: Polymerization



### 6.3.5 Synthesis and characterization of hydrophobically modified poly(vinyl alcohol)

Recently, hydrophobically modified polymers [HMPs] have emerged as excellent viscosity modifiers/thickeners in a wide variety of industrial applications. Amongst the many polymers, poly(vinyl alcohol) [PVA] has a great potential for hydrophobic modification because of the presence of reactive OH groups. Furthermore, it is commercially available at a cheaper price. In view of these advantages, hydrophobically modified poly(vinyl alcohol) [HMPVA] was synthesized using a gallic acid derivative namely, methyl 3,4,5 tris (octyloxy) benzoate [MOB], through trans-esterification reaction. Upon hydrophobic modification, the decreased solubility (due to small addition hydrophobic group) of HMPVA in aqueous fluid was regained by the subsequent reaction of HMPVA with 1,3-propane sultone. The sultone incorporates ionic charges on the polymer chain.



Viscosity-concentration plots showing dramatic increase in viscosity of HMPVAs

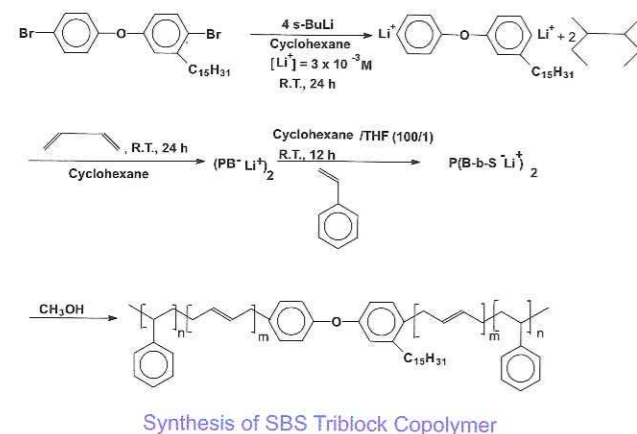
HMPVAs with three different contents of MOB were prepared and the structural characterization was performed by <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. The aqueous solutions of HMPVAs exhibited several fold increase in viscosity as compared to their unmodified precursors at the same concentrations (see Figure-1). The dramatic increase in viscosity of HMPVAs has been attributed to the formation of transient network as a result of the hydrophobic associations in the polymer chains. These materials show promising applications in paints, pharmaceuticals, cosmetics, and textile industries as viscosity modifiers/thickeners.

### 6.3.6 A new dicarbanionic initiator for the synthesis of telechelic polydienes, polystyrenes and SBS or SIS triblock copolymers in non-polar solvent without any additives

'Living' anionic polymerization is the most useful technique for the synthesis of block copolymers because of the absence of transfer and termination reactions. Among different block copolymers, ABA triblock copolymer is an important class e.g. the most well known being styrenic thermoplastic elastomers with two glassy end blocks connected to an amorphous polydiene block. One of the most versatile methods for the synthesis of such triblock copolymers is the use of a dicarbanionic initiator with a two-step sequential monomer addition sequence. However, one major difficulty met is the limited solubility of dicarbanionic initiator in non-polar solvent media that are required for the preparation of a polybutadiene or polyisoprene central block with a microstructure constituted of a high percentage of 1,4-polybutadiene or 1,4-cis-polyisoprene units, which is required for optimal elastomeric properties. Whenever high contents of 1,4-polybutadiene or 1,4-cis-polyisoprene units are desired, the anionic polymerization of dienes has to be conducted in non-polar solvent media, and with lithium as the counter-ion. *Sec*-butyllithium has proved to be an excellent monofunctional initiator. However, until now, no bifunctional initiator exhibiting carbon-lithium bonds, and yet soluble in non-polar solvent media without adding any additives has proved really satisfactory for the synthesis of polymers such as SBS or SIS thermoplastic elastomers or *μ*-difunctional polydienes possessing high percentage of 1,4-polybutadiene or 1,4-cis-polyisoprene units. Therefore, it is of great interest and importance to synthesise new bifunctional organolithium initiator soluble in non-polar solvents. Development of an ideal difunctional organolithium initiator, usable in hydrocarbon solvents for the anionic polymerization of dienes and/or vinyl aromatic hydrocarbon monomers has been a continuing effort since the past four decades. A new dicarbanionic initiator was discovered by lithium-halogen exchange reaction of 1-bromo-4-(4'-bromophenoxy)-2-pentadecyl benzene with *sec*-butyllithium. This dilithiated initiator is totally soluble in apolar medium in the absence of any additive and is



efficient to generate well-defined polybutadiene telechelics and poly (styrene-*b*-diene-*b*-styrene) triblock copolymers with high microstructure content of 1,4-units in polybutadiene and excellent mechanical properties. The dihalocompound *viz.*, 1-bromo-4-(4-bromophenoxy)-2-pentadecyl benzene used for synthesis for dicarbanionic initiator is derived from 3-pentadecyl phenol which in turn is obtained from cashew nut shell liquid (CNSL); a renewable resource material which is abundantly available and is inexpensive.



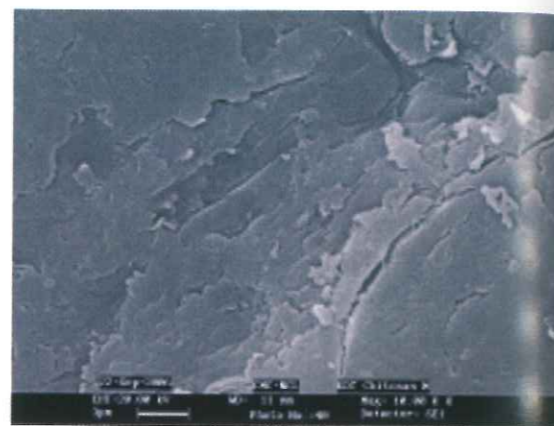
This work is that this is the first example of a dicarbanionic initiator totally soluble in non-polar media without any additives, which allowed us to synthesize well-defined polybutadiene telechelics with a high percentage of 1,4-PB units (91%). This initiator has proved to be very efficient in providing SBS triblock copolymers containing 91% 1,4-microstructure polybutadiene leading to high mechanical properties, e.g., ultimate tensile strength higher than 30 MPa and elongation at break of 1000%.

## 6.4 NATURAL POLYMERS AND BIODEGRADABLE POLYMERS

### 6.4.1 Crosslinking reactions of chitosan and their applications

This research looks at developing crosslinked chitin and chitosan reactions to arrive at new polymers that are dimensionally stable and can complex cations. Research into new types of crosslinking reactions with chemical structure modification can lead to new and improved materials for specific cation complexation, material for

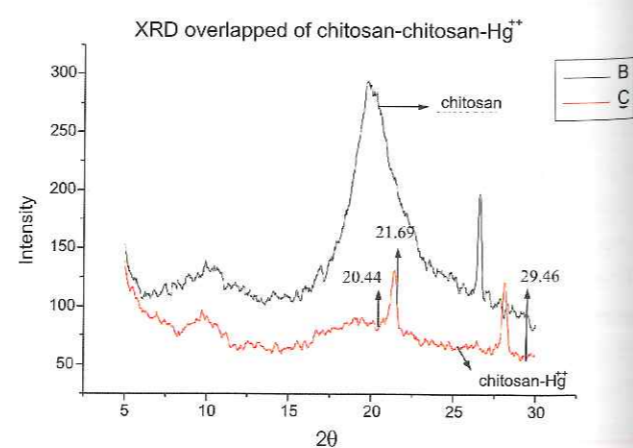
protein immobilization, protein-purification, and elucidation of structure-property relationships. Several new methods of crosslinking chitosan and applications based on the unique morphologies of these new materials were developed.



SEM of chitosan



SEM of crosslinked chitosan



WAXRD of chitosan and metal complexed chitosan



### 6.4.2 complexation of heavy metals by crosslinked chitosans

Chitin was crosslinked using diisocyanatohexane (HDI), trimellitic anhydride (TMA), and dibromodecane (DBD), then deacetylated in strong aqueous alkali. This led to a product with amine functional groups on the exposed surface of the crosslinked chitin, which could be utilized for complexation with heavy metals. Thus, a key feature of the crosslinked derivatives prepared was that only the hydroxy groups were utilized in the crosslinking reaction, and the acetyl amino groups of chitin were hydrolyzed only after the crosslinking was accomplished. This ensured that all amino groups of the chitosans so produced would be available for metal complexation, and not partially used up in crosslinking. This proposed advantage was proved by the similar binding observed for heavy metals like Hg (348-372 mg/g), Cu (91-119 mg/g), Zn (71-92 mg/g), Mn (3-10 mg/g), Cd (121-160 mg/g), and Pb (32-86 mg/g). Where as the control polymer (uncrosslinked chitosan powder) had complexation values for Hg (348-361 mg/g), Cu (100-106 mg/g), Zn (81-92 mg/g), Mn (4-7 mg/g), Cd (135 mg/g), and Pb (25-59 mg/g).

### 6.4.3 Morphological characterization of heavy metal complexes

Metal complexes of salts of Hg, Cu, Cd, Pb, Zn and Mn with chitosan and crosslinked chitosans were prepared, and their morphologies were studied using scanning electron microscopy and wide angle X-ray diffraction. The metal ions, which were specifically and strongly complexed to the amino functions of chitosans, like Hg, showed smooth surface morphology inspite of large number of ions complexed (360 mg/g of chitosan). The presence of metal ions on the surface of the chitosans could be detected with decrease in metal ion binding, in the following sequence Hg > Cu > Cd > Zn > Pb > Mn. Particularly in the case of Pb ions, the presence of these ions is clearly seen on the surface of the polymer by SEM. The number of ions of Mn complexed on the polymers were too few (5 mg/g of chitosan) to be visible. These results are also in agreement with the morphologies studies by WAXRD. The metal complexation data for each of these metal ions was also

### 6.4.4 Hydrolysis of metal complexes of crosslinked chitosans to produce chitooligosaccharides

The crosslinked chitosans were complexed with metals and then hydrolyzed using chitosanase enzyme. The hydrolytic rates and extent of hydrolysis was found to be significantly reduced. Thus while for chitosan about 840 µg/ml reducing sugar was produced in 4 hours time, and 780 µg/ml was produced for diisocyanatohexane crosslinked chitosan, only 400 µg/ml and 320 µg/ml was produced for cadmium sulfate with crosslinked chitosan and diisocyanatohexane crosslinked chitosan, respectively. Similar results are obtained for other crosslinking agents. Studies on preincubation of the metal with the enzyme show that of the metals studied, Mn has no effect on preincubation with the enzyme, Hg, Cd, Pb, and Cu completely deactivate the enzyme, while Zn reduces the enzyme activity by about 43.3%. Preincubation of the metal salts with the chitosan shows that Hg and Cu completely deactivate the molecule from enzyme hydrolysis, Cd and Zn inactivate it to the extent of 56.8% and 43.3% respectively, while Mn has no effect. Availability of the amino functions seems to be a key feature for the chitosanase to hydrolyze the chitosan polymer. This was also proved by the significant increase in the extent of hydrolysis for chitosan samples with 88% (final value 1120 µg/ml reducing sugar) and 85% deacetylation (final value 840 µg/ml reducing sugar). HPIC studies of the products show a variety of oligomers are produced in the chitosanase enzyme hydrolytic reaction.

### 6.4.5 Crosslinked chitosan as a matrix for selective adsorption and purification of lipase of *Aspergillus niger*

A series of ten crosslinked chitosans were synthesized with the specific objective of investigating the structure-property relationships for enzyme interactions, especially lipases, which are industrially most useful enzymes. Chitosan and its derivatives have been used as affinity matrices for purification of lipase from *Aspergillus niger* NCIM 1207. Ten derivatives of chitosan and crosslinked chitosan were evaluated for adsorption of lipase out of which trimellitic anhydride-crosslinked deacetylated chitin adsorbed lipase selectively.



Approximately 500 units of lipase were adsorbed per gram of trimellitic anhydride-crosslinked deacetylated chitin and 70% of the activity was eluted with increase in specific activity (63.17). These results suggested that trimellitic anhydride-crosslinked deacetylated chitin is an excellent substrate to get approximately 5.17 fold purification of the crude lipase with 70% yield for industrial applications

#### 6.4.6 Biomass to value-added lactic acid

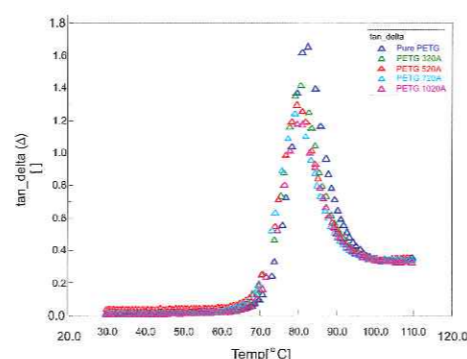
We studied the production of L(+) lactic acid from sugarcane bagasse cellulose, one of the abundant biomass materials available in India. The bagasse was chemically treated to obtain purified bagasse cellulose sample, which is much more amenable to cellulase enzyme attack than bagasse itself. This sample at high concentration (10%) was hydrolyzed by cellulase enzyme preparations (10 FPU per gram cellulose) derived from mutants generated in our own laboratory. We obtained maximum hydrolysis (72%) yielding glucose and cellobiose as the main end products. Lactic acid was produced from this bagasse cellulose sample by simultaneous saccharification and fermentation (SSF) in a media containing cellulase enzyme preparation derived from *P. janthinellum* mutant EU1 and *Lactobacillus delbrueckii* mutant Uc-3. The mutant Uc-3 was found to utilize high concentrations of cellobiose (50g per litre) and convert it in to lactic acid by homo-fermentative way. Considering that bagasse is a waste material available in abundance, we propose to valorize this biomass to produce cellulose and then sugars, which can be fermented to products such as ethanol and lactic acid.

### 6.5 ORGANIC-INORGANIC HYBRIDS

#### 6.5.1 Nanocomposites Based on Amorphous Copolyester and Layered Silicate

The effect of clay concentration on the properties of PETG/clay nanocomposites prepared by melt compounding PETG and organophilic clay (Cloisite 20A) at different clay loadings is studied. Dynamics of the nanocomposites are investigated over a broad range of temperatures and frequencies using DRS and DMTA. Variation in the  $\tan \delta$  as function of temperature in the range of 30 to 110°C for pure PETG and PETG20A nanocomposites containing different filler loadings is

shown in the figure. There is a steady decrease in the damping with increasing clay concentration in the nanocomposites as compared to the pure polymer. These results are attributed to favorable interactions between the polymer and the organically modified clay layers resulting in to immobilization of polymer chains. Furthermore, this immobilization of polymer chains may be due to the formation of a rigid amorphous phase resulting from the constrained amorphous phase (CAP).



Temperature dependence of  $\tan \delta$  for pure PETG and PETG20A nanocomposites over a temperature range of 30 to 110°C

The  $\tan \delta$  peak values and the normalized values of  $\tan \delta$  for PETG20A nanocomposites are shown in Table. The significantly lower values of  $\tan \delta$  than the normalized  $\tan \delta$  values in the nanocomposites indicate the existence of CAP.

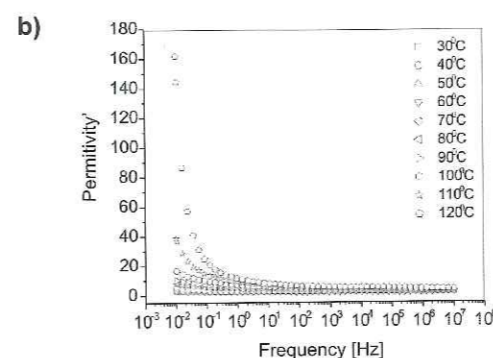
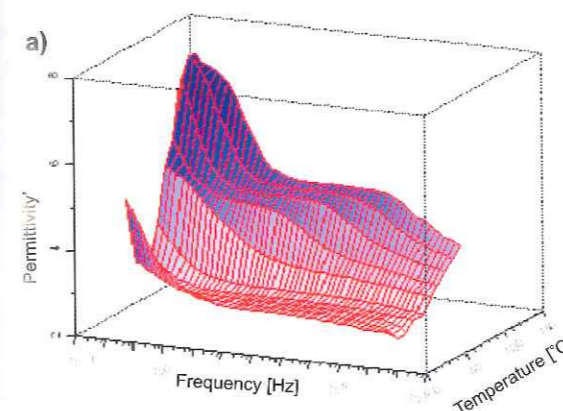
Table  $\tan \delta$  and normalized  $\tan \delta$  values at peak temperature for PETGCNT nanocomposites

Sample	Tan value	Normalized tan value
Pure PETG	1.6504	-
PETG20A3	1.4120	1.6008
PETG20A5	1.2962	1.5678
PETG20A7	1.2432	1.5348
PETG20A10	1.1792	1.4853

In dielectric analysis, the real part of the dielectric permittivity ( $\epsilon'$ ) for pure PETG and PETG20A7 as a function of frequency is measured and is presented in figure. The figure shows isothermal scans of  $\epsilon'$  extending over a temperature range of 30 to 120°C and over frequency from  $10^{-2}$  to  $10^7$  Hz. It can be seen from the figure that the permittivity of the pristine polymer does not increase much over the entire range of temperatures studied. However, there is a marked increase in the permittivity of the nanocomposites with increasing temperature, especially in the low frequency region. For



example, the permittivity of PETG20A7 nanocomposite at  $10^{-1}$  Hz is 160 at 120°C. This when compared to the permittivity of the pristine polymer, 7 at 120°C; gives an increment of 2285 % for PETG20A7. The significant increase in the permittivity is thus solely due to the nanoclay platelets. This demonstrates that the distributed nanocapacitance, which is hypothetically composed of MMT electrodes and a polymer insert in the clay interlayer, is responsible for the observed increase in the permittivity.



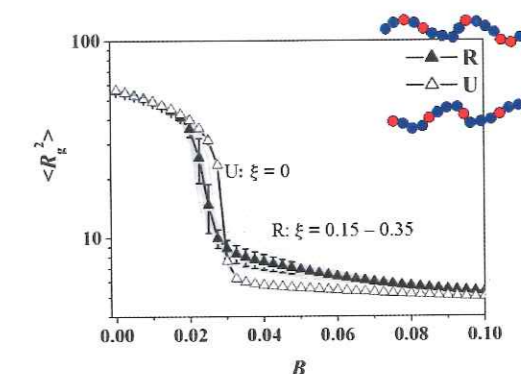
Experimental values of dielectric permittivity for (a) Pure PETG and (b) PETG20A7 as a function of frequency at various temperatures

### 6.6 STRUCTURE PROPERTY PERFORMANCE CORRELATION

#### 6.6.1 Coil-globule transitions in copolymers

When polymers containing "sticky" comonomer units collapse in dilute solution, the specific distribution of such units plays an important role in the route taken to the collapsed state. We have demonstrated that this route depends on the interplay of the entropy loss of the chain due to loop formation and enthalpic gain due to

comonomer aggregation as the comonomer units come together, forcing the polymer to collapse into a globule. This result has significant implications for the synthesis of single molecule nanoparticles by intramolecular collapse and for the protein folding problem.



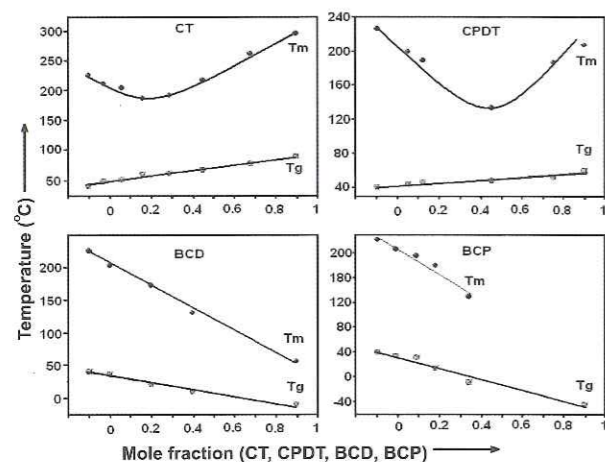
Simulations of the difference between the collapse behaviour of copolymers with uniformly (U) and randomly (R) spaced comonomers. comonomer

#### 6.6.2 Copolyesters based on poly (butylene terephthalate)s containing cyclohexane and cyclopentane ring

In an effort to understand the role of molecular structure on the thermal properties of polyesters and copolyesters, the following polyesters were synthesized: poly(1,4-cyclohexane dimethylene terephthalate) (PCT), Poly (butylene-1,4- cyclohexane dicarboxylate) (PBCD), poly (1,3-cyclopentane dimethylene terephthalate) (PCPDT) and poly (butylene-1,3-cyclopentane dicarboxylate) (PBCP). PCT and PCPDT are semicrystalline polymers with crystallization and melting temperatures higher than poly(butylene terephthalate)(PBT). However, PBCD and PBCP have lower glass transition temperature than PBT. The crystallization behavior of the polyesters depends on the molecular structure. The faster crystallization behavior of PBT and PCT compared with PCPDT may be attributed to their structures, i.e. planar structure of PBT and PCT vis-à-vis the non-planar cyclopentane of PCPDT. The non-planar nature of the cyclopentane ring inhibits the quick packing of the chains in the lattice leading to slower crystallization rates. Similarly, the PBCD and PBCP molecules are very flexible and highly non planar and hence could not easily pack in to a lattice for crystallization.



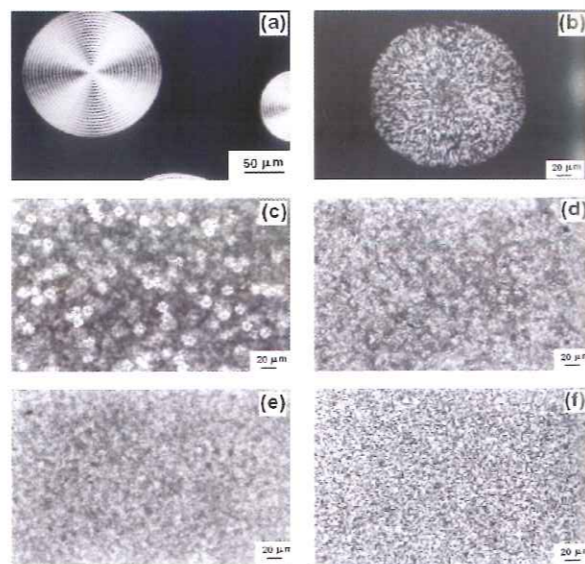
From these homopolymers a series of poly(butylene-co-1,4-cyclohexane dimethylene terephthalate) P(BT-co-CT), poly(butenes terephthalate-co-1,4-cyclohexane dicarboxylate) (P(BT-co-BCD), poly(butylene-co-1,3-cyclopentylene dimethylene) (P(BT-co-CPDT) and poly(butylene terephthalate-co-1,3-cyclopentane dicarboxylate) (P(BT-co-PBCP) random copolyesters were synthesized for the first time and their cocrystallization behavior was investigated using differential scanning calorimetry (DSC) and wide-angle X-ray diffraction (WAXD). The copolymers were found to be statistically random and crystallized in all compositions. The P(BT-co-CT) and P(BT-co-CPDT) copolyesters exhibited typical eutectic behavior in melting and crystallization, which indicated isodimorphic cocrystallization behavior. On the other hand, in the case of P(BT-co-BCD) and P(BT-co-PBCP) copolymers the melting and crystallization temperatures showed linear dependency with composition indicating isomorphous like crystallization behavior.



Dependence of glass transition and melting temperature on copolymer composition

Among the polyesters synthesized, PBT and PCT show high crystallization rates and very high nucleation density under crossed polars on crystallization from the melt. PBCP is an amorphous polymer and PBCD does not crystallize easily from the melt. However, PCPDT has lower crystallization rate and showed well-defined spherulitic morphology on crystallizing from the melt and provides an opportunity to study the effect of incorporating another monomer in the chain on the spherulitic morphology. The crystallization and spherulitic

morphology of PCPDT and the poly(BT-co-CPDT) copolyesters were observed using a polarized optical microscope. PCPDT exhibits well-defined banded spherulites, which were highly bi-refringent. Banded spherulites are also observed in poly(trimethylene terephthalate) (PTT). The banded spherulitic morphology changed with increasing comonomer content. When 20 % PBT was included as comonomer, the banded spherulitic morphology was highly distorted apparently due to the disturbance in the sequence of CPDT units by BT units. Other specific features are lower growth rates and increased nucleation density. For the sample PBT<sub>45</sub>CPDT<sub>55</sub>, the banded structure is extremely distorted and the excessive nucleation density reduces the size of spherulites also. The PBT rich blend, PBT<sub>78</sub>CPDT<sub>22</sub> shows spherulitic morphology similar to that of PBT. These results are consistent with the DSC and WAXS data presented in the preceding sections.



Polarized light micrographs of (a) PCPDT; (b) PBT15CPDT85; (c) PBT45CPDT55; (d) PBT78CPDT22; (e) PBT85CPDT15; (f) PBT

### 6.6.3 Phase behaviour of plate-like nanoparticles

Plate-like nanoparticles called laponite gel in water, viz. at low concentrations (around a few percent), they assemble into a network structure that does not flow. This is what gives materials like toothpaste their signature flow behaviour. We have been investigating how the addition of salts or organic modification of such plate-like nanoparticles can influence their gelation. We have



demonstrated that coating the plate edges with a hydrophobic organic compound leads to a significant change in the mechanism of gelation and in the gel structure formed. The other part of this investigation examines methods to inhibit gelation. For structures that are anisotropic, liquid crystalline phases would normally form above a certain critical concentration unless a non-equilibrium transition such as gelation interfered in the formation of this ordered phase. We have demonstrated the formation of low viscosity, free flowing liquid crystalline clay phases where gelation is postponed until much after the formation of the equilibrium liquid crystalline phase.

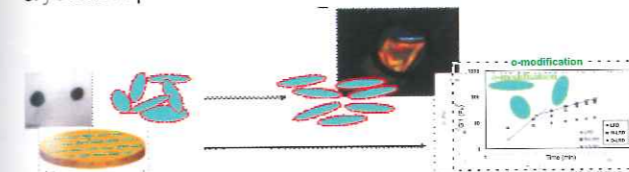
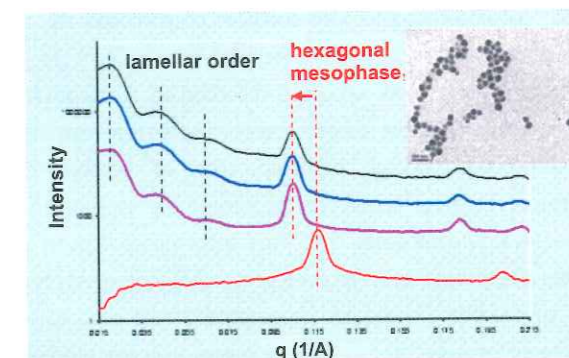


Plate-like anisotropic minerals normally gel, but can form birefringent liquid crystal phases if gelation is inhibited. They can also form gels with a novel structure on organically modifying their edges.

### 6.6.4 Dispersion of nanoparticles in surfactant liquid crystals

We have examined the organization of nanoparticles when they are dispersed in surfactant liquid crystalline phases with hexagonal smectic order. The characteristic length scale in our surfactant mesophases is around 6 nm. When the size of the dispersed nanoparticles is similar to the characteristic mesophase distance, we observe that an unusual phase forms in the ternary (surfactant-water-nanoparticle) phase diagram. The nanoparticles appear to form layered structures (viz. sheets of nanoparticles stack up) and these coexist with the surfactant hexagonal phase. This is unexpected and represents a novel region of the phase behaviour where the nanoparticle order is neither simply templated by the hexagonal phase nor determined purely by the free energy of elastic distortion of the mesophase. The intricate coexistence of lamellar and hexagonal structures has implications for design of new nanostructured materials.

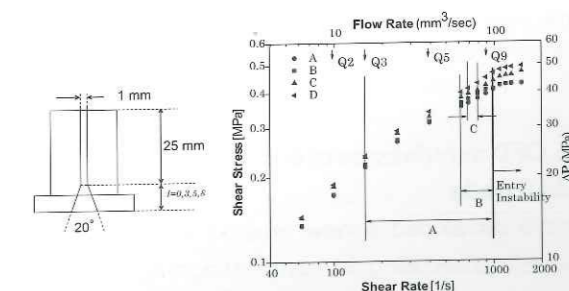


Small angle X-ray scattering from dispersions of nanoparticles (see TEM inset) in hexagonal liquid crystalline surfactant phases

## 6.7 RHEOLOGICAL STUDIES IN POLYMERS

### 6.7.1 A geometrical solution to sharkskin instability

We have studied the effect of die exit divergence on the sharkskin behavior, both experimentally as well as by using CFD simulations. Sharkskin or surface fracture is known to occur immediately after the die exit because of the large elongational deformation that polymer melt experiences as it exits the die. We show that the diverging taper at the die exit postpones or completely removes the occurrence of sharkskin. The corresponding computational fluid dynamic simulations of an equivalent K-BKZ fluid shows that the taper at the die exit significantly reduces the severity of the elongational flow thereby reducing the normal stresses as polymer melt leaves the die. We believe that in an extrusion operation, provision of a diverging taper at the die exit is one of the potential measures by which sharkskin instability can be eliminated on industrial scale.



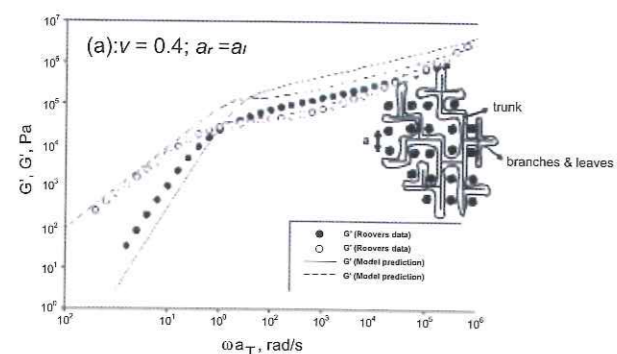
The graph on the right shows that as the length of the divergent section of an extrusion die exit (see schematic on the left) is increased the sharkskin defect is delayed and it is finally got rid of at a divergent section  $l/d$  of about 8.





### 6.7.2 Modeling the self similar dynamics of ring polymers

In our previous work we had developed a mean field coarse grained tube theory called the Pom-Pom Ring framework to model the dynamics of flexible ring polymers in two types of topologically constraining obstacle environments: (a) ring in a cross-linked gel devoid of solvent, and (b) melt of flexible rings. We have built upon this model to account for the self similar dynamics of ring chains. We propose that the dynamic response of a ring chain is composed of a linear superposition of independent relaxation modes corresponding to response of different length scales. This leads to the formulation of a mixing rule that captures the amoeba like self-similar dynamics of the ring chain. The proposed constitutive equation predicts a power-law dependence of the gain and loss moduli above the crossover frequency as expected from scaling arguments. The predictions of our model are found to be in semi-quantitative agreement with frequency sweep data for a poly(butadiene) ring melt available in the literature.

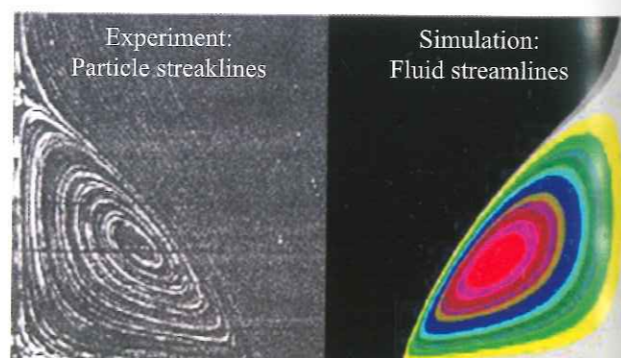


Comparison between experimental linear viscoelastic frequency response data of Roovers poly(butadiene) rings and PPR model predictions with dynamic self similarity

### 6.7.3 CFD simulations of contraction flow using a new ALE code

We have developed a new method for simulation of viscoelastic flows using an Arbitrary Lagrangian Eulerian (ALE) technique based finite element formulation. The ALE technique provides advantages of both Lagrangian and Eulerian frameworks by allowing the computational mesh to move in an arbitrary manner, independent of the

material motion. In our method, a fractional step ALE technique is employed in which the Lagrangian phase of material motion and convection arising out of mesh motion are decoupled. In the first step the relevant flow and constitutive equations are solved in a Lagrangian framework. The simpler representation of polymer constitutive equations in a Lagrangian framework avoids the difficulties associated with convective terms there by resulting in a robust numerical formulation. In the second step the mesh is moved in ALE mode and the associated convection of the stress is performed using a Godunov type scheme. This ALE technique is easy to implement and can accurately simulate the complex viscoelastic behaviour of transient polymer flow through complex geometries. We have studied steady flows through abrupt contractions of planar and axisymmetric geometries by performing transient flow simulations until steady state is achieved. The proposed method is validated with previously published numerical and experimental studies for polymer solutions obeying the Oldroyd B and Phan Thien Tanner (PTT) models. The simulated corner and lip vortex enhancement mechanism and flow behavior are in good agreement with experimentally obtained flow visualization photographs. The strength of the proposed method lies in its ability to simulate free surface flows such as swell and these will be discussed in a subsequent communication.



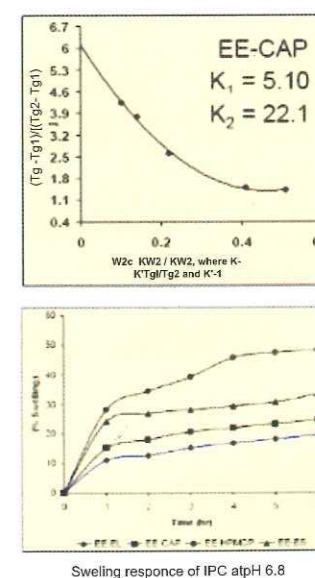
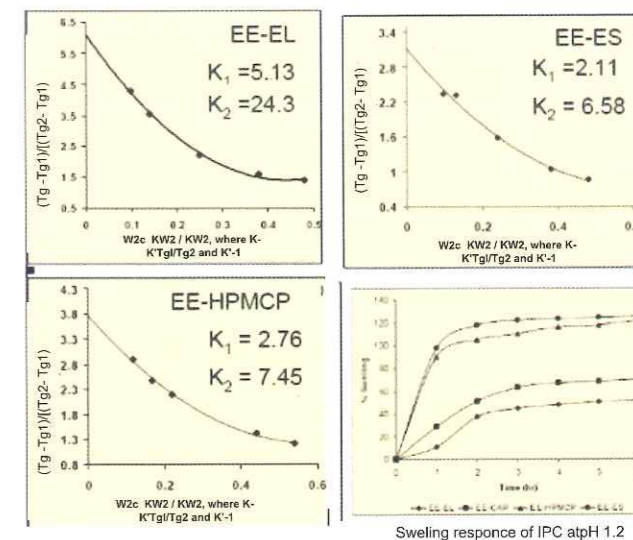
Comparison between experimentally observed particle streaklines in a 4:1 contraction flow of polyacrylamide solution and CFD simulations of our ALE code at  $We=3$ . The large salient corner vortex is quantitatively predicted by the simulations



### 6.8 MECHANISTIC INVESTIGATIONS OF PHASE BEHAVIOR IN EUDRAGIT®E BLENDS

Eudragit®E is the most widely used cationic polymer in pharmaceutical formulations. We recently reported investigations on blends of Eudragit®E with other polymeric excipients using thermal and spectroscopic methods and its implications for drug release. The probability of charge transfer is influenced by the functional group and favorable structural, and steric symmetry factors, which contribute to formation of hetero contacts. The higher basicity and spacer ethyl chain in DMAEMA groups from polymeric backbone in Eudragit E imparts greater mobility to form hetero contact with polyacids resulting in complexation. The thermal analysis showed that for polyelectrolyte complexes, the  $T_g$  values for blends showed positive deviations from additivity rule. The extent of interactions quantified in terms of parameters  $K_1$  and  $K_2$  of Schneider equation, decreased in the order  $EL > CAP > HPMCP > ES$ . The FTIR analysis was used to explain the nature of interactions in these polymers and also the presence or absence of free functional groups contributing to the observed phase behavior.

The evaluation of stoichiometry of EE-polyacid complexes helps select blend compositions containing a known excess of the particular blend component as to exhibit desired pH dependent swelling and release or a blend devoid of excess of any component as to yield the lowest swelling and pH independent release rate of the drug. The knowledge of degree of interaction in blend components will help select blend constituents and compositions with predictable swelling behavior for sustained release over the entire length of the GI tract. Since the polyelectrolyte complexes have  $T_g$ s above ambient temperatures and velocity of moisture penetration and the degree of swelling of the polyacid-polybase complexes is low, and can be manipulated by the choice of the blend components and composition, it may be possible to achieve swelling controlled release from blends forming polyelectrolyte complexes.





## 7 PROCESS DEVELOPMENT AND ENGINEERING

The Process development and engineering group undertook following activities during the year.

### 7.1 Downstream processing of lactic acid in Pilot Plant-II

Under this multidisciplinary project on polylactic acid funded by CSIR, various groups from NCL are working together towards the development of the process for polymer grade lactic acid and process development of poly-lactic acid. Biochemistry and Bio-chemical Engineering Group is responsible to study fermentation of sugarcane juice to calcium lactate, whereas Chemical Engineering and Process Development Group is mainly working on downstream processing of lactic acid and process development for polymer grade lactic acid. The Polymer Group is working towards polymerization of lactic acid, characterization and product development.

The basic process was developed for polymer grade lactic acid. Based on this process a pilot plant to produce 1 kg/hour of lactic acid is installed in Pilot Plant-II. The plant has following sections on the experimental skid:

- Acid splitting section to generate crude lactic acid solution followed by calcium sulfate filter.
- Crude lactic acid concentrator falling film evaporator.
- Reactive distillation set-up, which operates in a continuous mode to generate methyl lactate at 1.2 to 1.5 kg/hr, completely PLC based set-up with data logging facility.
- Methyl lactate fractionating set-up having approximately 50 theoretical stages.
- Methyl lactate hydrolysis set-up, which operates in a continuous mode to generate polymer grade lactic acid at 0.9 to 1.0 kg/hr, completely PLC based set-up with data logging facility.
- Agitated thin film dryer, spinning band column, Olsa dryer, centrifuge, vacuum pump, hot oil units, chilled water unit etc.

The entire experimental set-up is installed on a foldable experimental skid. The experimental skid is 21' tall structure having four different levels of operations. The skid is occupying approximately 250 ft<sup>2</sup> of floor space. The entire pilot plant was designed by NCL team, and was installed by a private firm as per NCL's design. These facilities will be used to develop a process

making polymer grade lactic acid and to generate enough material for polymerization study. The set-up will generate enough design details which will be of help for further scale-up.

#### The set-up has following benefits

- Complete know-how development for polymer grade lactic acid.
- As a demonstration unit.
- Data generation for further scale-up and commercial exploitation of the know-how.
- For any other reactive distillation activities this set-up can be used

### 7.2 BEP development for pilot plant to produce silicon tetrachloride at low cost

Silicon tetrachloride is a bulk and basic chemical used in various industrial applications on a large scale. M/s DuPont, USA is using silicon tetrachloride for vapor phase deposition of silicon dioxide on titanium dioxide particle. Silicon tetrachloride vapors are oxidized in-situ on the titanium dioxide particle to silicon dioxide. The other major use of silicon tetrachloride is in the optical fiber industry used in telephone and communication cables. Silicon tetrachloride is also used in making orthosilicates and polymers based on the orthosilicates, making high grade silica, fumed silica etc.

The project was sponsored by M/s DuPont, USA for the process development of low cost route to manufacture silicon tetrachloride for their captive consumption. The scale of operation and demonstration was 1 kg/hour of silicon tetrachloride. NCL successfully developed the process to make low cost silicon tetrachloride, which was demonstrated to the sponsor to their satisfaction. The sponsor was satisfied with the developed process and the quality of the material produced in the laboratory using commercial grade raw materials. M/s DuPont also reviewed process economics presented by NCL and was satisfied with the process economics. M/s DuPont further sponsored the basic engineering package (BEP) development activity for the pilot plant to produce 100 kg/hour of silicon tetrachloride. NCL's engineering team completed this task of BEP development activity in the stipulated time frame, and the BEP was submitted for the review of DuPont's engineering team.



The sponsor appreciated efforts put by NCL's team for development of total technology package.

### 7.3 Process development for alumina suitable for coating grade applications

Under this project sponsored by M/s DuPont, USA to develop a process for alumina suitable for the coating grade applications, the targets were set as stability of alumina in suspension form, suitability in the coating applications, economic alumina suspension and the scalability of the process. NCL's team developed the economical process to make alumina of desired grade and various samples were submitted to the sponsor for approval. M/s DuPont carried out the characterization study, stability study and the actual performance test. The sponsor was satisfied with samples submitted by NCL. NCL further prepared a report and submitted it to DuPont for review. The scalability of the operation was also addressed in the report. The total activity was completed in the stipulated time frame.



## 8 PUBLIC PRIVATE PARTNERSHIP PROGRAMMES

The New Millennium Indian Technology Leadership Initiative (NMITLI) envisages a symbiotic promotion and fostering of public-private partnership to enable Indian Industries to attain global leadership position in selected niche areas. The programme is backed by national determination to turn sound technological ideas into a reality through a systematic development of innovative projects. Over the last seven years, CSIR has evolved 50 projects involving over 71 industry partners and 250 R&D Institutions of India with an estimated outlay of about Rs. 400 Crores. Following projects are undertaken at NCL:

### 8.1 Polymers from biomass: cellulose, hemicellulose and lignin (Godavari Sugar Mills Ltd, Mumbai)

This project was started to utilize the vast agricultural biomass residues that are currently either wasted or grossly underutilized. For example, each year India produces about 50 million tons of dry bagasse. The idea was to fractionate biomass, with specific reference to sugarcane bagasse, into its component polymers cellulose, hemicellulose, and lignin. All these three polymers are industrially significant platform polymers, and this fractionation thus leads to excellent value-addition to an inexpensive organic resource. Thus, cellulose can be converted to cellulose acetate, a biodegradable plastic, in addition to water soluble cellulose ethers like hydroxyethylcellulose and carboxymethylcellulose.

After intensive and extensive experimentation involving several methods of fractionation, one process based on using a pressurized steam digester as reactor was shortlisted for further scaling up to a pilot plant level, in order to validate the laboratory generated data. The laboratory data had shown the feasibility of fractionating sugarcane bagasse into its component polymers cellulose, hemicellulose, and lignin. Several lab studies were made on the bagasse derived cellulose, hemicellulose, and lignin for further applications. Cellulose diacetate and triacetate were prepared and their membranes made for evaluation. Thermogravimetry was also used to assess these polymers for thermal stability in applications development. Results showed that the cellulose obtained in the process meets the requirements for conversion to cellulose derivatives, as

the cellulose acetates were soluble in organic solvents and could also be formed into membranes. During the year, the project activity was centred around procuring relevant pilot plant equipment and installing it the industrial site of GSML. The installation has been completed, and commissioning will start shortly. The estimate on the pollution load was sent to the Karnataka State Pollution Control Board.



### 8.2 Biotechnology of leather: Towards cleaner processing - Phase II (Spic Science Foundation, Chennai, CLRI, Chennai, IMTECH, Chandigarh, CCMB, Hyderabad, Madurai Kamaraj University, Madurai, Agharkar Research Institute, Pune, Indian Institute of Science, Bangalore, University of Delhi, Delhi, Pune University, Pune, Alagappa University, Karaikudi and CDFD, Hyderabad)

Production of NCL Protease 1 was scaled up in a 100L fermentor and further scaled in a 400L fermentor. Around three batches were taken varying the fermentor parameters such as aeration, agitation and media composition. Activities were low during the first 10h and slowly increased and reached maximum in 48-50h. Concentrated and stabilized enzyme was sent to CLRI for evaluation trials and demonstration of its application to leather industry.

The NCL Protease 3 from the extra cellular culture filtrate was purified to homogeneity by salting out using ammonium sulphate and DEAE ion exchange chromatography techniques. The crude culture filtrate was subjected to fractional ammonium sulphate precipitation. Nearly 70% activity and 45% protein were



recovered in 40-70% ammonium sulphate fraction. This fraction was dialyzed and loaded on DEAE-cellulose column previously equilibrated with 0.05 M phosphate buffer pH 7.0. The unbound enzyme was eluted with 0.05 M phosphate buffer pH 7.0 and with enzyme and protein recoveries of 38.6% and 3.85%, respectively. This sample showed a ten-fold increase in specific activity compared to the crude culture filtrate. The sample was concentrated by lyophilization and loaded on the cationic analytical PAGE (pH 4.3 system). A single protein band was observed on silver staining. The enzyme has a molecular weight of 28kDa as determined by SDS PAGE.

### 8.3 Biotechnological approaches for improvement of plant species with special reference to pulp and paper (IHBT, Palampur; CIMAP, Lucknow; NBRI, Lucknow; University of Lucknow, Lucknow; Osmania University, Hyderabad; FRI, Dehradun; KFRI, Peechi; ITC, Hyderabad; JK Paper, Raigada; and Ballarpur Industries Limited, Chandrapur)

The aims of the present endeavour are to exploit the existing *Leucaena leucocephala* and *Ochlandra travancorica* genetic diversity and also develop pulpwood plant species by genetic engineering of the target plants for altered lignin and cellulose content. Two full length genomic and cDNA clones of CCoAOMT have been cloned, sequenced and characterized. They show more than 85% homology at nucleic acid level and >90% homology at amino acid level. Full length genes have been cloned in expression vector pET30(b) within restriction sites Nde I and Xho I so as to express CCoAOMT protein with C terminus HisTag. The recombinant CCoAOMT protein has been expressed in *E. coli* strain BL-21 and its purification was done using Ni chelated column and also from inclusion bodies. Polyclonal antibodies were raised in rabbits which will be used for immunocytolocalization to study spatial and temporal expression. Two partial promoters of CCoAOMT have also been isolated, cloned and sequenced. They show all the essential elements of core promoter. QRTR PCR studies show that expression of CCoAOMT 1 gene is negligible in seedlings of one month age, but CCoAOMT 2 gene is expressed maximum in leaf with rachis, followed by root and least in stem. After isolation of full length genes of CAD, 4CL, CCoAOMT,

CCR, CAId5H and CBG, UTRs of these genes have also been isolated for differentiating among gene family. 4CL, CAD and CCR genes have been cloned in expression vectors for isolation of proteins and development of polyclonal antibodies. Transformation of *Leucaena* and tobacco is being done using *Agrobacterium* and biolistic gun approach with anti-sense and sense construct of the above genes. Transgenic *Leucaena* and tobacco plants are being analysed for expression of genes by QRT PCR and proteins by ELISA.

### 8.4 Development of novel fungicides (Indian Institute of Chemical Technology, Hyderabad, Rallies India Ltd., Bangalore, Institute of Microbial Technology, Chandigarh and MS University, Baroda)

In view of the need to develop novel fungicides to counter the resistance and to ensure environmental safety it is increasingly becoming essential to develop not only new chemical classes of compounds but also to identify novel targets or novel biological pathways that can be disrupted resulting in the effective control of fungal pathogens. This will ensure continuous production of wide variety of crops and sustainability of Indian Agriculture.

In this regard, nine targets have been identified for the development of target specific antifungal agents. A novel *in vivo* haploinsufficiency assay has been developed using mutants of *Saccharomyces cerevisiae*. The active compounds were used for plate assay with the target plant pathogens for validation. In the period of report, about 200 target specific compounds synthesized at NCL and IICT and 600 plus compounds from commercial libraries, were tested. Eight compounds which were target specific at 5 ppm concentration were identified. Two were specific against chitin synthase, an exclusive target for antifungal agents. While 60 compounds showed target specificity at 10 ppm concentration. The field performance testing is being carried out for these compounds.

Furthermore, in addition to the synthesis of organic molecules, different microorganisms (mesophiles as well as extremophiles) were isolated from a variety of soil samples which can be used as a potential source of enzyme inhibitors. One of the microbial products was found specific against ornithine decarboxylase. Four microbial extracts are being purified for further studies.



As chitinase could also be one of the targets for antifungal agents a rapid and sensitive method for screening of chitinase inhibitors using Ostazin Brilliant Red labelled chitin as a substrate for chitinase assay has been developed in NCL.

### 8.5 Lactic acid and lactic acid based polymers - establishment of a 300 TPA pilot plant for lactic acid production (Godavari Sugars Pvt. Ltd. (Somaiya Group of Industries), Mumbai and Indian Institute of Technology, Bombay)

In continuation of NMITIL project for lactic acid polymers, a new project entitled 'Lactic acid and lactic acid based polymers - establishment of a 300 TPA pilot plant for lactic acid production' was initiated. The mutant of *Lactobacillus delbrueckii*, Uc-3 was found to produce high amount of lactic acid with higher productivities (4g/l/h) in a medium containing low amounts of yeast extract than parental strain. This mutant also produces lactic acid (90g/L) from molasses sugar (102g/L) with higher productivity (5.1g/L/h). The mutant strain was also found to utilize cellobiose (100g/L) and converted it in to lactic acid (90g/L) within 40 h. These results showed commercial potential for this strain for conversion of cellulosic biomass to lactic acid. The initial experimentation on conversion of bagasse derived cellulose to lactic acid proved that the mutant could be a potential candidate for conversion of biomass to lactic acid. The mutant of *Lactobacillus delbrueckii*, isolated in the earlier stage will be scaled at a pilot plant at an industrial location. A plant for downstream recovery of the lactic acid of one kg / hour was established. Experiments are in progress in this pilot plant for sizing of the equipment for the 300 TPA plant.

### 8.6 Development of fuel cells based on hydrogen (Central Electrochemical Research Institute, Karaikudi, Central Glass and Ceramic Research Institute, Kolkata, Central Mechanical Engineering Research Institute, Durgapur, Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Petroleum, Dehradun, National Aeronautical Laboratory, Bangalore)

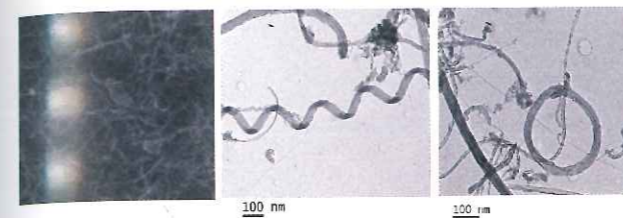
#### 1. Hydrogen generation

A program was initiated to develop an auto-thermal reforming (ATR) based fuel processor. ATR Fuel processor is expected to use all honeycomb monolith based catalysts. A catalyst evaluation facility for ATR catalysts has been built and a separate dedicated facility for water gas shift catalyst testing has been created. In addition, various experimental facilities required for wash coating of monoliths such as high power ball mill, viscometer etc have been set up. Two hybrid (SR+CPOX) catalysts that are supported on ceria-mixed oxide support, containing Rh, Pt and Pd were prepared. This catalyst was initially evaluated for about 400 hours by passing the LPG feed through a sulphur trap. Subsequently, the testing was done for various periods with and without sulphur trap in the LPG line. Many other catalysts based on perovskite structures having Pt and Rh were tested.

A new start-up procedure for ATR fuel processor operation was designed. A small quantity (5 cc) of Pt-Alumina (preferential oxidation catalyst) was loaded above the monolith catalyst. Hydrogen and air in stoichiometric quantities was passed in the ATR and the quantities were increased to get 400°C temperature at the monolith outlet. LPG/ methane was then started in small quantity and increased at regular intervals while hydrogen was decreased and the temperature was maintained constant. A fuel processor with 300 LPH of hydrogen was tested for further scale-up

#### 2. Hydrogen storage

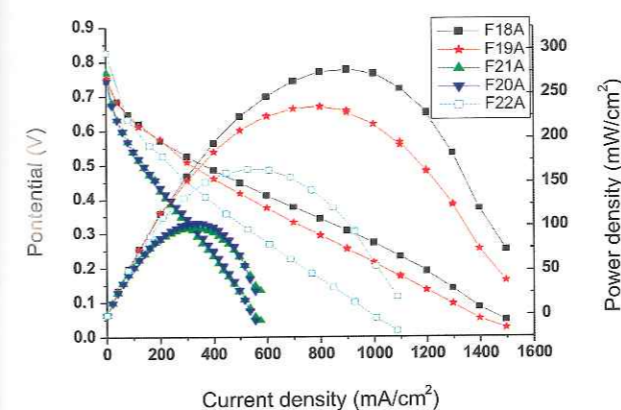
Carbon-based nanostructured materials are attractive systems for reversible hydrogen storage. A new catalyst material was prepared from a mixture of transition metals and inorganic oxide support ( $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ ,  $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and  $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ ). The yield of carbon deposit depends on the textural properties and the new catalyst yielded very high amount of carbon deposit in contrast to the low yields for Fe-Mo catalyst.



Methane decomposition on Fe-Co-Ni catalyst produced uniform CNTs in high abundance with well-defined structures and high aspect ratio. The diameter of multiwalled CNTs was in the range of 20-50 nm as shown by TEM images.

#### 3. Hydrogen utilization: PEM fuel cells

Fabrication of membrane electrode assembly (MEA) is one of the key processes in fuel cell technology. In order to have a systematic study of MEA fabrication for PBI as an alternative for the expensive nafion membrane based fuel cells, a  $2^{7-3}$  fractional factorial optimization was started. After completing two sets of 16 factorial experiments the results were analysed through Yates analysis. Six optimization experiments using PBI membranes were designed. The polarization plots obtained in these optimization experiments are shown below. The PBI based MEA showed equivalent performance to values reported in the literature.

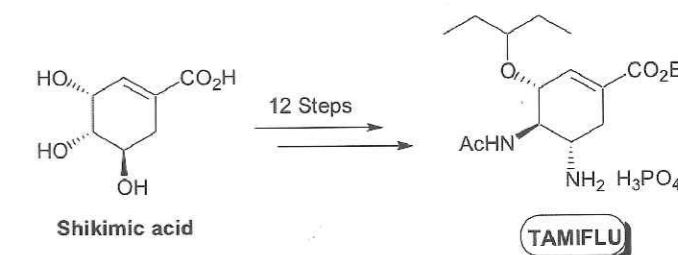


Polarization plots for the optimal designs of membrane-electrode assemblies obtained ( $2^{7-3}$  factorial design) design 18 to F22 at 160°C

Injection moldable composite bipolar plates were also developed. The design of the mould has been finalized.

#### 8.7 Process development for Tamiflu Antiinfluenza drug

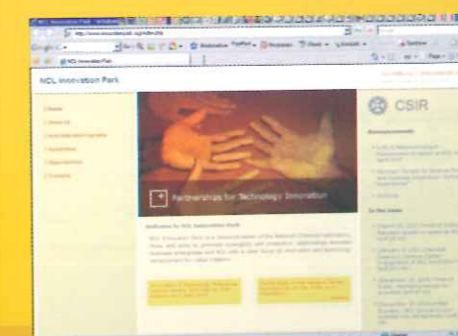
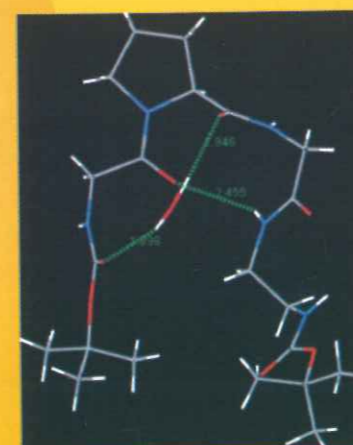
Roche's 954104 (Oseltamavir) and available in market as Tamiflu®, is recommended as the best choice amongst the currently available antiinfluenza drugs as it is active against about 3000 types of influenza virus. A laboratory scale process starting from shikimic acid was developed along with establishing a couple of novel routes for the synthesis of advanced intermediates of tamiflu® process. The required analytical HPLC and/or GC methods for monitoring each reaction, to establish the purity of intermediates and final products were developed. The less number of tedious purifications like chromatography, and coupling of two synthetic steps together for operational simplicity characterize the process established.



# NOTES

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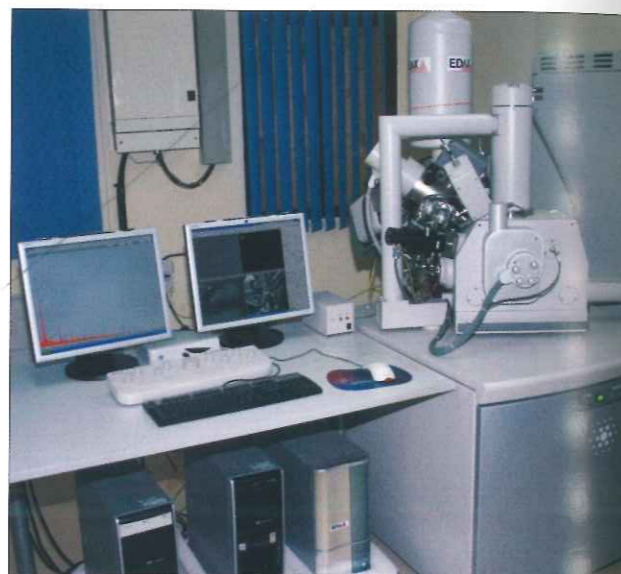
### CENTER FOR MATERIALS CHARACTERIZATION

Center for Materials Characterization (CMC) houses some of the most sophisticated equipments utilized for R & D projects of the Laboratory. The Center is run by core member scientists of the Center as well as by the affiliate scientists from other divisions of NCL. This is perhaps the only Center in India having this wide range of facilities under one roof. The facilities that houses Transmission electron microscope, Scanning electron microscope, MALDI-TOF-MS, LC-MS/MS-TOF, High resolution mass spectrometry, SMART APEX single crystals x-ray diffractometer, Electron spectrometer for chemical analysis, vibrating sample magnetometer is at the heart of the research projects from government funding agencies, Indian and overseas industries, academic institutions, universities and even some small scale industries around the area. This year Quanta 200 3D Scanning Electron Microscopy was added to the list.

#### Quanta 200 3 D scanning electron microscopy

A new scanning electron microscopy (SEM) facility has been commissioned at CMC. The equipment The Quanta 3D DualBeam® is a combination of two systems: i) An environmental scanning electron microscope (ESEM) A tungsten electron column capable of producing high resolution electron micrographs (3nm resolution at 30KV) both at high vacuum conditions as well as at low vacuum or environmental sample chamber conditions (1- 20 Torr). It allows seamless transition from one vacuum mode to the other, and ii) A focused ion beam microscope (FIB) -- an ion beam system that is capable of fast and precise milling of the specimen material, revealing the structure under the surface layer, making cross sections, deposition layers, etc. The ion system produces high-resolution images as well. FIB/SEM workstations provide an expanded range of capabilities not possible with separate FIB and SEM tools. The system makes it possible to image, section and analyze a wide range of conducting as well as non-conducting samples. It offers the capability for in-situ dynamic experiments, 3D imaging and analysis and transmission electron microscope (TEM) sample preparation for more in-depth analysis. NCL has undertaken major research initiatives in the area of nano-materials, biomaterials, organic-inorganic hybrid materials as well as soft materials (polymer gels, swollen networks, controlled release polymeric carriers, porous

polymers, metal nano-particles in various environments, etc.). These areas of research will benefit significantly as the Quanta 200 3D will enable the scientists to develop fundamental understanding on structure, composition, morphology and porosities of these novel materials. The equipment will prove to be an asset in many of the NCL's collaborative network research projects. It will also develop as an important characterization tool to be used by neighbouring educational Institutes as well as industries.



#### GLIMPSES OF CURRENT RESEARCH 1 SINGLE CRYSTAL X-RAY DIFFRACTION

The existing Oxford Cryostream, which has the temperature range of 80 - 400 K was replaced with the new Oxford Cryostream Plus system. The new accessory has an extended temperature range of 80-500 K. The new system will help to undertake the research work on crystals at temperatures higher than 200 °C to study phase transitions, solid-state reactions and structural features over a wider dynamic range.



Oxford cryostream plus installed at Bruker SMART APEX single crystal X-ray diffractometer

#### 1.1 Crystal-to-crystal transformation among polymorphs

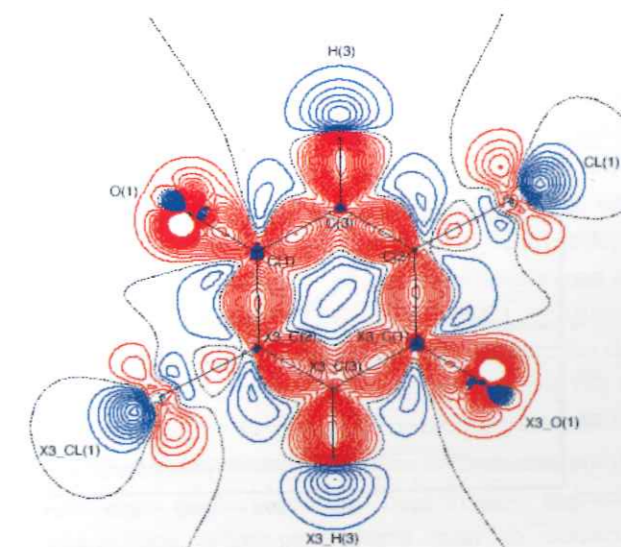
Temperature induced crystal-to-crystal phase transitions in molecular solid compounds are of high importance as they provide rather rare cases in which one crystal lattice can transform to the other molecular organization within the same solid phase. The thermal induced transformations amongst polymorphs are of great interest because of the stabilities of pharmaceutical crystalline solids. While working on solid-state chemistry of inositols, a few interesting cases of thermally induced crystal-to-crystal transformations amongst polymorphs were encountered. One such case, 2-O-tosyl-4,6-di-O-benzoyl-myo-inositol-1,3,5-orthoformate (I), which produced three polymorphs (plates and needles) at room temperature under different crystallization conditions is presented here. Interestingly, all the three forms upon heating undergo crystal-to-crystal irreversible phase transformation into the high temperature (fourth) form. These are conformational polymorphs having different orientation of the tosyl group due to freedom of rotation around O-S bond, as also observed in a few other cases. As the conformationally flexible substituents e.g., tosyl group here, are often present in pharmaceuticals compounds, such as spiro, the studies reported here become highly relevant.

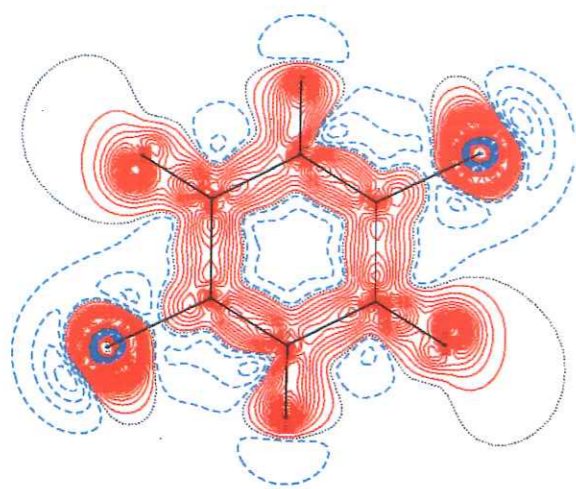


Four conformational polymorphs of (I), forms A-C occur concomitantly, all of them transform to D upon heating

#### 1.2 Experimental charge density measurements to study weak intermolecular interactions

Due to pioneering work of Philip Coppens and coworkers, crystallographic measurements at high angles allow to measure charge deformation densities to understand the intra and intermolecular interactions in a crystal. Evaluation of weak intermolecular interactions has become one of the most researched areas, which provides an insight into problems of chemistry, material science and biology. Charge density analysis is one of the direct experimental tools that allow to observe and quantify these interactions. In continuation of earlier work on halogen bonding, a compound 2,5-dichloro-1,4-benzoquinone containing strong halogen bonding contacts was taken up for charge density studies, a theoretical and experimental static deformation densities are shown.



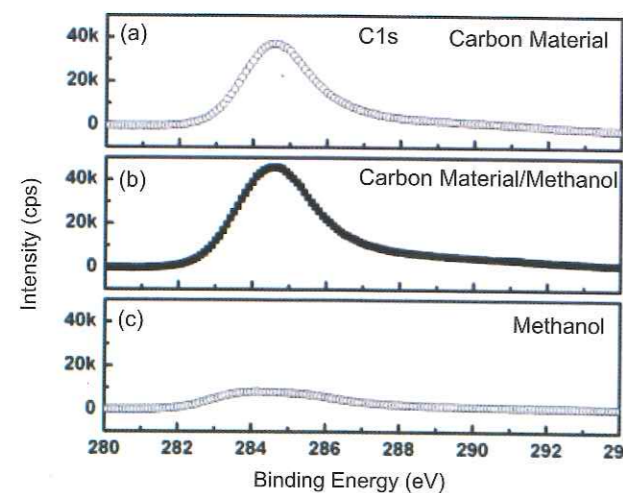


Static deformation density maps form, A) theoretical structure factor and B) experimental structure factor for (II)

2 ESCA (XPS)

2.1 Methanol adsorption on soybean oil lamp created carbon nanomaterials

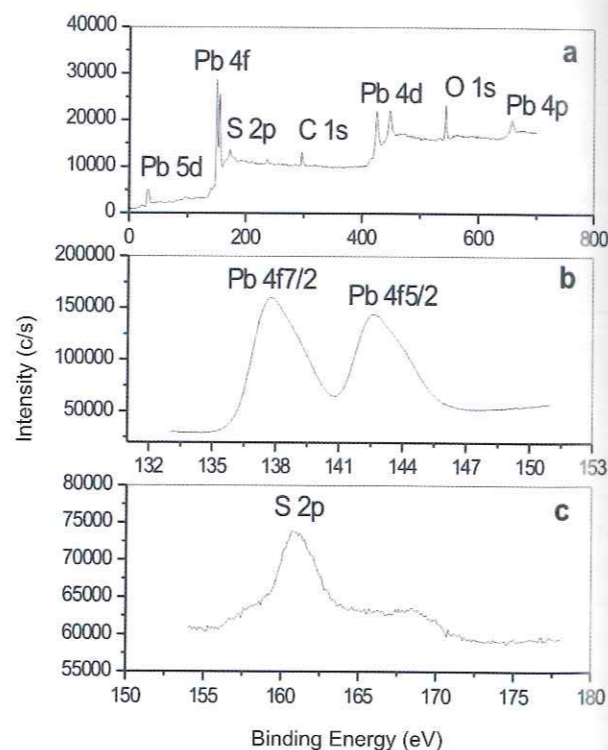
Interaction of organic molecules with inorganic materials is a hot topic today due to its relevance in many technological applications. Adsorption of methanol on soybean oil lamp created carbon nanomaterial that has been studied by X-ray photoelectron spectroscopy (XPS). XPS of the carbon material was done before and after methanol adsorption using VG Micro-Tech ESCA 3000. Part (a) of figure shows the spectrum before methanol adsorption, part (b) shows the spectrum after methanol adsorption and part (c) shows the contribution



from methanol alone. This result confirmed that the increased integrated area of XPS peak is indeed due to methanol adsorption.

2.2 Synthesis of fine pbs and pbse powder from

Lead sulphide and lead selenide are narrow band gap semiconductors useful in many applications such as infrared detectors, solar cells and optoelectronics devices. Lead sulphide and lead selenide have been synthesized via an in situ reduction of S and Se in aqueous N, N-dimethylformamide (DMF) and sodium formaldehydesulphoxylate (SFS). The quantification of the XPS peaks showed that atomic ratio of the Pb:S is approximately 49.34 : 50.66 and therefore it is believed that the formation of PbS is stoichiometric.



3. VIBRATING SAMPLE MAGNETOMETER

Among the various nanosystems under active investigation in the biological and pharmaceutical sector, magnetic nanoparticles are possibly at the forefront because of the range of their potential applications in drug delivery systems, hyperthermia applications,

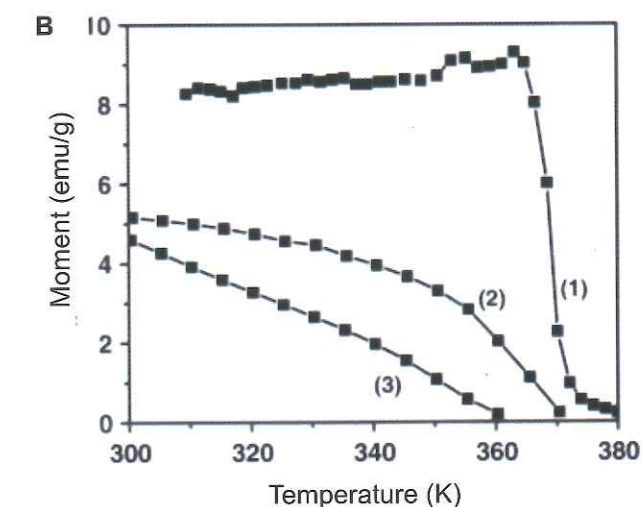
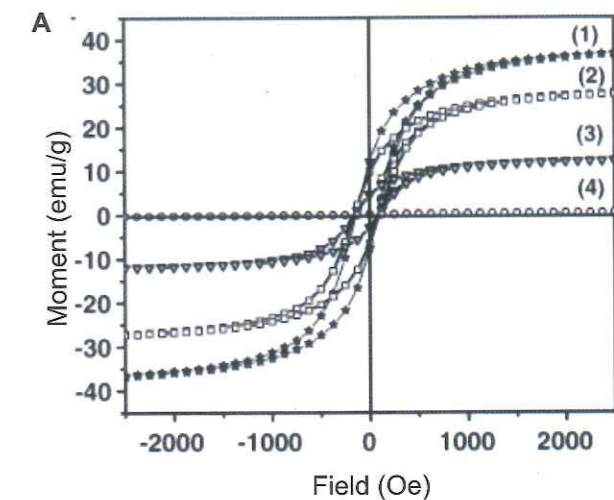


magnetic resonance imaging, contrast imaging, magnetic separation, and magneto-fluids. The ability to control and manipulate magnetic particles by a remote magnetic force, the penetrability of bio organisms/ systems to magnetic field and some unique properties of magnetic nanoparticles offer interesting application avenues for such particles in biomedicine

3.1 Magnetic nanoparticles as hyperthermia agents

LSMO nanoparticles are evaluated as possible candidates for hyperthermia applications. Since, the basic LSMO system has a Curie temperature of ~ 365 K, it promises self-control over rise in temperature, which is a highly desirable property from the point of safe hyperthermia. Cerium doped  $La_{0.7}Sr_{0.3}MnO_3$  ( $La_{0.7-x}Ce_xSr_{0.3}MnO_3$  with  $0 \leq x \leq 0.7$ ) nanoparticles were synthesized by citrate-gel route (in collaboration with Agharkar Research Institute, Pune) and the magnetic behavior of the system was studied by vibrating sample magnetometer. Figure A, shows the hysteresis loops for (1) LSMO (2) LCSMO10 (3) LCSMO40, and (4) CSMO samples taken at room temperature. The data for pure LSMO show saturation magnetization of 36 emu/g. The saturation moment is seen to decrease progressively with increasing Ce concentration. With Ce doping, segregation of  $CeO_2$  nanoparticles clusters is observed with a systematic decrease in the saturation magnetic moment at room temperature. Figure B, shows the dependence of magnetic moment on temperature for (1) LSMO, (2) LCSMO10, and (3) LCSMO40 samples. It can be clearly seen that the moment reduces with increasing Ce in the composition. A broad nature of transition can be attributed to stoichiometry imbalance and chaotic magnetic structure.

These nanoparticles were evaluated for hyperthermia treatment and toxicity. It was found that they serve the purpose of hyperthermia agent well, but the corresponding toxicity is acceptable only at low dose values. Thus, cerium doping in LSMO leads to dramatic improvement in toxicity tolerance without compromising the microwave absorption and the related heating effects of interest to hyperthermia.

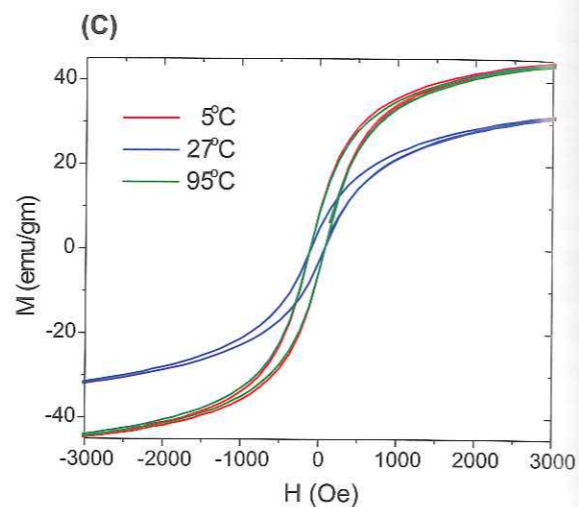
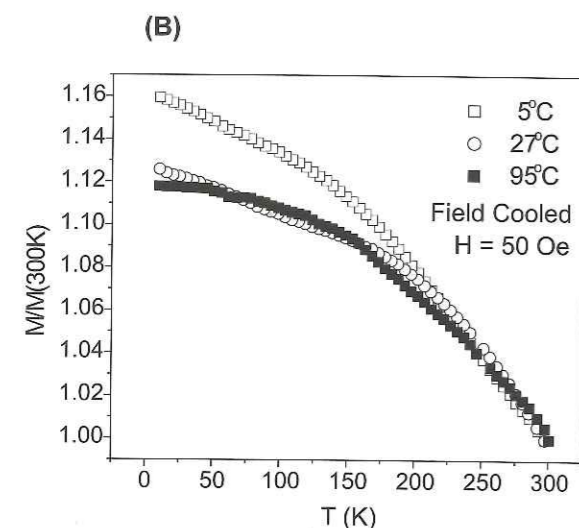
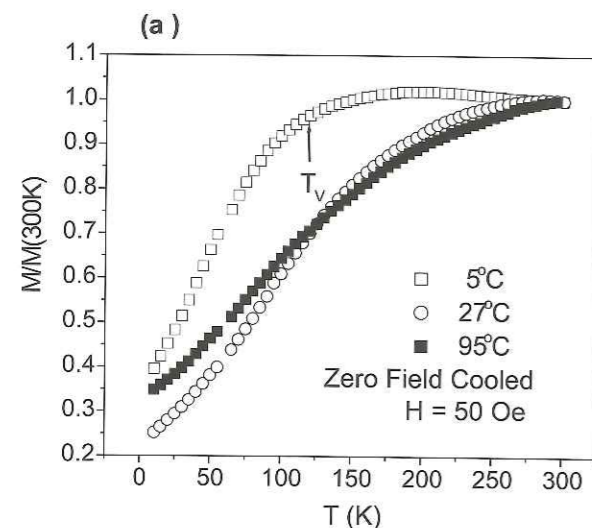


3.2 Magnetic studies on low temperature synthesized magnetite/maghemite particles

Synthesis of iron oxide nanoparticles by a simple chemical protocol was developed and the magnetic characterization was studied on VSM, EG&G PAR4500 system. The nanoparticles synthesized at the lowest temperature of 5°C exhibited magnetite phase, while increase in the growth temperature to 95 °C leads to pure maghemite phase. The results of field cooled and zero-field cooled (FC and ZFC) magnetic measurements are shown in figure a and b. The data were normalized at room temperature to bring out the differences in the three cases. The blocking temperature in all the cases is found to be close to room temperature. The origin of this effect can be attributed to contact interactions which effectively lead to collective behaviour and apparent



Larger blocking temperatures. The room temperature hysteresis loops for all the three samples are shown in figure c. The fact that the nano particles synthesized at all the three temperatures showed finite coercive field at room temperature implies that the blocking temperature TB is higher than 300 K, which, as mentioned earlier, can be attributed to the collective behaviour of superparamagnetic particles in contact. As the temperature of synthesis is varied, the value of saturation magnetization (Ms) is seen to change. This work was carried out in collaboration with chemistry department of Pune University.



Analytical and testing facilities

CMC also coordinated the analytical services from within CMC and other divisions. Elemental analysis, MS, surface area measurements (BATE), etc. were extended as research/ technical aid to various industries, research students and research institutes. The facilities like elemental analysis, XRD, NMR, etc. have been used for drug identification and drug-master file making by many pharmaceutical companies and rest for research purpose in characterization of various compounds of high importance and interests. These include ceramics, catalysts, ferrites, polymers, etc.

A summary of annual utilization report (1st April 2006 to 31st March 2007) of these services is tabulated below:

	In-house	Outside	Total
No. of Samples	11811	446	12257
Amount (Rs.)	—	15.20Lacs	15.20 Lacs



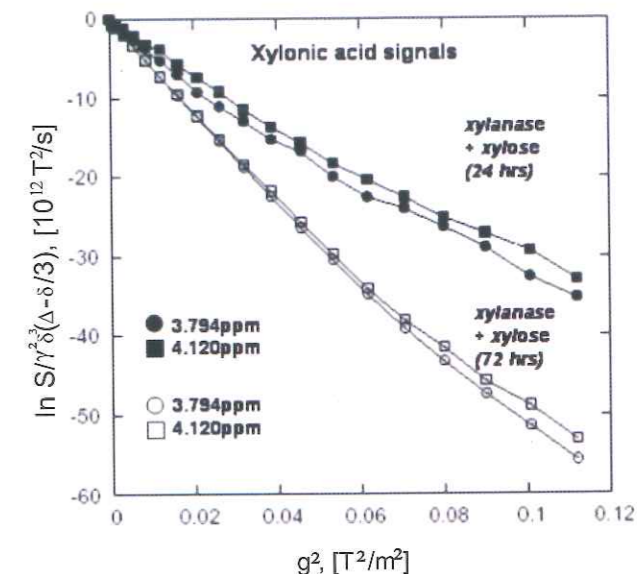
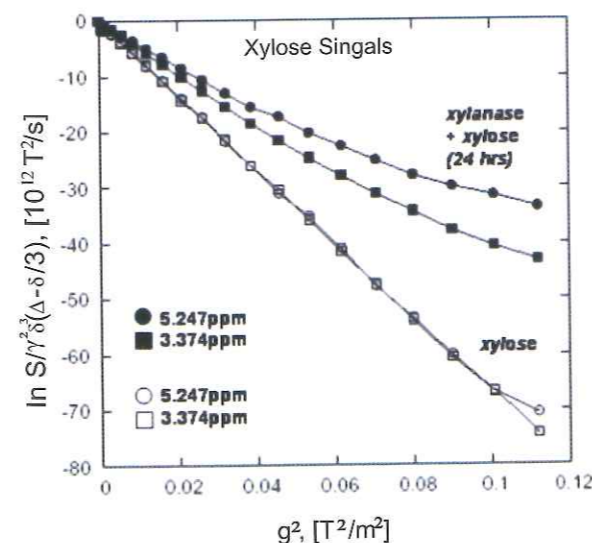
CENTRAL NMR FACILITY

1. STRUCTURAL CHARACTERIZATION

1.1 Binding of xylose to xylanase

Protein-Carbohydrate interactions are very important for many biological processes such as synthesis or hydrolysis of polysaccharides, intercellular trafficking, signaling, carbohydrate based cellular recognition etc. Xylanases are carbohydrate active enzymes with possessing various binding modules and a variety of mono-, di- and oligosaccharides can bind to these modules. Binding of small ligands to proteins can be conveniently studied by NMR spectroscopic techniques either by examining changes in protein spectra or ligand spectra. NMR experiments can provide information about the conformation as well as the movement of the ligand in the binding site.

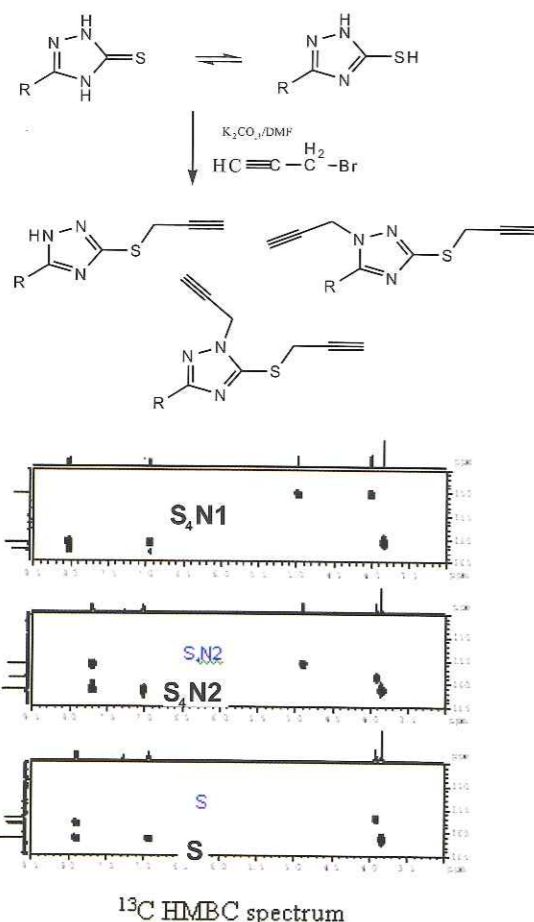
Binding of xylose with xylanase, obtained from an alkalophilic *Bacillus* (NCL 87-6-10), has been followed by NMR spectroscopic techniques with special emphasis to the measurement of self-diffusion coefficients. The investigation showed that xylose initially binds to xylanase and undergoes an oxidative transformation to xylonic acid which get detached from the protein molecule with time. The *in situ* transformation of xylose to xylonic acid was also followed by various NMR spectroscopic techniques



1.2 Structural studies on propargylated triazole thiols

1,2,4-Triazoles are very stable compounds and show wide range of biological activities such as antifungal plant growth regulator, coronary dilator, broad spectrum antiviral activity. Alkylated products such as the propargyl derivative of triazoles are key intermediates for the synthesis of different heterocycles. In substituted 1,2,4-triazole-3-thiol, which itself exhibits thiol-thione tautomerism, the differences in reactivity of N1, N2 and N4 atoms are of particular interest. In alkylation of triazole thiols, multiple nucleophilic sites are available for an incoming electrophile, as sulphur donates proton to annular system and complicates prototropy further. Propargylation of 3-substituted-1,2,4-triazole-5-thiols with propargyl bromide in K<sub>2</sub>CO<sub>3</sub>/DMF at room temperature furnished three products which have been characterized by <sup>1</sup>H, <sup>13</sup>C, <sup>15</sup>N NMR, 1D and 2D NMR techniques. The NMR investigations unambiguously established the formation of S, N1 and S, N2 dipropargyl products in the reaction.

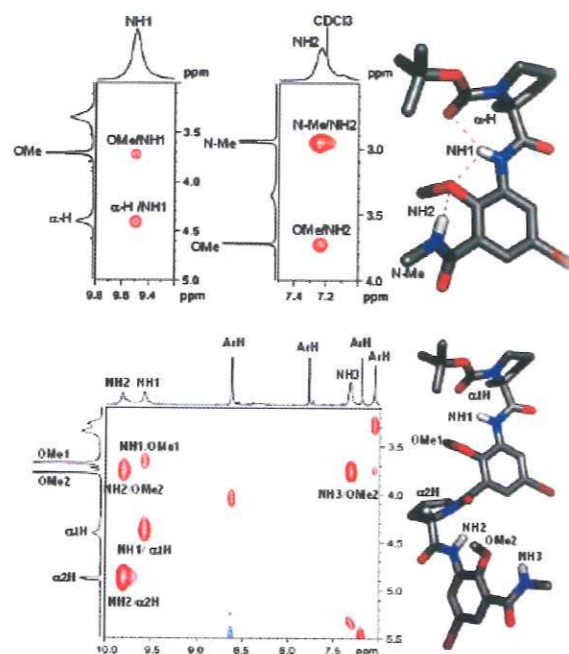




### 1.3 NMR studies on synthetic foldamers

Foldamers are molecules of oligomeric size that folds into a conformationally ordered state in solution. They are stabilized by non-covalent interactions between non-adjacent monomer units. Study of foldamers has both practical and fundamental applications and is an emerging field, which holds promise for new medicine, materials and greater insights into molecular folding. NMR techniques are used to study the structure and conformational flexibility in foldamers of various types. Studies of molecular conformation is being carried out by applying homonuclear methods such as NOESY, ROESY, TOCSY etc together with heteronuclear experiments involving natural abundance  $^{13}\text{C}$ . NMR investigations were carried out on a novel hybrid foldamer, derived from a conformationally constrained aliphatic-aromatic amino acid conjugate. NMR studies show that the foldamer adopts a well-defined, compact, three-dimensional structure, governed by a combined conformational restriction imposed by the individual

amino acids from which the foldamer is composed. NMR conformational studies were also carried out on another novel foldamer system which was found to display periodic gamma-turn conformations stabilized by intramolecular bifurcated hydrogen bonds.

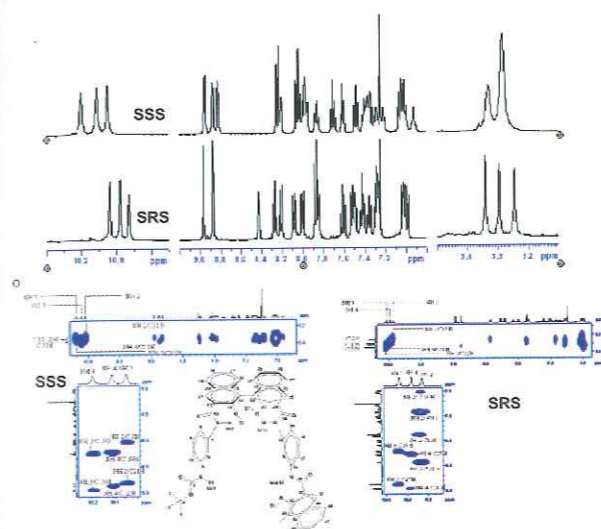


### 1.4 Conformational studies on two-dimensional aromatic foldamers

Extensive NMR studies have been undertaken to investigate the conformational preferences a novel class of foldamers viz two-dimensional aromatic foldamers in solution. We also developed BINOL-pyridine-based hybrid foldamer structures, which differ only in their chirality, yet diverge distinctly in their structural architecture. Structural investigation by NMR studies showed that they differ markedly in their conformation which is also in line with the *ab initio* calculations of these systems carried out at the HF/6-31G\* level (This work has been carried out in collaboration with Institut für Biochemie, Universität Leipzig, Leipzig, Germany).

### 1.5 Role of water in a GPGGX mimic

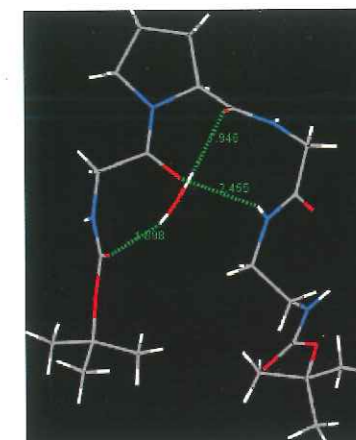
Spider Flagelliform silk, having more than 200% extensibility, is one of the most elastic natural materials



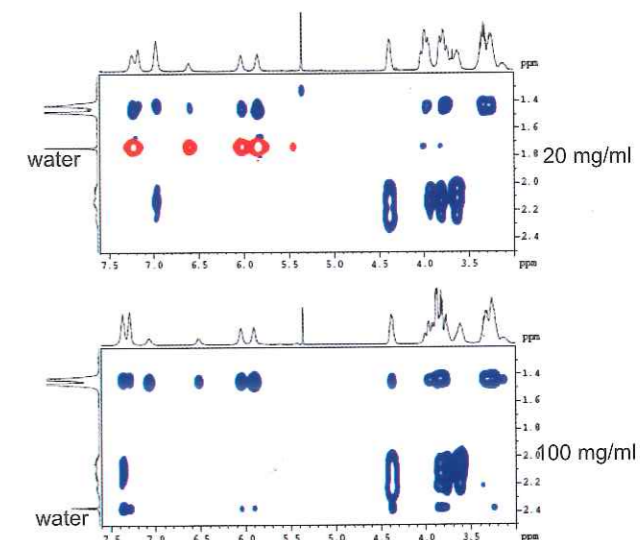
known. This amazing biopolymer contains a repeat pentapeptide sequence (Gly1-Pro2-Gly3-Gly4-X5aa) $_n$ . The "turn site" ( $\beta$ -turn) in each pentapeptide sequence, having an embedded water molecule, is thought to be providing the protein its characteristic elastic property. The backbone hydration at the turn site is suggested to be strongly influencing the physical property of this silk form, although clear evidences for such a proposition are yet to be obtained. In order to gather evidences to this *hydration hypothesis* at the turn site, we recently made several derivatives of the repeat pentapeptide sequence by amidating the C-terminal of Gly4 with various amines. One of the analogs of the flagelliform pentapeptide sequence (Gly1-Pro2-Gly3-Gly4-X5aa) $_n$  having a reduced glycine at the fourth position, crystallized relatively easily. This analog was found to have a water molecule inserted at the *turn site* of the peptide backbone, according to crystal structure studies. Conformational studies by NMR in solution-state clearly confirmed the existence of the  $\beta$ -turn conformation at the Pro-Gly site and also the presence of water molecule. Interestingly, several shorter analogs of this peptide sequence showed an unusual three-centered hydrogen bonding interaction, confirmed by both single crystal X-ray and NMR studies.

### 1.6 Dynamics of protein and RNA in a protein-RNA complex

In an effort to understand the role of molecular flexibility in the intermolecular recognition process, the internal dynamics of both interacting partners in a protein-RNA



NOESY in DCM 298K with 1.25 s Mixing time



Single crystal X-ray structure showing binding of water to the peptide backbone

complex was investigated by heteronuclear NMR relaxation rate measurements at multiple fields. The system examined is a complex of an eighty one residue protein (sterile alpha motif domain of *Saccharomyces cerevisiae*) and a twenty-three nucleotide stem-loop RNA. Longitudinal and transverse relaxation rates along with heteronuclear NOE and transverse CSA/dipole cross correlation rates were measured for the backbone  $^{15}\text{N}$  nuclei of the protein in its free form and when complexed to the RNA.  $^{13}\text{C}$  longitudinal and transverse relaxation rates together with heteronuclear NOE were measured for the base and sugar moieties in the RNA. In addition spin-lock field dependence of transverse



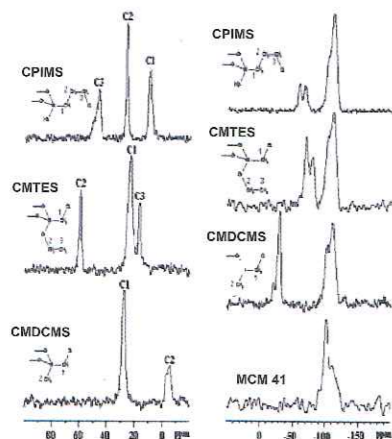
addition spin-lock field dependence of transverse relaxation rates in the rotating frame was measured to gain insights into slow motions in the RNA. (This work has been carried out in collaboration with Institute for Molecular Biology and Biophysics, ETH, Zurich, Switzerland).

### 1.7 Studies on organic-inorganic hybrid systems

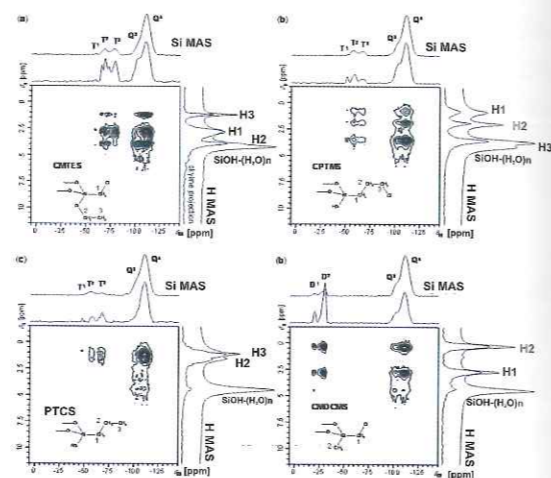
The major challenge in the study of functionalized-MCM-41, is to know the type of environments that are formed. For their structural characterization, X-ray diffraction is rather restrictive and other spectroscopic methods are of no avail. Solid state NMR, using  $^{29}\text{Si}$  and  $^{13}\text{C}$  as probe nuclei, has been effectively employed to provide molecular level inspection at the functionalized and non-functionalized sites. Analysis of the solid state NMR data provided valuable insights about the nature of functionalization, as well as the degree of functionalization. Deeper insights on the type of covalent linkages could be delineated from 1D and 2D solid state NMR. Further,  $^{29}\text{Si}$  chemical shielding could be determined experimentally and compared with calculations based on quantum chemical methods for the structural characterization of the MCM-41 derived materials.

### 1.8 Studies on transitional aluminas

The thermal decomposition of aluminum hydroxides yields a series of alumina phases, collectively referred to as transitional, or active, 'aluminas', in a well defined dehydration sequence resulting in  $\alpha\text{-Al}_2\text{O}_3$  as the end member. At the root of all transitional aluminas lie the



$^{13}\text{C}$  and  $^{29}\text{Si}$  CP-MAS spectra of functionalized MCM-41

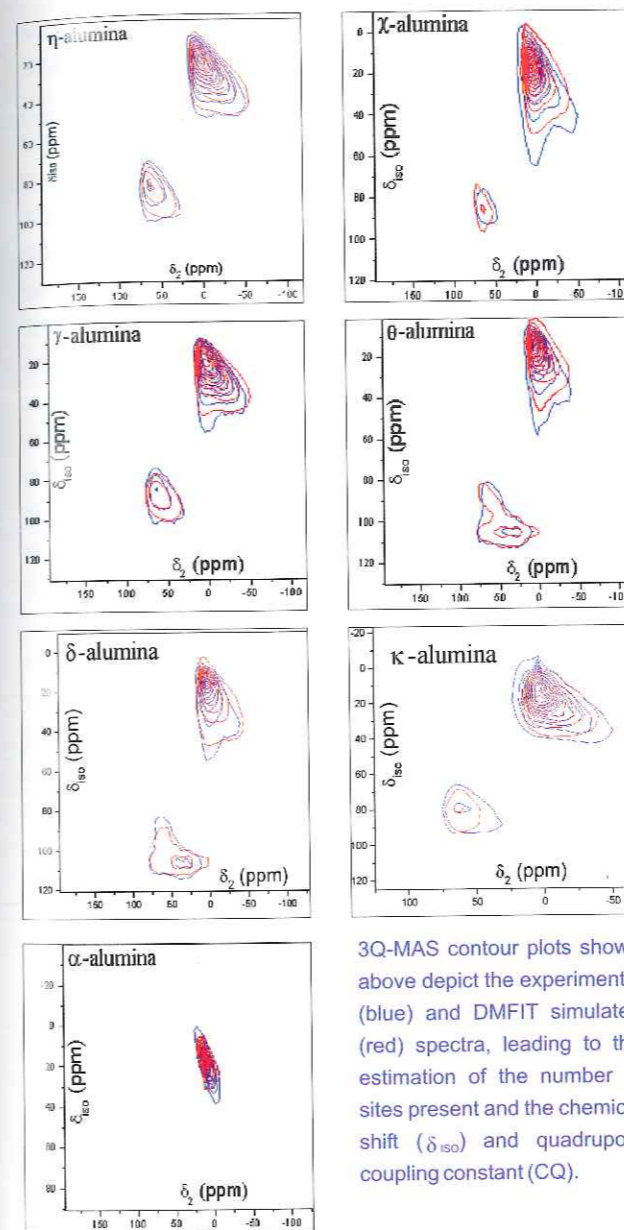


$^1\text{H}$ - $^{29}\text{Si}$  HETCOR data on functionalized

three starting materials, namely, gibbsite, bayerite and boehmite. Their controlled thermal decomposition yields the various alumina phases. Gibbsite decomposition generates  $\chi$ - $\kappa$ - $\alpha$  phases, in contrast to the  $\eta$ - $\theta$ - $\alpha$  phases generated from bayerite and the  $\gamma$ - $\delta$ - $\theta$ - $\alpha$  phases from boehmite. Each of the intermediate phases so generated exhibited unique structural characteristics, in terms of texture, morphology, particle size, cation vacancies and crystallinity and hence places them among the most widely used materials as catalysts, refractories, adsorbents, desiccants and binders. Proper characterization of these materials is of utmost importance to understand its properties. A complete NMR characterization of the all the transitional aluminas, derived from the thermal decomposition of gibbsite, bayerite and boehmite, based on  $^{27}\text{Al}$  3Q-MAS experiments and their analysis in conjunction with  $^{27}\text{Al}$  MAS experiments conducted at the same magnetic field strength have been carried out.

### 1.9 HRMAS NMR studies on breast cancer tissues

Breast cancer is the most frequent form of cancer in women and improved diagnostic methods are desirable. Malignant cells have altered metabolism and metabolic mapping might become a tool in cancer diagnostic. High-resolution magic angle spinning (HR-MAS) MR spectroscopy of tissues biopsies provides information on metabolic composition. Preliminary investigations by various 1D and 2D experiments on the



3Q-MAS contour plots shown above depict the experimental (blue) and DMFIT simulated (red) spectra, leading to the estimation of the number of sites present and the chemical shift ( $\delta_{iso}$ ) and quadrupole coupling constant (CQ).

breast cancer tissue samples by HRMAS and PCA extracts by conventional solution state NMR techniques have been carried out for identification of metabolites and the molecular markers. (This work has been carried out in collaboration with Ruby Hall Research Centre/ Jehangir Hospital, Pune).

## 2 APPLICATION OF SOLID-STATE NMR FOR THE STUDY OF ADVANCED MATERIALS

### 2.1 Spinel nanoparticles

Spinel ferrites are a class of chemically and thermally stable materials suitable for a wide variety of applications including magnetic recording media, magnetic storage

including magnetic recording media, magnetic storage and retrieval of information, information technology, telecommunication, sensors, pigments, catalysts etc. Nano-meter sized ferrite particles offer great advantages and applications in many important areas. For many of its applications, high surface area, small crystalline size and special active sites are greatly desired. "Nanosize" powder particles (a few nanometers in diameter, also called nano-particles) are potentially important in ceramics, powder metallurgy and because of their interesting magnetic properties. Therefore, in the recent years, the synthesis and study of the nanometer-sized ferrite particles have been the focus of intense fundamental and applied research with special emphasis on their size-dependent properties. Decreasing size of the ferrite particles to nanometer size will change the surface to volume ratio and this will strongly influence the magnetic properties of these materials. Normally, degree of the distribution of the ions in the tetrahedral and octahedral sites cannot be predicted in the case of the nanoparticles. Therefore, studying and understanding the coordination and distribution behavior of the different metal ions in the ferrite nanoparticles are very important. However, it is very difficult to get this information from the usual structural characterization techniques. Solid state NMR is a powerful technique to obtain information on local structural variations. However, it is extremely difficult to analyze magnetic materials using NMR. One of the options is to synthesize nanoparticles of a non-magnetic model compound having similar structure as that of a ferrite and study its structural characteristics using solid state NMR and then to extrapolate the results to magnetic spinels. Magnesium aluminate, is the most suitable candidate for such studies as the  $^{27}\text{Al}$  nuclei can be probed by NMR. Thus, we have carried out the  $^{27}\text{Al}$  NMR analysis of  $\text{MgAl}_2\text{O}_4$  of different sizes and have estimated their cation distributions.

### 2.2 Polymer dynamics and morphology

The mechanical properties of polycarbonate copolymers depend on the molecular and segmental motions that are present in the system. The aim of this project is to detect and measure the molecular and the segmental motions of polycarbonate copolymers by solid-state NMR techniques and then correlate it with other macroscopic techniques like the Dynamical Mechanical Analysis



(DMA). In solid-state NMR, there are different experiments which probe different time-scales of motion. In this project, we have used the conventional solid-state NMR techniques like relaxation studies and new techniques like the separated local field (SLF) and the center band only detection of exchange (CODEX). Using these techniques, we have been able to measure a wide range of frequencies of motion with  $^1\text{H}$  relaxation methods able to detect motion in the MHz region and the CODEX able to detect motion in the range of 0.1 Hz to 1 KHz (please rewrite this sentence). The other modern technique, SLF is able to measure motions in the intermediate regime of the order of a few hundreds of KHz and SLF in combination with CODEX promises to give us further information on the polymer dynamics. The CODEX experiments were carried out in collaboration with University of Halle, Germany.

In semicrystalline polymers like Polyoxymethylene (POM), the crucial factor that determines the mechanical property like stiffness is their crystalline to amorphous ratios. Solid-state NMR is a powerful tool for the determination of the morphology and we have explored NMR methods like the  $^{13}\text{C}$  MAS, Inversion recovery cross polarization (IRCP) and  $^1\text{H}$   $T_2$  for the accurate determination of the morphology.

### 2.3 Functionalized materials

Heterogenization of homogenous catalytic materials has been an effective strategy to overcome the difficulties involved in the separation, purification and reusability of homogenous catalysts. One of strategies that have been adopted for the same is the encapsulation of the homogenous catalytic molecules into porous materials. Heteropolyacids (HPA) like phosphotungstic acid (PTA) are promising catalysts for many acid catalyzed reactions like benzylation of phenol. PTA can be heterogenized by impregnation or encapsulation on porous supports like silica. But due to its weak bonding interaction with the silanol group, leaching will occur. We have immobilized PTA on the surface of fumed silica by means of chemical bonding with certain organic groups like amines, imidazole and methyl imidazole. This chemical bonding was done by an alkoxy silyl group. We expect that this will result in the strong anchoring of PTA in the support and will prevent leaching. Solid-state NMR is the most important characterisation technique that can

confirm the organic modification of silica or the mesoporous materials. We have carried out a NMR investigation with  $^{29}\text{Si}$ ,  $^{13}\text{C}$ ,  $^1\text{H}$  and  $^{31}\text{P}$  solid-state NMR. Comparison of  $^{31}\text{P}$  CPMAS spectra of anchored PTA and neat PTA showed the confirmation of anchoring. Among the three catalysts, i.e., amine modified, imidazole modified and methyl imidazole modified catalysts, the catalytic activity may differ due to the difference in substituent groups. In addition, leaching will be less for that group which is strongly bonded to HPA. In order to get a better insight into the interaction between the support and HPA, we are planning to study a detailed NMR investigation using advanced techniques like heteronuclear correlation (HETCOR), rotational echo double resonance (REDOR), center band only detection of resonance (CODEX), separated local field (SLF) experiments.



### COMBI CHEM-BIO RESOURCE CENTER

#### Isolation of bioactive natural products from plants using high throughput screening

High throughput screening (HTS) group of Combi Chem-Bio Resource Center is involved in identifying targets, development of HTS protocol and running HTS programs. Anti-tubercular development is a priority area because of the alarming situation at the national and international level with the concurrent increase of multi-drug resistant strains of virulent *Mycobacterium tuberculosis* and HIV. Glutamine synthetase and nitrate reductase were chosen for developing HTS protocols and screening. Glutamine synthetase was reported to be essential for the survival of pathogenic mycobacteria whose extracellular activity could be targeted for antitubercular development. Two HTS protocols were developed in microplate format to find inhibitors against this enzyme based on its transfer as well as biosynthetic activities. A library of 2000 plant extracts and fractions was screened to validate these protocols and few samples were identified inhibiting glutamine synthetase activity. A parallel work on nitrate reductase had shown that specific inhibitors have better killing effect on dormant *M. smegmatic* than metronidazole. This enzyme is considered as a marker for dormant stage of *Mycobacteria*. Using this enzyme as biomarker, an HTS assay was developed to identify antitubercular inhibitors on *Mycobacterium bovis* BCG. These protocols are already being used for screening of in-house libraries. Apart from identifying hits, NCL has assays ready for checking specificity and general cytotoxicity on different bacterial cultures and mammalian cell lines. These assays are also being used in bioactivity guided purification of taxol derivatives where mammalian cell lines are being used.

As part of an industrially sponsored project to screen Indian medicinal plants for skin care (trypsin, tyrosinase, COX-I, COX-II and ZPT inhibition activities), 103 extracts of different Indian medicinal plants and their parts were fractionated using state-of-the-art Flash Chromatography System. About 2200 fractions were obtained and screened against trypsin, tyrosinase, COX-I, COX-II and ZPT. Fifty-four samples were identified inhibiting trypsin and tyrosinase and initially, five lead molecules are under further tier-II clinical evaluations. This study was undertaken in collaboration with Regional Research

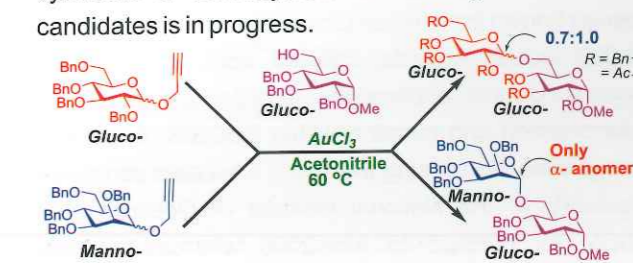
Laboratory, Jammu and Central Drug Research Institute, Lucknow.

#### Isolation of bioactive natural products from plants using flash chromatography

In an effort to obtain bioactive compounds from medicinal plants for use in pharmaceuticals, agrochemicals and other areas, two medicinal plants have been identified viz. *Lagascea mollis* and *Detarium senegalense*. Several extracts of both the plants have been prepared and isolation of bioactive constituents is in progress. Some extracts of *D. senegalense* have shown promising protease inhibition activity and isolation and structure elucidation of the active constituents are in progress.

#### Propargyl glycosides as stable glycosyl donors

Chemical synthesis of glycoconjugates using a novel transglycosylation methodology exploiting gold catalyst is demonstrated. A competing reaction in diversity oriented syntheses pathway development programme enabled to identify the peculiar behaviour of propargyl group in the presence of Au(III) salts. Extrapolation of this observation led to a novel transglycosylation protocol for the glycoside and disaccharide synthesis. The procedure developed facilitates conversion of stable propargyl glycosides to transglycosylated products in the presence of catalytic quantity of  $\text{AuCl}_3$  in acetonitrile. The utility and efficacy of the transglycosylation is demonstrated using various aglycones and synthesized respective glycosides and disaccharides. It can be envisioned that transition metal mediated activation of propargyl glycosides would be advantageous as propargyl glycosides can be (i) synthesized from aldoses by modified Fisher glycosidation, (ii) stable to diverse chemical manipulations, (iii) directly used for saccharide coupling, and (iv) chemoselectively activated. Improving the stereoselectivity of the glycosylated product, exploiting the transglycosylation protocol for the synthesis of carbohydrate-based drugs and vaccine candidates is in progress.





**DIGITAL INFORMATION RESOURCE CENTER**

Digital Information Resource Center (DIRC) provides a centralized support for the information infrastructure. This includes an excellent campus wide local area network with more than 750 computers, a range of servers, internet connectivity, access to a range of digital resources including databases like Chemical Abstracts, Current Contents, Chemical Business Newsbase on the intranet and online access to a large number of electronic journals (including back volumes for many) from leading publishers like Elsevier Science, American Chemical Society, Royal Society of Chemistry and Wiley Interscience.

**Research and development programs**

Besides infrastructure activities, we are actively involved in research and developments programs in "Scientific Informatics"-primarily Chemical Informatics and Biodiversity Informatics. Some recent work is highlighted below:

**Biodiversity Informatics**

Biodiversity informatics encompasses collection, collation, analysis, prediction, and dissemination of knowledge about biotic resources. The efforts in this area are aimed at developing tools, standards, and protocols that would help improve infrastructure and capacity building leading to acceleration of national and regional progress in this emerging new discipline.

**Indian Ocean node of ocean biogeographic information system**

Indian Ocean node of ocean biogeographic information system (IndOBIS) is one the seven southern regional nodes of the ocean biogeographic information system (OBIS). Through its web portal <http://www.indobis.org>, IndOBIS advanced the agenda of collation and dissemination of data and information on biotic resources of the Indian Ocean. Currently, IndOBIS Catalogue of Life disseminates baseline information on over 40,000 species known from Indian Ocean. It currently holds over 84,000 locality records, collated from 150 years of modern scientific publications. In order to expedite the data collation and curation within IndOBIS, three data camps were held during the year. One data camp was organized at the National Institute of Oceanography (NIO), Goa during 5-16 June 2006, whereas two data

camps were organised at NCL during 10-24 July 2006 and 14-25 August 2006.

**Manthan** - In order to collate data from the public domain web based resources on continuous basis, Manthan, a marine biodiversity search engine was developed using distributed computing architecture. Using the Google API based robot, Manthan crawls URLs to index the content from marine biodiversity related portals, as well databases.

**IndOBIS DUF** - In order to invite collaborations and contributions from taxonomists and potential data holders, IndOBIS Data Upload Facility (IndOBIS DUF) was developed. This facilitated in mobilizing the data at increasing rate.

**Digitization of NIO Collection** - NIO holds valuable and rich collection of biological specimens especially the herbarium collected from various regions along Indian coast and waters. Over 800 specimens have been digitized using IndCollections, and the curated data has been upwardly linked to OBIS, through DiGIR provider. Sacred groves information system (SaGRIS) for North East India (pilot project) collated data on nearly 101 sacred groves.

**Electronic catalogues of known biota**

Information and communication technologies are being used to create collaboratory environment for biologists and ecologists ensuring that rate of exchange and sharing of information on our biotic resources improves. Electronic catalogue of known Indian fauna - Electronic Catalogue (ECAT) of (IndFauna) has collated baseline information about 94,000 known Indian faunal species (<http://www.ncbi.org.in/>). This has created a virtual pool of "Taxon Editors" who volunteer to authenticate and validate the data. It demonstrated that such a catalogue would provide a platform for collaboration within the taxonomic and ecological community. It further brings together taxonomic treatments from authors and institutions to provide a centrally collated system for Indian fauna. Other than single click access, ECAT would play the role of central registry of names of known organism, as it would provide much required baseline data for taxonomic scrutiny or revision.



IndCollections currently disseminate data associated with nearly 1500 specimens from 5 collections.

**Indian Biodiversity Information Facility (IBIF) prototype**

One of our objectives is to ensure free and open access dissemination of biodiversity knowledge to anyone, anyplace, anytime. In order to seek interoperability with cross discipline databases such as genetic, molecular, ecosystems, species, climate, geospatial, and environment as well as social and economic ones, we are

attempting to employ web services architecture. Using the open source resources such as Gremoris registry, DiGIR provider and Crawler, mySql dRDBMS prototype portal of "Indian Biodiversity Information Facility (IBIF)" accessible at <http://www.ibif.net.in/> was developed. IBIF currently provides nearly 500,000 data records provided by seven distributed databases.

**NCL Centre for Biodiversity Informatics**

Select Language: **Beta**

- Indian Biota
  - IndFauna
  - IndFlora
  - IndFungi
  - IndViruses
  - IndMicrobes
  - Threatened
  - Invasive
- Special Ecosystems
  - Sacred Groves
  - SaGRIS for NE
- Natural History
  - SAMPADA
  - IndCollections
  - Collections
  - ABCD of Indian Origin
- Traditional Knowledgebase
  - IndTMK
- Tools, Protocols, Services
  - IBIF
- Outreach & Capacity Building
  - New! BIR
  - Indian Taxonomists
  - South Asian Taxonomists
  - Indian Ocean Taxonomists
  - National Networks
  - Organizations
  - Geospatial Data Repository

Created on: 8 Aug 2003  
Updated on: 8 Oct 2007

**Gontse Gaden Rabgyeling Gompa Forest - 1**

Gontse Gaden Rabgyeling Gompa Forest - 1 is located 0.2 kilometers off Bomdila Bazar in the West Kameng (Bomdila) district of Arunachal Pradesh. This grove which extends over an area of 1 sq. km is owned by Village community and managed by Village community. The grove is dedicated to the deity Buddha by the Monpa community. The vegetation of the grove can be classified as Temperate mixed. So far, 10 species have been recorded from this grove.

Climate	
Min. temperature (°C)	N.A.
Max. temperature (°C)	N.A.
Annual rainfall (mm)	N.A.
Min. humidity (%)	N.A.
Max. humidity (%)	N.A.

**Biodiversity**

Category	Count
Microbes	0
Fungi	0
Plants	10
Animals	0

Altitude (m): 1795  
Water Sources: 2  
Threat status: Low

Deity: Buddha  
Motive: Religious  
Community: Monpa  
Festivals: 3

SaGRIS collates biological, ecological, social data on sacred groves



### NATIONAL COLLECTION OF INDUSTRIAL MICROORGANISMS

National Collection of Industrial Microorganisms (NCIM) preserves nonpathogenic, industrially important microbial cultures and provides authentic cultures to research institutes, colleges, universities and private organizations on request. The center generated an ECF of about Rs. 39 lakhs during the year by providing cultures to industries and research institutes including testing of samples.

#### Preservation of microbial cultures

The center maintains approximately 3500 microbial cultures of bacteria, yeast and fungi using regular transfer and lyophilization methods. This year the center has received 500 microbial cultures from several laboratories for preservation in response to the Network project on microbial diversity. The cultures, which are in frequent demand, are tested for their purity and biochemical performance.

#### Lyophilization of microbial cultures

The center has about 1100 microbial cultures under lyophilized form. Lyophilization of ten cultures (60 vials each) was done for a project sponsored by Biological E. Limited, Hyderabad.

#### $\alpha$ -Galactosidase from *Bacillus stearothermophilus*

An extracellular, thermostable  $\alpha$ -galactosidase from *Bacillus stearothermophilus* (NCIM-5146) was purified to homogeneity with 389 fold purification. The molecular weight of the purified enzyme as determined by SDS-PAGE and gel filtration was 79.9 and 165.9 kDa, respectively, suggesting its dimeric nature. The purified  $\alpha$  galactosidase is a non-glycosylated protein with a pI value of 4.9. The partial N-terminal sequence of  $\alpha$ -galactosidase showed remarkable homology (80 % similarity) with earlier reported  $\alpha$ -galactosidase from *Bacillus stearothermophilus* NUB 3621. The secondary structure of the enzyme determined by circular dichroism (CD) spectroscopy and analyzed by prediction method, exhibited  $\alpha/\beta$  class of protein. The pH and temperature optima for the purified enzyme are 6.5-7.0 and 65 °C, respectively. The  $\alpha$ -galactosidase is stable over a broad pH range (3-9) and its half-life of inactivation ( $t_{1/2}$ ) at 70 °C is 30 minutes. The enzyme exhibited strict anomer specificity towards the substrates and hydrolyzes  $\alpha$ -1-3-,

$\alpha$ -1-4-, and  $\alpha$ -1-6- galactosidic linkages and not the  $\beta$ -galactosidic linkages. Synthetic substrates pNPG and oNPG had lower  $K_m$  (higher affinity) and higher  $K_{cat}$  (higher rate of hydrolysis) as compared to natural substrates, melibiose, raffinose, and stachyose. Among the three natural glycosides, a disaccharide, melibiose was hydrolyzed at higher rate than the trisaccharide, raffinose, and tetrasaccharide, stachyose. The chemical modification studies indicated the role of carboxylate, lysine and tryptophan in the catalytic site of the enzyme.

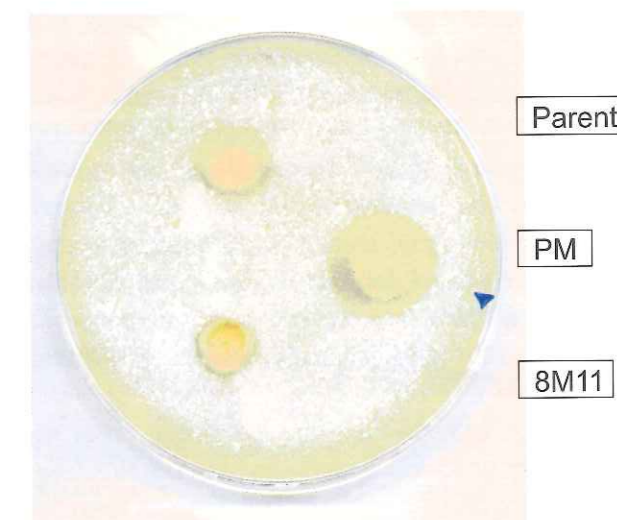
#### Phytase from *Aspergillus niger* NCIM 563

The mutation was carried out by subjecting spore suspension of *Aspergillus niger* to EMS (1%v/v) treatment followed by UV-irradiation, which resulted in 99 % killing of the spores after exposure for 4 min. Criteria for further selection of mutant are: (a) Mutants with enhanced zone of hydrolysis by phytase on calcium phytate containing plates compared to parent strain, (b) Mutants resistant to antifungal compounds like bavistin (carbendazim), and Mutants resistant to sodium azide. Easiest method of isolation of hyper secretory mutant is to spread UV mutated spores on 0.5 % calcium phytate containing plates and look for higher zone of hydrolysis. This method is also used to isolate phytase producing strains from soil. About 400 colonies of mutants were checked on calcium phytate plates for enlarged zone of hydrolysis of phytate than the parent strain. About 9 strains were selected and screened under submerged fermentation for phytase production. However, phytase activity was not enhanced than the parent strain. So UV mutation was followed by further selection method. Mutants resistant to antifungal compounds like nystatin, carbendazim (benomyl) have been reported to overproduce microbial metabolites. Attempts are being made to isolate carbendazim resistant mutants. Initial experiments demonstrated that the parent strain does not grow on carbendazim containing even at 1  $\mu$ g/ml concentration. About 12 colonies were selected which were resistant to carbendazim. Evaluation for phytase production under submerged fermentation is in progress.

Mutants of *Aspergillus niger* resistant to sodium azide are reported to secrete higher levels of ribonuclease. Mutants of the parent strain resistant to 0.025 mM sodium azide were isolated. About 16 mutants are



isolated and further streaked on calcium phytate plate to compare phytase production in comparison with parent strain. Further studies on evaluation of these mutants under submerged fermentation conditions are in progress.





NCL INNOVATIONS

The creation of NCL Innovations, a new resource center of NCL, was formally announced on 19 February 2007. The mission of NCL Innovations is to successfully exploit new ideas and to find means and ways to help the birth of new technology ideas and assist and support their translation into products and successful exploitation. The immediate goal of NCL Innovations is to build various component parts of a world-class ecosystem supporting the development and enrichment of commercially and socially useful knowledge (technology), protection and capture of value, exploitation of know-how, and the setting up of new commercial and social enterprises based on NCL know-how. Thus, NCL Innovations will bring a fresh and renewed focus to and champion the cause of technology development and acceleration, technology commercialization (in concert with Business Development Division) and new venture development.

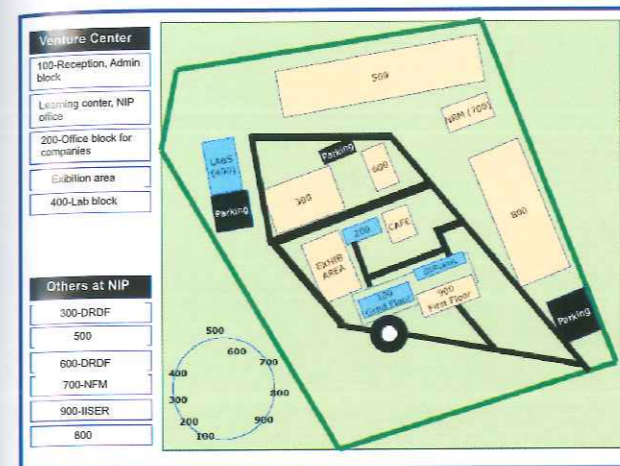
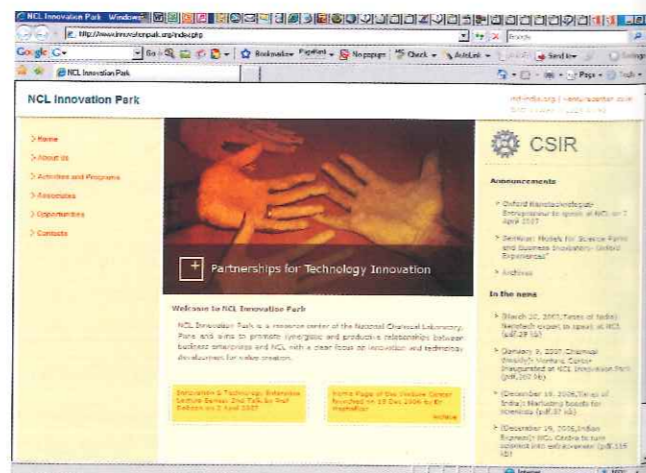
The activities of NCL Innovations:

- NCL Innovation Park (a physical and mind-space where industry and NCL will work in close concert on technology based innovation) and industry program
- Venture Center (technology business incubator) and new venture creation program  
Inspiration and learning program: Inspirational lectures and professional programs focusing on entrepreneurship, intellectual property and innovation management.
- Technology acceleration and stewardship program: Nucleate and enrich technology development activities within NCL targeting product platforms.
- Institutional mechanisms and systems: Contribute to efforts at the CSIR and NCL level to change rules and procedures so as to facilitate and be more supportive of technology development, entrepreneurship and public-private partnership.
- External projects: Project-mode engagements with external clients in the area of technology and innovation strategy and planning.

The NCL Innovation Park

The year 2006-2007 witnessed several changes in the erstwhile MERADO campus (in the close vicinity of NCL) and its transformation into and re-christening as the NCL Innovation Park. The campus also underwent a facelift with several renovations, modifications and infrastructure development. The website of the NCL Innovation Park ([www.innovationpark.org](http://www.innovationpark.org)) was launched in November 2006.

Deepak Nitrite Limited (DNL), Pune and the NCL entered into a memorandum of understanding (MoU) that allowed DNL and NCL to work closely together in identifying and pursuing research and technology development opportunities in selected areas of mutual interest, particularly relating to fine chemicals via homogeneous catalysis and contemporary methods of organic synthesis. As part of this MoU, DNL has set up an R&D centre called the Deepak R&D Foundation (DRDF) within the NCL Innovation Park. The DRDF was inaugurated on 10 March 2006 by Dr. R. A. Mashelkar, the then Director-General, CSIR. Dr. S. Sivaram, Director of NCL, Dr. M.M. Sharma, Chairman of NCL's Research Council, besides Dr. L.K. Doraiswamy and Dr. Paul Ratnasamy, both, former Directors of NCL were present on the occasion. DRDF, currently located at 300 and 600, NCL Innovation Park, is expected to move into their new research campus planned in the outskirts of Pune by 2008.



National Repository of Molecules (NRM), an intra-preneurial venture of NCL relocated its operations to its new facilities 700, NCL Innovation Park in February 2007. NRM aims to build a powerful physical library of small molecules, leveraging NCL's strong research programme in organic chemistry, along with a complementing library of research information relating to these molecules. This repository can be a significant resource for new drug development and other activities always on the lookout for new and interesting molecules

Inspiration and learning program

NCL Innovations has begun a prestigious lecture series and a seminar series during the year. These are the Innovation and Technology Enterprise Lecture Series and the NCL Innovations Seminar Series.

The Innovation and Technology Enterprise Lecture Series, which is a public lecture series, aims to present exemplary cases of research-based innovation translated into business ventures the associated ideas, the people and the experiences in order to inspire, energize and inform Indian scientists, technologists and business people. Professor Sir Richard Friend delivered the inaugural lecture of this series on 18 December 2006 on "Company start-up in Cambridge: From science to technology to products".

On the other hand, the NCL Innovations Seminar Series presents talks by people who have excelled in building institutions and institutional mechanisms/ systems to promote technology, technology commercialization and new venture development goals that are important for "NCL Innovations".

Institutional mechanisms and systems

One of the goals of NCL Innovations is to participate in and contribute to the shaping of policies, procedures and rules at the CSIR and NCL levels that have a direct impact on technology development and acceleration, technology commercialization and new venture development. NCL contributed in significant ways in shaping the scheme for setting up incubation centers in CSIR laboratories (16 June 2006).

# NOTES

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## BUSINESS DEVELOPMENT

Business Development Division (BDD) takes care of various aspects of business planning, contracts management, strategy consulting, intellectual property and event management. Significant portion of NCL's budget is generated through contract R&D services, consultancy and technology licensing. The division is staffed with engineers and management graduates who work as technology facilitators interfacing with scientists, industries, government, financial institutions, other statutory agencies, etc.

### Business facilitation

NCL is constantly exploring opportunities to work with industrial customers on challenging research problems which have an impact on their performance. NCL realizes that it is the industrial customer that keeps research relevant to and focused on real world problems and opportunities. Great emphasis is placed, therefore, on understanding customer's needs, clearly defining deliverables and meeting customer's expectations.

The BDD undertakes a mapping of skill sets and patent portfolio available at NCL and contacts industrial customers relevant under the context. It then plays a technology facilitation role through discussions related to project proposals, pricing issues and contracts management. NCL believes in the credo that NCL wins only if its customer wins. Consequently, NCL constantly aims at building a win-win relationship with all its customers. During the year NCL worked with 45 Indian and 22 foreign customers.

### Intellectual property management

The IPR unit looks after the protection of Intellectual Property Rights mainly prosecuting and securing patents for inventions in NCL. The unit is involved with scrutinizing the drafts submitted by scientists, finalizing the complete specifications and coordination with the Intellectual Property Management Division of CSIR. Ninety-five foreign and thirty-two Indian patent applications were processed during the year. IPR unit in collaboration with IPMD also oversees filing and securing patents in foreign countries including United States, Europe and other countries covered under Patent Cooperation Treaty.

### Events management and exhibitions

Business Development Division assists in planning, coordination and organisation of various types of events organized at NCL. NCL also actively participates in the exhibitions related to scientific achievements organized by other agencies at various places throughout the country.

### Exhibitions

NCL participated in the "Chemspec India 2006" held at NSE Complex, Mumbai during 5-6 April 2006, "Workshop-cum-exhibition on safe drinking water" held at National Agricultural Science Center (NASC) complex, Pusa Campus, New Delhi on 14th August 2006, "Science Expo-2006" held at Nehru Science Centre, Mumbai during 13-17 January 2007, and "Science and society exhibition" held at Mumbai University during 20-23 January 2007.



Dr Kharul delivering the popular science lecture on "Applications of membrane science and technology" at Nehru Science Centre, Mumbai



School students visit NCL stall at Nehru Science Centre, Mumbai



### Training and HRD programme

CSIR Programme on Youth for leadership in Science (CPYLS) for standard X meritorious students was organized on 27-28 December 2006 at NCL, besides faculty improvement and motivation training programme for high school and higher secondary school teachers from Solapur district at Suyash Gurukul, Solapur on 17-18 November 2006.



CPYLS-2006

### NCL'S CUSTOMERS

#### Global customers

- Alcoa Inc.
- BASF
- Biotechnology Consulting and Research Inc.
- Dow Chemical Company
- E. I. Du Pont de Nemours and Company
- DuPont Titanium Technologies
- GE Corporate Research & Development
- INVISTA Inc.
- Johnson and Johnson Vision Care Inc.
- Lanxess Deutschland GmbH
- Lyondell
- New Century Lubricants Inc.
- Nikem Research S.r.l.
- PPG Industries Inc.
- Reviva Pharmaceuticals Inc.
- Rasayan Inc.
- Scios Inc.
- Solvay Advanced Polymers L.L.C.
- Solvay Solexis S.p.A.
- Thai Organic Chemicals Company Ltd.
- The Proctor & Gamble Company
- UCB Pharma

#### Indian customers

- Ajeet Seeds Ltd.
- Alkyl Amines Chemicals Ltd.
- Ankur Seeds Pvt. Ltd.
- Aquapharm Chemicals P. Ltd.
- Arch Pharma Labs Ltd.
- Aristo Pharmaceuticals P. Ltd.
- Atul Ltd.
- Beck India
- Biological E. Limited
- Bioasset technologies
- Biosynthetics
- Cipla Ltd
- Clutch Auto Ltd.
- Deepak Nitrite Ltd.
- Dr. Reddy's Laboratories Ltd.
- Emcure Pharmaceuticals Ltd.
- Emmeellen Biotech Pharmaceuticals Ltd.
- FDC Ltd.
- FleetGuard Filters Pvt. Ltd.
- GE India Technology Centre Pvt. Ltd.
- Gujarat State Fertilizers and Chemicals Ltd.
- Gujarat Dyestuff Manufacturers Association
- Hinoday Industries Ltd.
- Hindustan Lever Research Centre
- Honeywell International Inc.
- Hyca Technologies Ltd.
- Innovasynth Technologies (India) Ltd.
- Kard Scientific India P. Ltd.
- Lupin Research Park
- Arun P. Kaulgud & Co.
- National Thermal Power Corporation
- PNP & Associates Pvt. Ltd.
- Reckitt Benckiser (India) Ltd.
- Reliance Industries Ltd.
- RPG Life Sciences Limited
- Schenectady Herdillia Ltd.
- Shasun Chemicals & Drugs Ltd.
- SC Johnson Products Pvt. Ltd.
- Tata Chemicals Ltd.
- Tata Steel Ltd.
- Thing Pharma
- Transmetal Limited
- Transpek-Silox Industry Ltd.
- Unichem Laboratories Ltd.
- USV Limited





## INFORMATION DIVISION

The Information Division (ID) has the responsibility to design and manage the information infrastructure of the laboratory. The division is continuing to make effective use of Information technology (IT) to provide the infrastructure - in terms of access to a wide range of Information resources located within NCL as well as in outside world, to enable the NCL scientists to perform better and to maintain its leadership position.

### ICT Systems

NCL has been in the forefront of deploying information technologies to help its scientists to excel in their chosen area of research. NCL has an excellent campus wide local area network (LAN) with about 750 computers, a range of servers to host databases, e-mails systems, web services and a good connectivity to the internet. The laboratory has considerable strength in the areas of computational chemistry, molecular modeling, CFD as well as simulation and modeling of chemical systems. The ICT plan of the laboratory is closely dovetailed to the IT vision of NCL.

Some of the highlights of this year are: Upgraded divisional uplinks to gigabit speed with a failover, Deployment high performance core switch, and Upgradation of Internet links

For transparent access to information NCL has local home page called ncl@home for campus wide information dissemination. NCL Staff Recreation Club conducts its annual elections online successfully. ncl@home has the pages for: Director's podium, DG's desk, Submission of online APAR, Finance and Accounts, Staff welfare club, Resources for employees, Students and career, NCL alumni association, Medical services, etc

### Library and information services

Library services are aimed at satisfying scientists' requirement of scientific information. NCL library acquires and disseminates the information by various ways and means by providing printed material and access to online version of documents. During 2006-07, Library procured 591 books, the cost being Rs 43.82 lakhs from various grants. This is the highest number of books purchase done after many years. The total library collection is 1,35,414 which includes books and bound volumes of journals.

A book exhibition of latest scientific and technical books was organized in Aug 2006 for three days. This provided an opportunity to scientists and students to browse the

new books and recommend for purchase. A very good response of the students and scientists was received, 232 books worth Rs. 14 lakhs are purchased.

NCL subscribed to 250 journals for the year 2007, Rs. 332.57 lakhs were spent which includes electronic journals and databases. Access is provided to NCL scientists to over 4400 journals of 11 publishers, through CSIR E Journals consortium project. Library is subscribing to major publisher's back files collection, Access to Web of Science, Delphion, UMI Proquest Dissertation Database, Springer Chemistry and Materials Science E books is provided.

NCL library organized a training program for students and scientists to enhance the usage of e journals facility provided under NISCAIR, CSIR E journals Consortium Project. The usage statistics of the E journals of all the CSIR labs shows that NCL is on the top, availing maximum usage of the facility.

This year an information festival was organized in which various E Products of renowned scientific publishers were exhibited. This provided an opportunity to scientists and students to get acquainted with the e resources and to know the usefulness. Springer E books- Chemistry and Materials Collection was subscribed, which includes Springer books published during 2005-2007 of the subject. Library provides document delivery service to industrial clients. These industrial clients avail library services namely photocopies of journal articles available and not available at NCL library. Library has approx. 340 students in and around Pune as non NCL members, 20 corporate members using facility of CA on CD, and 40 small scale industries using the library membership.

Compact shelving mobile storage system was installed in one of the basement rooms to shelve lab record books and theses. Fifteen library computer terminals were replaced by new ones. Library homepage was updated continuously providing latest information to the users. A project of digitization of NCL theses is in progress. Theses submitted to library since 1950 will be fully digitized and will be made available to the users in electronic format.



### Management information system

MIS Group handles all activities related to Project Management System. The activities can be broadly classified as follows:

- Assistance to scientists in preparation of project proposals as per CSIR guidelines.
- Coding of New projects and preparation of new project Initiation note for circulation to all concerned departments.
- Allocation of funds to the projects and circulation of challan to all concerned.
- Preparation and raising of invoices for Industrial Projects.
- Extension of projects in consultation with scientists.
- Issuing of completion Certificate of Projects.
- Calculation and payment of service tax for consultancy and technical services projects to Central Excise Department.
- Maintenance of service tax records as per CSIR guidelines for consultancy and technical services projects.
- Providing audit Information on NCL projects.
- Laboratory budget preparation/ allocation / monitoring
- Preparation of financial and performance reports of NCL.
- Developing appropriate systems for MIS functions.
- Providing Information on projects to MC/RC Meetings.
- Management of NCL Research Foundation and its activities
- General assistance in the management and smooth functioning of the Laboratory.

Efforts are being made continuously to streamline the procedures relating to project initiation, monitoring and closure. Many of the activities have been computerized. There is an efficient system to track the receipt of funds for various projects, monitoring cash flows, project monitoring, publication profiles etc.

A web enabled project management information system was developed in-house to support the activities of the group. This system takes care of the financial aspects (receipts, budgeting) of projects from initiation to completion. It stores all the important information about the project:

- Project information
- Funds receipt
- Party information
- Staff deployed
- Project installments

The systems provides for generating a range of reports to enable the management to review the status. The MIS portal offers access window to PMIS for the scientific staff, project leader, HOD's and management teams. The site offers hierarchical login to different users. This enables to control the information depending on the requirements of the user and prevents unauthorized viewing. Apart from PMIS, the site also provides information on NCL performance, Divisional performance, various proforma for downloading, about NCL research foundation activities etc. This portal will be the driving force for providing financial information to NCL Scientists.

PMIS is a centralized document management system holding all project records at one place. The project records are available to the concerned scientists through MIS website (24 x 7 hours). MIS group creates all the project records internally and same is made available on the MIS website to the scientists. The scientists are provided with a login and password to access their project records directly from their desktops. All project documents like agreement, project proposal, project initiation, challans, funds received and due are available on the fly as and when the records are created by MIS group. In addition, there is an upload facility for scientists to upload interim and final reports submitted to the client and project output summary into the PMIS system.

Therefore all financial and scientific reports are centralized and stored in MIS server and all project records can be created as when required. PMIS creates important reports for management for decision making. The External cash flow reports, Lab reserve earnings, detailed project break up, dollar earnings, funds due from project are some of the important management reports available to HOD's and Director. In addition, queries can be created to pull out information from the database as and when required. PMIS sends alert mails, whenever a payment is due. This helps MIS group to raise invoice and collect the funds in time. The alert mail is also sent to the scientists, whenever a report to the client is due and scales



up the alerts to HOD and Director, if the request is not complied.

#### Budget Planning

Budget Planning is a significant management tool adopted by the laboratory to manage & control the resources of the laboratory. It helps to utilize the resources for the development and growth of the laboratory to achieve the aims set by the management of the laboratory.

MIS is responsible for the budgeting exercise of the laboratory. MIS along with Director make a detailed plan to meet the overall budgetary requirements of the laboratory. They are further broken down to different budget heads and the expenditure is matched with the available resources of the laboratory.

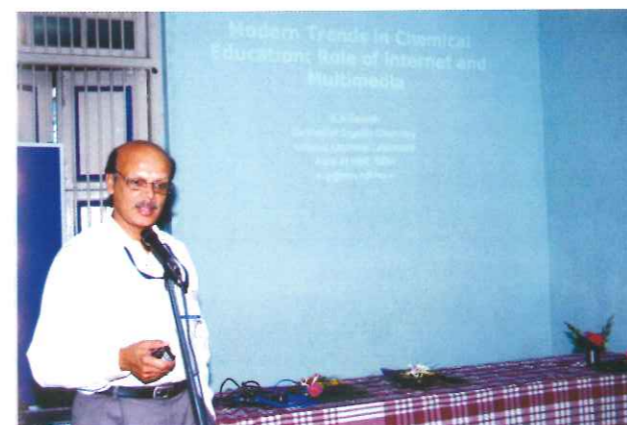
With over all plan in hand, MIS calls for the budgeting requirements known as "Operational Budget" for the divisions and resource centers at the beginning of the financial year. The budget mainly covers Equipment maintenance within the divisions and common equipments for the laboratory, divisional office requirements for office equipments, consumables and small scientific equipments required in the divisions. The requirements are compiled into appropriate formats and studied. The allocations are made based on the resource planning and overall budgeting principles developed within the laboratory. The budgets are then projectised with project codes and then released to budget centers. The Budgets are booked through stores, which maintain the expenditure for all budget centers. MIS along with Director monitor the expenditure twice in a year in the months October and March. Corrective measures are undertaken if the expenditure is more or too less than the allocated resources.



#### HUMAN RESOURCE MANAGEMENT

##### CSIR HRDG faculty training programme for science teachers

NCL, Pune as a part of CSIR HRDG programme to motivate and to promote interest, excitement and excellence in science education among the science teachers conducted a two-day "Hands-on training-cum-workshop and demonstration of micro-scale experiments in chemistry" for science teachers from high schools and higher secondary schools from Solapur district of Maharashtra at Suyash Gurukul, Solapur during 17 - 18 November 2006. About sixty teachers both from rural and urban areas actively participated in the training programme. Shri Keshav Shinde, Director of Suyash Gurukul welcomed the guests and thanked the organizers for giving opportunity to host the workshop for science teachers at Solapur. Professor K.N. Ganesh, Director, Indian Institute of Science Education and Research, Pune delivered inaugural address on "Modern trends in chemical education: Role of Internet and multimedia". Prof. Ganesh enumerated the need of advancement in teaching science with simplicity with creativity using modern methods available in IT era. Prof. S. P. Kamat, Department of Chemistry, Goa University and his colleagues conducted technical training-cum-workshop using specially made micro-scale laboratory kits and gave hands on training in use of micro-scale experiments in chemistry.



Prof. Ganesh delivering inaugural address



Prof. Kamat demonstrating micro-scale experiments

##### Training programme on "integrated supply chain management"

Indian Institute of Materials Management, Pune conducted in-house Training Programme on "Integrated Supply Chain Management" for Stores & Purchase staff of NCL in two batches. This two-day programme, organized on 7 & 8 Feb. and 13 & 14 Feb. 2007, was attended by 26 staff members in each batch.

##### Users' training workshop-CSIR e-journals consortium

NISCAIR, New Delhi under CSIR e-journal consortium has agreements with thirteen publishers to access more than four thousand international S & T journals with 5 to 10 years back files. With a view to enhance the usage of all e-journals NISCAIR organized one-day users' training workshop at NCL on 13 September 2006. About thirty-five students and scientists attended the training programme. Publishers' representatives/ vendors provided the training. The training covered presentations, facilities and functionalities in details of the products from respective publishers.

##### Student academic programme

NCL introduced and implemented revised guidelines to Ph.D. admission from January 1, 2005, to streamline the admission process. With over 400 students pursuing their doctoral degree in Chemical and allied sciences, there was a necessity to introduce new guidelines. As per the guidelines, students were admitted through centralized interview, where candidates, qualified in NET under CSIR - UGC examination, are eligible to appear. The advertisements were sent twice a year, following the announcement of CSIR - UGC NET examination results.



Candidates were selected depending on vacancy and requirements of research guides for the five broad disciplines of physical and materials chemistry, polymer science and engineering, organic chemistry, life sciences, and catalysis. Admission to the Ph.D. program through direct Senior Research Fellowship (SRF) program of CSIR continued as per usual procedures.

Every batch of students joining the Ph.D. program from 2005 at NCL undergoes a two-day orientation session, which provides an introduction to the laboratory, its systems, procedures and functioning, safety, security, scientific ethics, scientific record keeping and access to scientific information. Participation in the orientation program is compulsory. Additionally, each student (JRF as well as selected through direct SRF scheme) was required to complete at least one credit course that is offered by

NCL, appropriate to his/ her research area. These are offered with a view to bridging the gap between Masters Education and what is required for Ph D research. This is waived in case of students is registered with IIT- Mumbai or MUICT. The resource persons were drawn from the staff of NCL, neighboring Institutions as well as outside Pune. This course work was made compulsory for all students, joining from 1 July, 2004.

Students also present two seminars, one general seminar on topic of research (overview) to be preferably completed before registration, second one on research theme to be completed before synopsis submission. An academic committee comprising research guide, internal NCL member and an external expert evaluates the seminars and periodically assess the progress of the student.



## THESIS

### M.Sc. Degree : Pune University (2006)

Author	Title	Guide
Gaydhankar, T.R.	Synthesis Characterization and Catalytic Applications of MCM-41 Type Mesoporous Materials	Rajiv Kumar
Taralkar, U.S.	Influence of Synthesis Parameters on the Characteristics of the Mesoporous Materials	Rajiv Kumar

### Ph. D. Degree : Pune University (2006)

Author	Title	Guide
Aland, G.R.	Aminoethyl (alpha- alpha- Dimethyl) Glycyl PNAs: Synthesis and Interaction Studies with DNA and Gold Nanoparticles	Ganesh, K.N
Arora, K.K.	A Study of Design and Non-Covalent Synthesis of Supramolecular Assemblies	Pedireddi, V.R.
Bala, T.	New Methods for the Synthesis of Magnetic Nanoparticles	Sastry, M.& Prasad, B.L.V
Bansal, V.	Fungus-Mediated Biosynthesis of Oxides Nanoparticles and Composites	Prabhune, A.(Ms) & Sastry, M.
Bharathy, P.V.	In Vitro Embryo Rescue Plant Regeneration and Genetic Transformation studies in Grapevine	Agrawal, D.C.
Chavan, S.P.	Synthetic Studies Towards Taxol and Development of Synthetically Useful Methodology	Chavan, S.P.
Damodaran, K.	Spatially Dependent Interaction Tensors Determined Through Novel Methods of High Resolution Solid State NMR	Ganapthy, S.
Deka, S.	Studies on the Magnetic and Electrical Properties of Nanosized Transition Metal Oxides and Ferrites	Joy, P.A.
Deshpande, S.G.	Studies on the Synthesis of New Hexopyranosyl Thymines	Pathak, T.& Sashidhar, M.S.
Deshpande, S.S.	Rate Enhancement of Diels-Alder Reactions in Salt Solutions and Ionic Liquids	AnilKumar
Devaraj, S.	Synthetic & Mechanistic Studies Related to Rigid Derivatives of Cyclitols	Sashidhar, M.S.
Dumbre, S.G.	Design and Synthesis of New Azasugars: B Lactam-Azasugars Hybrids, 1-Deoxy-D- Galactohomonojirimycin and 1- Deoxy -D Glucohomonojirimycin as Glycosidase Inhibitors	Pandey, G
Easwar, S.	Enzymes as a Reagent in Organic Synthesis: an efficient Resolution of key Intermediates of Pharmaceutically important Compounds and Synthesis	Argade, N.P.
Gnaneshwar, R.	Synthesis & Characterization of Functional Polymers by Living Polymerization Methods	Sivaram, S.



Author	Title	Guide
Gonnade, R.G.	Structural Studies of Molecular Crystals of Inositol Derivatives and their Inclusion Complexes	Bhadbhade, M.M. & Shashidhar, M.S.
Jagtap, S.S.	Study of Cellulolytic and Hemicellulolytic Enzymes from a Novel Alkalothermophilic Thermomonospora Sp.	Rao, M.(Ms)
Joshi, B.P.	To Design and Develop Brewster Angle Microscope Coupled with LB Through for Observing and Analyzing Monolayers Formed at Air Water Interface	Gowariker, S.R., Sastry, M. & Lyer, N.
Joshi, H.M.	Surface Modification of Nanoparticles for Biological Applications	Sastry, M.
Joshi, M.A.	Synthetic Studies towards Total Synthesis of Lactacystin Analogue and the related Beta-Lactone Omuralide Analogue	Gurjar, M.K.
K.Sankar	Synthetic Studies Toward Manzacidins, Pondaplin and Some Applications of Cyclopropylmethyl Radicals	Gurjar, M.K.
Karandikar, P.R.	Synthesis, Modification and Catalytic Evaluation of Mesoporus Molecular Sieves	Chandwadkar, A.J.(Ms)
Karmakar, S.	Synthetic Studies towards Pseudotheonamides, Herbarium III, Bicyclic Thiohydantoin and Oxazolidinone -5- One	Gurjar, M.K.
Khaire, S.S.	Synthesis Characterization and Catalytic Activity of Ordered Mesoporous Metallosilicate Catalysts	Sivasanker, S. & Kumar, R.
Khan, F.	Purification and Characterization of a Lectin from <i>Fusarium</i> SP. LR11 having Complex Sugar Specificity	Khan, M.I.
Khobragade, D.A.	Synthesis of Biologically Active Compounds	Chavan, S.P.
Kulkarni, G.M.	Transition Metal Nitrenes-Synthetic Applications in Aziridination and Bicyclic N-Heterocycles and use of Nitrogen Ligands in Heck Suzuki Coupling and Amination Reactions	Iyer, S.
Kumar, R.S.	Investigation into the Structure and Activity of Conjugated Bile Salt Hydrolase and Related Penicillin Acylase	Suresh, C.G.
Maddanimath, T.M.	Preparation, Characterization and Applications of Custom Designed Nanoparticles and their Organised Assemblies	Vijayamohan, K.
Madhusudanrao, J.N.	Applications of Support Vector Machines to Process Engineering Systems	Kulkarni, B.D.
Maheswar, K.	Studies Toward the Synthesis of a Novel Carbocyclic Nucleoside, FR 901483, TAN 1251 (A, B, C&D) and Cheimonophyllon E	Gurjar, M.K.
Menjoge, A. ,R.	Enhancing Bioavailability of Drugs	Kulkarni, M.G.
Mittal, A.	Controlled Synthesis of Acrylic Polymers	Sivaram, S.
Mondal, D.	Studies Towards the Enantioselective Synthesis of Oxazolomycin and Litsea Verticillols A-H	Gurjar, M.K.
Nair, S.S.	Studies on the Development of Structure and Morphology in Nylons	Ramesh, C.



Author	Title	Guide
Pedduri, Y.	Synthetic Studies towards Peloruside a Clavosolides and Temperature dependent Isomerisation versus Net Fragmentation of secondary Allylic alcohols with Grubbs Catalyst	Gurjar, M.K.
Priya, R.	Structural and Biophysical Characterization of Penicillin V Acylase from <i>Bacillus Subtilis</i> and Comparison with Related Hydrolases as well as Study of Selected Proteins from Malarial Parasite	Suresh, C.G.
Raikar, S.	New Synthetic Strategy for Optically Active trans-Hydrindane: Application Towards the Synthesis of Vitamin D3	Pandey, G.
Raj Sankar, C.	Studies on the Structural Magnetic and Electrical Properties of Non-Stoichiometric and Related Rare Earth Manganites	Joy, P.A.
Ramgir, N.S.	Synthesis and Characterisation of Tin Oxide and Zinc Oxide Nanostructured Materials for Gas Sensors	Vijayamohan, K. & Mulla, I.S.
Reddy, J.P.	Non Covalent Synthesis of Supramolecular Assemblies	Pedireddi, V.R.
Renukdas, N.N.	Development of Transgenic Papaya and Its Analysis	Rawal, S.K.
Roy, D.	Studies in Catalysis and Reaction Engineering on Multiphase Hydrogenation Reactions	Chaudhari, R.V.
Sanyal, A.	Use of Inorganic Composites for the Synthesis of Nanoparticles	Sastry, M.
Satyanarayana, L.	Structural Studies on Phycocyanins from Three Cyanobacterial spp. and a Xylanase from an Alkaliphilic <i>Bacillus</i> Sp.	Suresh, C.G.
Sawant, D.P.	Studies in Heterogeneous Catalysis: Supported Heteropolyacids Catalyzed Organic Reactions	Halligudi, S.B.
Shah, S.N.	Biotransformation in Synthesis of Bioactive Molecules, 19-Hete and 20-Hete, from Arachidonic Acid	Prabhune, A. (Ms)
Sharma, J.	Synthesis and Assembly of High Aspect Ratio nanostructures of Silver and Gold	Vijaymohan, K.
Sharma, P.	Synthesis of Biologically Active Compounds: CCG and its Derivatives, Mitralactonine and Development of Synthetic Methodologies	Chavan, S.P.
Shetti, V.N.	Studies on Reactive Oxo Intermediates Generated During Selective Hydrocarbon Oxidations Over Metallosilicate and Mixed Metal Oxide Catalysis	Srinivas, D.
Shingte, R.D.	Synthesis of Processable High Performance Polymers	Wadgaonkar, P.P.
Shylesh, S.	Synthesis and Characterization of Organo Modified Metal Containing Mesoporous Material for Oxidation Catalysis	Singh, A.P.
Singh, A.	Metal Nanoparticles in Therapeutic and Sensor Applications	Rao, M.(Ms)
Sonawane, R.S.	Preparation and Characterization of Modified Tio2 Thin Films for Photocatalytic applications	Dongare, M.K.



Author	Title	Guide
Srinivasan, A.	Chickpea - <i>Helicoverpa armigera</i> : A System to Elucidate Plant - Insect Pest Interactions	Gupta, V.S.(Ms)
Subramanyam, U.	Synthesis Structure and Property Studies of Polyolefins Prepared Using Late Transition Metal Catalysts	Sivaram, S
Sunil Kumar, G.	Chemical Studies on Pyrrolidine Derivatives: Synthesis of Bulgecinine and Aminomethyl Prolyl Peptide Nucleic Acids	Ganesh, K.N.
Tanwar, A.	Density Based Reactivity Descriptors: Relation to Molecular Properties and the Strength of Chemical Interactions	Pal, S.
Telang, M.	Molecular Analysis of Plant-Pest Interaction with Special Reference to <i>Helicoverpa Armigera</i> and Proteinase Inhibitors from Host and Non-Host Plants	Gupta, V.S. (Ms)
Thakkar, M.	Studies Towards Synthesis of Beta-Herbertenol and Other Biological Active Molecules	Chavan, S.P.
Thirunavukkarasu, K.	Molecular Beam Studies of Nitric Oxide (NO) Reduction Reactions on Pd(111) Surfaces	Gopinath, C.S.
Tillu, V.H.	Synthesis of Thiaprostaglandins and some Organic Transformations like Oxidative Halogenation Protection Deprotection and Multicomponent Reactions	Wakharkar, R.D.(Ms)
Umashankara, M.	Synthesis and Biophysical Studies of 4-Substituted Proline Containing Collagen Peptides: Effect of Substituents on Triplex Structure	Ganesh, K.N.
Varughese, S.	Design and Synthesis of Supramolecular Assemblies of Organic and Coordination Complexes	Pedireddi, V.R.
Vijayaraj, M.	Heteroatom Alkylation Reactions of Aromatic Compounds over Metal Oxides	Gopinath, C.S.
Vinod, V.P.	Structural and Mechanistic Insights into Hydrolytic Enzymes/Inhibitors with Special Reference to Aspartic Proteases	Rao, M.(Ms)



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Dr. Waghmare, Kashinath	Pune
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### PUBLICATION AND SCIENCE COMMUNICATION

The Publication and Science Communication (PSC) unit develops, maintains and manages bilingual business website, academic website and Intranet webpages, press releases, digitisation of archives, NCL publications, in-house and CSIR films, video and photography, software development, annual reports and its publication, liaison with CSIR and providing overall in-house support.

#### NCL websites and conference management system

The unit coordinates and updates the contents of business site (NCL website) thereby providing the latest information to the user on modules like 'research publications', 'patents', 'reports and press releases', 'NCL in news', 'R&D feature', 'major events', 'tenders', 'job vacancies', 'scientist's information' etc. RTI page in Hindi version was made. The updating and maintenance of both English and Hindi version of websites is done periodically. As a part of software development activity and for assisting the organisers of the conference to manage various aspects required by the organisers the *conference management system (CMS)* was set up. The system consists of a website exclusively for a particular conference containing static as well as dynamic pages. Conference information is provided by static pages and interactive dynamic pages including online registration, upload of files, evaluation of abstract, mass email, registration fee, hotel accommodation and any other information required by the organisers. The organisers are also given continuous support in terms of printing of name badges, abstract books, customised stationary items. Softcopies of the abstract book are uploaded on the website. Wi-fi enabled internet surfing in and around the auditorium and lecture hall of main building have also been made available to the participants.

NCL scientists are encouraged to develop their own homepages and these are uploaded at NCL academic site. The CMS was provided for the following events during the year:

- Macro-2006 - 9th National conference on "Polymers for advanced technologies",
- 6th International symposium on "Catalysis in multiphase reactors (CAMURE-6) and 5th international symposium on multifunctional reactors (ISMR-5)",
- International conference on chemo-informatics,

- 13th National magnetic resonance society of India (NMRS) symposium,
- International conference on "Biology of yeasts and filamentous fungi", and
- DST-JSPS Asia academic seminar on "Molecular and supramolecular materials with designed functions".

#### Intranet and ncl@home

A new Admin Control is built for the home portal (*ncl@home*), which follows the policy of distributed administrative control with a Central Admin Control for monitoring it. Individual web portal of different divisions containing specific information related to the division were developed. Each section of the web portal was provided with an application oriented search tool, enabling the users with an easy, efficient and effective searching option.

In addition to the facilities available in Resource Centers, NCL has a large number of high-end instruments / equipments under direct control of scientists. Many of these equipments are made available to the common user from the laboratory, provided the user gets training to operate the equipment. To effectively manage the available time slots an *instrument booking system* was developed. The moderator (one who is in-charge of monitoring the instrument) defines time slots per day in order to allot the specific time to complete the operation. The user (one who wants to use the instrument) may register the instrument while the moderator accepts the user registration after providing formal training to the user. Registered users of the instruments can book the time slot up to two weeks in advance. The moderator is given a special privilege to book the instrument up to a month in advance. In case of a break down or preventive maintenance the moderator has the right to block the instrument. The system is working properly and many instruments are being added by the scientists for making them available to the users. Presently seventeen equipments are made available under this system. The system is also being upgraded to accommodate the booking of time slots for adding video conferencing. The unit provided regular support for the maintenance of *NCL-India server, home server, APAR server, library server* and the various *software applications* available on these servers.



Besides redeveloping and automating the applications already present on the ncl@home, many new applications like *NCL directory* for providing all the essential information of NCL members, *Picture Gallery* a repository for photo albums and movies of various events frequently held at NCL, *Discussion Forum*, *Help*, *Safety Webpage* etc were developed. The archive page is continuously updated by archiving various reports, science day posters, etc. Apart from the above activities an important task of the unit has been preparation of *press releases* covering important events and publication of NCL Annual report. The unit also communicates with CSIR and gives valuable inputs to 'CSIR News', 'CSIR Samachar' and 'CSIR annual report' published by CSIR. The unit also brought out the NCL annual report 2005-06. In addition the unit responds to the press enquiries from local media, provides customised reports to magazines dedicated to chemical industries, etc.

A report covering NCL R&D activities was also prepared for inclusion in the background paper prepared on the science and research of India's premier institutes and labs for the delegates attending 12th Technology Summit and Technology Platform (TECHSUMMIT 2006) on the 6-7 November at New Delhi.

The unit co-ordinated the video shootings for CSIR films and also for the Science Safari, a television program created in partnership between the Ministry of Science and Technology, and the National Geographic Channel. The program aimed to showcase innovative science solutions developed by Indian Scientists. The video shooting was organized to cover the ultra filtration membrane based water purifier units installed at Vigyan Ashram, Pabal, off Pune-Nagar Road.

The screenshot displays several web pages from the NCL website. At the top, there is a banner for 'MACRO-2006 Polymers for advanced Technologies 9th National Conference' organized by the Society for Polymer Science, India, Pune Chapter, held on December 17-20, 2006. Below this, there are sections for 'CHEMOINFORMATICS' (International Conference on January 2007) and 'NMRS-2007' (Special Symposium on 'Current trends in Solid State NMR Methodology and Practice' at the 13th National Magnetic Resonance Society Meeting, February 05-08, 2007). The pages include details about themes, objectives, dates, and registration information. A navigation menu on the left lists various site sections like Home, Pains, and Latest Updates.



## RESEARCH PLANNING & AUDIT UNIT

Research Planning & Audit Unit (RP & A) has been involved in areas of project planning, project monitoring, budget, liaison with CSIR, etc. Technical and scientific audit of all on-going projects is a key activity.

### In-house projects

RP&A Unit is associated with the screening, evaluation and providing funding for the new projects within the lab. During the year, fresh proposals were invited and reviewed. In addition, monitoring and review of existing in-house research programs was undertaken. During the year 2006-07, four review meetings / seminars were conducted to audit the technical and scientific performance of about thirty ongoing projects.

As a policy of the laboratory, start-up grant of Rs. 6 lakhs per year was provided to the six newly joined scientists. In addition, start-up grants for previously joined five scientists were continued for the subsequent year. The total funding to all in-house projects along with the start up grant during 2006-07 was Rs. 95 lakhs.

### Projects under X Five-year plan

RPA acts as a nodal agency for the coordination and implementation of the network projects within NCL, with CSIR and other participating labs. RPA unit organizes for the receipt and allocation of funds, reviews, monitors the scientific and financial progress and provides the necessary data support for the procurement of equipments and instruments. NCL has a participation in 12 network projects with other CSIR labs, including two projects where NCL is the nodal lab.

### Projects under XI Five-year plan

The formulation of the XI Five Year Plan (FYP) for NCL has been one of the major activities of RPA during the year. The entire research programmes of NCL were clubbed in frontier areas of chemistry and biology and for capacity building, network programmes, centers of excellence, etc. that would meet the S & T demands / requirements of the next decade. The research proposals, complete with concepts, deliverables, requirements for equipments, financial requirements etc. were compiled and put forward to CSIR. Similar and converging competencies were identified in other CSIR laboratories and projects within the network mode were proposed. The document also included the achievements and outcomes of NCL during

the X FYP projects and other projects supported by different agencies. The proposals were screened, evaluated and discussed at various levels within NCL and at CSIR. Another highlight of the XI FYP was the preparation of the Annual plan (2007-08) document.

### Interface with auditors

The unit interacted and provided detailed supporting information for submission to the external audit of CSIR. It also interfaced with the audit parties from the Principal Director of Audit, Scientific Department (Mumbai) on matters relating to research projects at NCL. During the audit for 2006-07, with the quantity and quality of information provided, many existing and outstanding objections were dropped.

### Research Council meetings

The Unit has been involved in arranging and conducting Research Council meetings at NCL. A meeting was conducted during the last year and actions taken to follow-up and implement the recommendations. Presentations on the "Status of in-house projects 2005-06" and "Analysis of major publicly funded projects during 2005-06" were made at the RC meeting. The tenure of the RC ended in December 2006.

### Liaison with CSIR

The Unit liaises with CSIR in providing timely information on many aspects of the laboratory. Moreover, the consolidated performance reports on two major network projects and research utilization data of NCL was sent to CSIR on a quarterly basis. This involved providing current status on the on-going projects, highlighting the work done, major achievements in basic and applied science, outputs (patents - applied for and granted) and funds generated through technical services, etc. Response to certain queries under RTI was also sent to CSIR.



### SAFETY MANAGEMENT

The concern for health and safety is a matter of paramount importance to NCL. Efforts are made to motivate, bring in safety awareness and imbibe safety culture amongst the staff and students of NCL.

NCL has a standing committee on Lab Safety, including member representations from all divisions. Besides this, divisional safety committees also exist with member representations from scientific staff and research students. During the year, meetings were held under the chairmanship of Director NCL, while the divisional subcommittees on lab safety held meetings every quarter to review the status on compliance of safety norms. A review of various activities and initiatives taken during the year is as under:

#### Orientation courses

Two orientation courses were organized for the new research students, project assistants and scientists during the year. The objective was to sensitize them of the safety in a chemical laboratory, initiatives taken by the safety unit, information sources and facilities; their duties and responsibilities.

#### Fire Safety

Live demonstration and hands on practical training for tackling small fires and the use of portable fire extinguishers, was organised thrice during the year and more than 300 students including scientists were trained.

#### Up gradation of systems and infrastructure

The health, safety and environment is protected and the systems are refined and upgraded on a continuous basis. Many locations in the laboratory have been equipped with gas detectors for sensing leakage of gases, in addition to procurement of portable gas detectors. The safety features in the ovens and furnaces have been upgraded with the fitting of additional high temperature cut off switches. CD ROM's containing MSDS and other safety related information were procured and posted on the intranet. Fourteen new fume hoods were installed while many more labs have been equipped with nine eye wash fountains and safety showers. The solvent disposal facility is being upgraded and a tie up with licensed vendors for the disposal of hazardous chemicals is being worked out.

#### Assistance to outside agencies

Timely assistance is provided to outside agencies in the

event of an accident or a crisis in a chemical accident. Public awareness programmes and lectures on various aspects of safety, accident prevention and mitigation, disaster management are also organized for various educational and industrial establishments.

#### Fire at polymer science and engineering building

A fire broke out at Room No. 936, one of the laboratory rooms located in the Polymer Science and Engineering building on March 2, 2007 at about 10.30 am. At the time of incident the laboratory was occupied by scientists and staff. As soon as the fire was noticed, precautionary steps were taken to evacuate the occupants of the building and alert the Pune Municipal Corporation (PMC) fire brigade. The fire brigade immediately responded with the fire tenders and the fire fighters. The fire was brought under control by about 12.30 pm.

A fact finding committee with Dr. M.K. Gurjar, Head, Organic Chemistry Division as Chairman and Dr. P.P. Barve, Scientist, Chemical Engineering and Process Development Division, as members along with two external experts specialized in the area of Fire and Safety, namely, Shri I.G. Dudhani, Senior Manager (Health, Safety & Environment), Alfa Laval (India) Ltd., Pune and Shri Chandra Mohan Bisen, Chief Engineer (Fire & Safety), Rashtriya Chemicals & Fertilizers Ltd, Chembur, Mumbai conducted an inquiry into the cause of fire. The committee interviewed all the individual members who were present in the laboratory at the time when fire broke out, inspected the site, examined the electrical wirings, fittings and assessed the nature of damage caused.

There was no major injury to humans except for a minor burn injury on the hands of the student and one fire fighting staff. There was no significant loss of the laboratory research data and records, as these were kept at another location. The laboratory, however, was completely gutted. The lab Room No. 936 did not house any expensive equipment. The book value of the loss of equipment, furniture, etc. was approximately Rs. 39 Lakhs. Out of this, about Rs. 18 Lakhs worth of assets were purchased before 2001. The committee after its in-depth investigation, based on the eyewitness accounts and technical evaluation unequivocally excluded the possibility of sabotage or any intentional act as the cause of the accident. The fire was caused during the distillation of a hydrocarbon solvent. Based on the suggestions made by the committee, a comprehensive revamp of safety systems in NCL is currently under implementation.



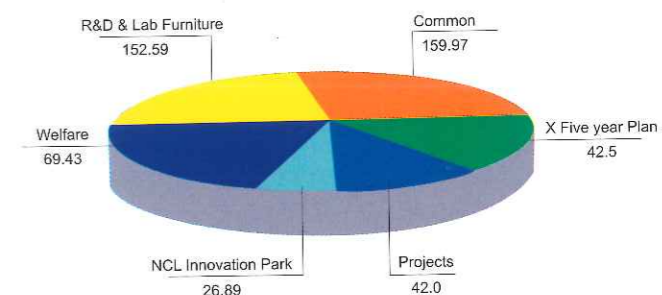
### ENGINEERING SERVICES UNIT

Engineering Services Unit (ESU) carried out several activities such as modifications and renovations of many labs and offices in the campus with respect to civil and electrical works during the year. This included: (1) Replacement of elevators in Main building, (2) Renovation of Guest House rooms, Entomology lab and Bio-tech lab, (3) Laying communication cable to Guest House, (4) Illumination on road from Main Gate to Main Building, and (5) New Board Room facility in Chemical Engineering Building. The foundation stone for the construction of a new building "Polymers and Advanced Materials Laboratory" was laid down on 18 December 2006 and the construction is in progress.

A separate DG Set was installed to provide power back-up to CMC building that houses sophisticated equipments like TEM, XRD. Old MERADO campus was modified further to create more space for NCL Innovation Park. Storage space facility was also created for National Repository of Molecules (NRM) in the same campus. A major task of modifying the existing facilities to provide necessary infrastructure for IISER was completed. The Old Hostel of NCL was converted to IISER student hostel with all modern amenities.

The Glass Blowing Unit carried out about 15,000 jobs of various nature that included special projects that required glass apparatus with innovative ideas (140), new fabrication work like distillation sets and filtration sets (1500), new jobs like manufacturing of round bottom flasks, columns, viscometers, special stirrers (5000), maintenance work like repairing of broken glasswares (3000) and minor jobs (5000). The Unit provides the training to the students in glass blowing. Every batch of students is trained for a period of three years. At present, four students are being trained as scientific glass blower. The Unit is also in the process of framing the guidelines for a regular trade in this connection at NCL in consultation with Regional Directorate of Apprenticeship Training, Mumbai as such a trade in glass blowing is unavailable within the Maharashtra State.

Expenditure : Rs. 493.39 Lakhs



Illumination of streetlights from entrance gate to main building



A view of renovated laboratory



Prof Richard Friend laying foundation stone of new building for "Polymer and Advanced Materials"





## COMMUNICATION GROUP

Values added services as listed below were added to the Alcatel Omni PCX Enterprise Communication System which was commissioned in August 2005:

- Voice message facility for the staff with an ability to programme the length / time of message to be recorded, and
- Integration of fax server for desktop fax facility for scientific staff for immediate access and replies to faxes from anywhere in the world.

Divisional conference rooms were equipped with Alcatel digital telephones for audio conferencing purpose. NCL guest house and NCL Innovation Park were also connected onto the Omni PCX Enterprise System.

An important feature of Omni PCX Enterprise - a server gateway technology has been utilized and that is the disaster management or total redundancy of Omni PCX

Enterprise. The total redundancy has been executed over optic fiber cable over a considerable distance. By this Business Continuity Plan (BCP) for NCL has been executed.

Communication system is functioning for 950 direct lines with calling line identification (CLI) facility. Implementation of call billing software for extensions with outward dial facility has made a great impact on the monthly NCL telephone bill

Video Conferencing (VC) system was commissioned with connectivity on IP, ISDN BRI and ISDN PRI lines. The conferencing can be done with maximum three parties at a time anywhere in the world with a facility to share PC presentations and document camera presentations. Omni PCX Enterprise BRI lines have been utilized for BRI connectivity for VC functioning.



## प्रशासन

वित्त एवं लेखा विभाग  
निष्पादित कार्य :

वित्त एवं लेखा विभाग ने निदेशक, एनसीएल, प्रमुख, ग्राहक सन्तुष्टि मूल्यांकन यूनिट, प्रमुख, सूचना उत्पाद अनुसंधान एवं विकास यूनिट तथा निदेशक, भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान को वित्तीय सलाह प्रदान की।

- भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान के खातों (प्राप्त राशियों, भुगतान की गई राशियों तथा इससे सम्बन्धित अभिलेखों) का हिसाब रखा गया।
- नियंत्रक तथा महालेखापरीक्षक के उन्नीस में से नौ लेखापरीक्षा पैरा निपटाए गए।
- बाहरी वित्तपोषित 500 से अधिक परियोजनाओं का वित्तीय एवं लेखा प्रबन्धन किया गया।
- करारों, कार्य प्रस्तावों, वेतन नियतन मामलों, वैयक्तिक फाइलों, प्रतिनियुक्ति तथा न्यायालय से सम्बन्धित विभिन्न प्रस्तावों की वित्तीय दृष्टिकोण से समीक्षा की गई।

- सम्पूर्ण खातों (इम्पैक्ट) तथा इससे सम्बन्धित रजिस्ट्रों का रखरखाव किया गया तथा इम्पैक्ट आँकड़े प्रत्येक मास/वर्ष में सीएसआईआर मुख्यालय को प्रस्तुत किए गए।
- बैंक समाधान विवरण को अद्यतन किया गया। समायोजित कुल राशि- रु.1189.265 लाख तथा लेनदेन की कुल संख्या - 1208
- इण्टरनेट बैंकिंग का प्रभावी कार्यान्वयन प्रगति पर है।

## निधि की उपयोगिता :

## 1 (क) सीएसआईआर अनुदान राशि (दि. 31.3.2007 तक)

	परियोजनाएँ	राशि (रु. लाखों में)
(1)	नेटवर्क	361.215
(2)	गैर-नेटवर्क	4960.756
(3)	आईआरआर (आईसीटी)	151.156
(4)	आईआरआर (निर्माण)	15.840
(ख)	प्रयोगशाला आरक्षित निधि	675.874
(ग)	नमिटली परियोजनाएँ	442.079
(घ)	ईएमआर एवं वैज्ञानिक पूल	414.235
(च)	बाहरी वित्तपोषित परियोजनाएँ	1799.602
(छ)	आगे ले जाई गई अनुदान राशि (30.09.2006 तक)	
(1)	नेटवर्क	40.593
(2)	गैर-नेटवर्क	300.000
(3)	आईआरआर (आईसीटी)	45.500
	कुल योग	(1)9206.850

2	(क) वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर से भिन्न) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	167.784
	(ख) अन्य लेखाशीर्षों से	522.147
	कुल	(2)689.931
	(ग) निवेश का अन्तिम शेष 2006-2007	3011.000



## 3 आपति-पुस्तिका मदों का निपटारा

(रु. लाखों में)

	सरकारी	निजी	टीए/एलटीसी	स्थानीय
वर्ष के दौरान किए गए समायोजन	1.000	2374.175	48.752	40.237
कुल राशि	2464.164			
मदों की संख्या	771			

## 4 निम्न प्रकार के वाउचर तैयार किए गए :-

	एनसीएल	ग्रा.सं.मू.यू.	भा.वि.शि.अ.सं.	कुल
भुगतान प्राप्त राशि	18765	155	724	19644
टी.ई.	4886	5	38	4929
कुल	408	2	-	410
कुल	24059	162	762	24983

## भण्डार एवं क्रय

भण्डार एवं क्रय अनुभाग एनसीएल के लिए रसायनों, विलायकों, उपभोग्य वस्तुओं, अतिरिक्त पुर्जों आदि के अलावा अत्याधुनिक उपकरणों की खरीद करके उन्हें उपलब्ध कराता है। यह विभाग सामग्री प्राप्त करने, उसे जारी करने, उसका हिसाब रखने, सामग्री का अभिलेख रखने एवं अनुपयुक्त मदों/वस्तुओं के निपटारे हेतु वर्षभर अपनी कार्ययोजना पर कार्य करता है। भण्डार एवं क्रय विभाग ने सुचारु रूप से कार्यनिष्पादन हेतु विभिन्न विभागों एवं एजेंसियों जैसे - सीमा शुल्क एवं केन्द्रीय उत्पाद शुल्क से छूट हेतु डीएसआईआर के साथ, चुंगी (ऑक्ट्रॉई) से छूट प्राप्त करने के लिए पुणे नगर निगम, आयातित सामग्री समय पर प्राप्त होने के लिए सीमा शुल्क प्राधिकारी, मुम्बई/पुणे के साथ समन्वय स्थापित किया तथा भारतीय स्टेट बैंक एवं माल वहन करने वाले एवं कार्गो क्लियरिंग एजेंटों के साथ भी समन्वय बनाए रखा ताकि प्रयोगशाला हेतु खरीद/प्राप्त की जाने वाली सामग्री समय पर उपलब्ध हो सके।

## मूल्य (रुपयों में) के साथ संख्यात्मक संकेतक

मद	संख्या		मूल्य (रु. करोड़ में)	
	2005-06	2006-07	2005-06	2006-07
कुल प्राप्त एवं निष्पादित माँगपत्र	2322	2098	34.03	32.28
कुल दिए गए ऑर्डर (आयातित)	763	763	26.72	15.38
कुल दिए गए ऑर्डर (स्वदेशी)	1258*	1125*	8.04	13.89
कुल प्राप्त सामग्री (आयातित)	917	962	24.04	25.13
कुल प्राप्त सामग्री (स्वदेशी)	2112	2012	7.79	8.41
स्थानीय खरीद (ऑनलाइन आर सी सहित)	8458	9502	2.30	1.011
भण्डार से जारी की गई कुल सामग्री	35517	36928	0.79	0.99
समायोजित बकाया शेष			24.46	24.40
सीमा शुल्क से छूट प्राप्त राशि का उपयोग			21.64	21.60
उत्पाद शुल्क से छूट प्राप्त राशि का उपयोग			1.59	3.28

\*- ऑनलाइन रेट कौन्ट्रैक्ट मदों को छोड़कर



## खरीदे/खरीद हेतु ऑर्डर दिए गए प्रमुख उपकरण

क्र.सं.	मदों के नाम	लागत(रु.लाख में)
1	कम्प्यूटर	61.00
2	सैन, नैस, टेप लाइब्रेरी, ब्लेड सर्वर आदि	115.00
3	हाईपावर एक्साइमर लेसर फॉर पल्स्ड लेसर डिपोजिशन	67.00
4	मल्टिपर्पज हेस्टलॉय रिऐक्टर	31.00
5	हाई पर्फार्मन्स कम्प्यूटिंग क्लस्टर सिस्टम	130.25
6	डाइनामिक मेकैनिकल एनालाइजर (डीएमए)	75.00*
7	जेटा साइजर	40.00
8	ए सिंगल सिस्टम फॉर(एसएनओएम/सीएसएफएम/एएफएम)	90.00*
9	फ्लुरोसेन्स स्पेक्ट्रोफोटोमीटर	26.00*
10	इंजेक्शन मोल्लिंग मशीन	25.00*
11	टेबल टॉप ईजीएक्सआरएफ	25.00*
12	प्लाज्मा क्लीनर फॉर एचआरटीईएम	40.80
13	माइक्रोसॉफ्ट पेपर लाइसेन्स	78.40
14	टाइम रिजाल्ड फ्लुओरोसेन्स स्पेक्ट्रोमीटर	59.00
15	अपग्रेडेशन ऑफ डीआरएक्स५०० एनएमआर	98.81
16	वैक्स गोनिओमीटर	46.96
17	स्टीम एक्सप्लोजन रिऐक्टर	67.50
18	लैक्टिक अम्ल हेतु उपकरण	40.00
19	एचपीएलसी क्लस्टर सिस्टम	130.25
20	३डी लेजर लाइट स्कैटरिंग इक्विपमेन्ट	61.75
21	मल्टिपास रिओमीटर	80.00
22	लेबोरेटरी वर्क बेंचेज	40.50*

\*- उक्त उपकरणों की खरीद/प्राप्त करने की कार्रवाई जारी है।

## अनुपयुक्त वस्तुओं का निपटान :

वर्ष के दौरान दो बार अनुपयुक्त वस्तुओं का निपटारा किया गया। अप्रैल एवं जून 2006 के मध्य किए गए वस्तुओं के निपटान से रु.22,21,271 की राशि प्राप्त हुई जबकि अक्टूबर एवं दिसम्बर 2006 के बीच किए गए वस्तुओं के निपटान से रु.22,74,345 प्राप्त हुए।

## अभिलेखों का निपटान :

वर्ष 1974-75 से 2002-03 की अवधि की क्रय से सम्बन्धित फाइलों को अलग-अलग करके उनमें से 25775 फाइलों का निपटारा किया गया जिससे प्राप्त रु. 8750/- की राशि रोकड़ अनुभाग में जमा की गई।

## भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान हेतु खरीद :

भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान, (आईआईएसईआर) पुणे की स्थापना हेतु उनके लिए आवश्यक सामग्री एवं अन्य प्रशासनिक सेवाएँ उपलब्ध कराने का कार्य एनसीएल को सौंपा गया है। इस निर्णय के आधार पर एनसीएल के भण्डार एवं क्रय अनुभाग ने आईआईएसईआर के निदेशक/शासी मण्डल द्वारा इस कार्य हेतु निर्धारित समय सीमा के अन्दर उन्हें सौंपा गया कार्य निष्पादित करने की तैयारी कर ली है। उक्त अनुभाग द्वारा आईआईएसईआर के लिए आवश्यक सामग्री आदि की खरीद/प्राप्ति निम्न प्रकार से की गई है:



मद	संख्या	मूल्य (रु. करोड़ में)
	2006-07	2006-07
कुल प्राप्त एवं निष्पादित माँगपत्र	135	2.169
कुल दिए गए ऑर्डर (आयातित)	10	0.578
कुल दिए गए ऑर्डर (स्वदेशी)	128	1.915
कुल प्राप्त सामग्री (आयातित)	9	0.598
कुल प्राप्त सामग्री (स्वदेशी)	176	2.187
स्थानीय खरीद (ऑन-लाइन रेट कॉन्ट्रैक्ट सहित)	135	0.162
<b>भण्डार से जारी की गई कुल सामग्री</b>		
समायोजित बकाया शेष	4	0.220
सीमा शुल्क छूट से प्राप्त राशि का उपयोग		0.665
उत्पाद शुल्क छूट से प्राप्त राशि का उपयोग		0.169

#### सूचना उत्पाद विकास एवं अनुसंधान यूनिट :

सूचना उत्पाद विकास एवं अनुसंधान यूनिट हेतु वर्ष के दौरान रु. 75.00 लाख की सामग्री खरीद करने की प्रक्रिया पूरी की गई।



#### ADMINISTRATION

##### Finance and accounts department

##### Highlights of the work

- Finance and accounts department provided financial advises to Director, NCL, Head, CSE Unit, Head, URDIP and Director, Indian Institute of Science Education and Research (IISER-Pune).
- Accounts of IISER (receipts, payments and its related records) were maintained.
- Maintained GPF/CPF accounts of all individual, Issue of Annual Closure statement to individual on the 1st day of New Financial Year
- Nine out of nineteen CAG Audit paras were settled.
- Finance and accounts of more than 500 externally funded projects were dealt.
- Various proposals from financial angles related to agreements, works proposals, pay fixation cases, personal files, deputation and court attachments were scrutinized.
- Full accounts (IMPACT) and its related registers were maintained and IMPACT data was submitted to CSIR H monthly/ annually.
- Bank reconciliation statement was updated: Total amount adjusted -Rs. 1189.265 lakhs and number of transactions- 1208.
- Effective implementation of Internet Banking is in progress.

##### Funds Utilization :

1

a)	CSIR Grant (by 31.3.2007)	Amount (Rs. in lakh)
	Projects	
i)	Network	361.215
ii)	Non network	4960.756
iii)	IRR (ICT)	151.156
iv)	IRR (Const.)	15.840
b)	Laboratory Reserve	675.874
c)	NIMITLI Projects	442.079
d)	EMR & Scientist Pool	414.235
e)	Externally funded projects	1799.602
f)	Carry forward grant (by 30.9.2006)	
i)	Network	40.593
ii)	Non network	300.000
iii)	IRR (ICT)	45.500
	<b>Grand Total (1)</b>	<b>9206.850</b>



2	Generation of Lab Reserve (a) through earning of interest on investment of surplus funds (other than CSIR) during the year.	167.784
	(b) From other heads	522.147
	Total (2)	689.931
	(c) Investment closing balance 2006-07	3011.000

## 3 Clearance of OB items

(Rs. in lakh)

	Govt.	Private	TA/LTC	Local
Adjustment. made during the year	1.000	2374.175	48.752	40.237
Total Amount Rs.	2464.164			
No. of items	771			

## 4 The following types of vouchers were generated:

	NCL (nos.)	CSEU (nos.)	IISER (nos.)	Total (nos.)
Payment	18765	155	724	19644
Receipt	4886	5	38	4929
TE	408	2	-	410
Total	24059	162	762	24983



## Stores and Purchase

Stores and Purchase Department procures highly sophisticated instruments for NCL, besides chemicals, solvents, consumables, spares etc. The department works with plan of action throughout the year to procure the materials, issuing, accounting, record maintenance and disposal of unserviceable items. The department co-ordinated with various other department/ agencies like DSIR for Custom Duty & Central Excise Duty exemption, Pune Municipal Corporation for obtaining Octroi Exemption, Mumbai/ Pune Customs Authorities for timely clearance of imported consignments and co-ordinating with State Bank of India and Freight forwarding and Cargo Clearing Agents.

## Numerical indicators along with value (in Rupees)

Item	Numbers		Value (Rs. in Crores)	
	2005-06	2006-07	2005-06	2006-07
Total indents received and processed	2322	2098	34.03	32.28
Total orders placed (imported)	763	763	26.72	15.38
Total orders placed (indigenous)	1258*	1125*	8.04	13.89
Total consignments received (imported)	917	962	24.04	25.13
Total consignments received (indigenous)	2112	2012	7.79	8.41
Local Purchases (including on-line RC)	8458	9502	2.30	1.011
<b>Total Stores Issued</b>	35517	36928	0.79	0.99
Outstanding balance adjusted			24.46	24.40
Utilization of Custom Duty Exemption			21.64	21.60
Utilization of Excise Duty Exemption			1.59	3.28

\*- Excluding on-line rate contract items

## Major equipment procured/ processed

S.No.	Name of the Items	Cost (Rs. in lakhs)
1	Desktop PCs	61.00
2	SAN, NAS, Tape Library, Blade Servers etc.	115.00
3	High Power Excimer Laser for Pulsed Laser Deposition	67.00
4	Multi-Purpose Hastelloy Reactor	31.00
5	High Performance Computing Cluster System	130.25
6	Dynamic Mechanical Analyzer(DMA)	75.00*
7	Zeta Sizer	40.00
8	A single system for (SNOM/CFM/AFM)	90.00*
9	Fluorescence Spectrophotometer	26.00*
10	Injection Moulding Machine	25.00*
11	Table Top EDXRF	25.00*
12	Plasma Cleaner for HRTEM	40.80
13	Microsoft Paper License	78.40

Table cont'd



Table cont'd from previous page

S.No.	Name of the Items	Cost (Rs. in lakhs)
14	Time Resolved Fluorescence Spectrometer	59.00
15	Upgradation of DRX500 NMR	98.81
16	Wax Goniometer	46.96
17	Steam Explosion Reactor	67.50
18	Equipment for Lactic Acid	40.00
19	HPLC Cluster System	130.25
20	3D Lazer Light Scattering Equipment	61.75
21	Multipass Rheometer	80.00
22	Laboratory Work Benches	40.50*

\*- Files are in process

**Disposal of unserviceable items:**

On two occasions unserviceable items were disposed off during the year. A sum of Rs.22,21,271 was realized from the disposal between April and June 2006 whereas a sum of Rs.22,74,345/- was realized from the disposal between October and December 2006.

**Disposal of records:**

Purchase files accumulated from 1974-75 to 2002-03 were segregated and 25775 files were disposed off and an amount of Rs.8750/- was deposited with the cashier.

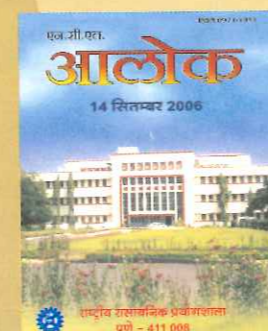
**Procurement for IISER:**

NCL has been entrusted with the responsibility of procurement of materials and other administrative services for setting up of Indian Institute for Science Education & Research (IISER) at Pune. Based on this decision, NCL Stores & Purchase has been geared up to meet the time target set by the Board of Directors/ Governors of IISER. The following are the Accomplishments related to IISER.

Item	Numbers	Value ( Rs.in Crores )
	2006-07	2006-07
Total indents received and processed	135	2.169
Total orders placed (imported)	10	0.578
Total orders placed (indigenous)	128	1.915
Total consignments received (imported)	9	0.598
Total consignments received (indigenous)	176	2.187
Local Purchases (including on-line RC)	135	0.162
<b>Total Stores Issued</b>		
Outstanding balance adjusted	4	0.220
Utilization of Custom Duty Exemption		0.665
Utilization of Excise Duty Exemption		0.169

**Procurement for URDIP** procurement worth Rs.75.00 Lakhs was processed during the year for URDIP.

Research Papers Published	176
Foreign Patents Granted	202
Indian Patents Granted	204
Books/ Chapters In Books	208
Academic Collaborations	209
Deputations Abroad	213
Lectures/ Seminars Delivered By Visitors	217
Invited Talks/ Lectures Delivered By NCL Scientists	221
Conferences/ Seminars/ Workshops Organized	223
Awards/ Recognitions	224
Member, Board Of Directors, Industry	225
Editor/ Editorial Board Members Of Journals	226
NCL Research Foundation	228
Venture Center	233
राजभाषा	235
Dateline NCL	238
Committees	240





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Process for preparation of optically active azabicyclo heptanone derivatives	Joshi, R.R., Prabhune, A.A., Joshi, R.A., Gurjar, M.K.	EP 1348765
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An improved process for preparation of cumene	Bokade, V.V., Kharul, U.K.	194304



Title	Inventors	Patent No
A process for the transesterification of keto esters using solid acids as catalyst	Keshavaraja, A., Ramaswamy, A.V., Chavan, S.P., Dentale, S.W., Zubhidha, P.K.	194311
A process for the preparation of substituted 6-[6-benzyl-5-oxo-3-phenyl-(3S, 7S,7aR)-perhydroimidazo[1,5-C][1,3] thiazol]-7yl	Chavan, S.P., Chittiboyina, A.G., Kamat, S.K., Kalkote, U.R., Ravindranathan, T.	194355
An improved process for the preparation of an optically active 6-hydroxymethyl-4-(tert-butylidimethylsilyloxy)-(4R,6S)-tetrahydro-2H-2-pyranone	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	194362
An improved process for the preparation of 1,2,4, trichlorobenzene	Sharma, S., Singh, A.P.	194594
An improved process for the preparation of sulphate immobilized zirconia based superacids	Mulla, I.S., Vijayamohan, K.P.	194595
An improved process for the preparation of diphenylmethanes	Pandey, A.K., Singh, A.P., Ramaswamy, A.V.	194597
An improved process for the treatment of black liquor waste from paper mills	Moghe, P.P., Kotasthane, M.G., Pol, A.V., Bahirat, P.K.	194598
An improved process for the selective separation of copper ions	Skaria, S., Ghadge, V.B., Ponrathnam, S., Rajan, C.R.	194601
A process for the preparation of thin film composite membranes	Kulkarni, S.S., Mudaliar, J.M.	194602
A process for the preparation of optically active azabicyclo heptanone derivatives	Joshi, R.R., Prabhune, A.A., Joshi, R.A., Gurjar, M.K.	194686
A process for the ortho hydroxylation of monohydroxy aromatic compounds	Robert, Raja, Halemane, S.T., Chandwadkar, A.J., Ratnasamy, P.	194689
An improved process for the recovery of tartaric acid and other products from tamarind pulp	Kulkarni, M.G., Thakar, M.J., Gaikwad, B.G., Nene, S.N.	194699
A process for the preparation of branched poly(Arylcarbonate)s	Sivaram, S., Hait, S.B.	194790
An improved process for the preparation of dialkoxy methanes	Deshmukh, A.R.A.S., Bhawal, B.M., Gumaste, V.K.	194804
An improved process for the preparation of a one piece insert useful for an artificial foot	Nadkarni, V.M. (Ex.), Patil, P.S., Pandit, S.B., Yemul, O.S., Rajan, C.R.	194808
A process for the preparation of a novel 3-tetrahydro-2H-2-pyran-5-yl-5-(tert-butylidimethylsilyloxy)-(1S,3R,5R)-cyclohexylacetate useful as an intermediate for 6-hydroxymethyl-4-(tert-butylidimethylsilyloxy)-(4R,6S)-tetrahydro-2H-2-pyranone	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	195688
A process for the separation of lignin from black liquor waste of paper mills	Moghe, P.P., Kotasthane, M.G., Pol, A.V., Bahirat, P.K.	195692



Title	Inventors	Patent No
An improved process for the preparation of ethanol	Prabhune, A.A., Chandwadkar, A.J., Baliga, S.A., SivaRaman, H.	195695
A process for production of modified polypropylene moulding compounds having high impact strength	Radhakrishnan, S., Khare, A.A., Saujanya, C.	195696
An improved process for the complete oxidation of carbon monoxide using partially stabilized zirconia	Keshavaraja, A., Katdare, S.P., Ramaswamy, A.V.	195758
A process for the preparation of a novel 3-tetrahydro-2H-2-pyran-5-yl-(tert-butyl dimethylsilyloxy)-(1S,3R,5R)-cyclohexan-1-ol- useful as an intermediate for 6-hydroxymethyl-4-(tert-butyl dimethylsilyloxy)-(4R,6S)-tetrahydro-2H-2-pyranone	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	195793
An improved process for the preparation of Linear Alkylbenzene	Robert, Raja, Ratnasamy, P., Sivasanker, S.	195808
An improved catalytic process for the production of pyridine and picolines	Rajiv Kumar, Joshi, P.N., Chaphekar, G.M., Niphadkar, P.S., Agarwal, A., Verma, P.K., Singh, K.S.	195827
A process for the preparation of S(-) Amlodipine salts	Joshi, R.R., Joshi, R.A., Gurjar, M.K.	196770
A process for the preparation of 1,4 butenediol from 1,4 butynediol using a nanosized noble metal catalyst	Rode, C.V., Telkar, M.M., Chaudhari, R.V.	196828
An improved process for the preparation of meta-phenoxy benzaldehyde	Ratnasamy, P., Chavan, S.A., Halligudi, S.B.	196831
A process for the acylation of aromatic compounds using a reusable solid catalyst comprising indium halide	Choudhary, V.R., Jana, S.K., Patil, N.S.	196834
An improved process for the preparation of tetrahydrofuran	Chaudhari, R.V., Jaganathan, R., Chaudhari, S.T., Naik, R.V., Vaidya, S.H., Rode, C.V.	196977
A process for preparation of zirconium containing aluminosilicate molecular sieve	Raksh, B.P., Ramaswamy, A.V., Ramaswamy, V.	196987
An improved process for the preparation of crystalline titanate molecular sieve	Das, T.K., Chandwadkar, A.J., Sivasanker, S.	197034
An improved process for the preparation of poly(ester carbonate)s	Hait, S.B., Sivaram, S.	197048
A process for the preparation of an improved copper chromite catalyst	Chaudhari, R.V., Jaganathan, R., Chaudhari, S.T., Rode, C.V.	197205
An improved single step process for preparation of p-Aminophenol	Chaudhari, R.V., Divekar, S.S., Vaidya, M.J., Rode, C.V.	197210
A process for the preparation of thermally conducting polymer composite useful for mounting thermistors on metal substrates	Radhakrishnan, S.	197219



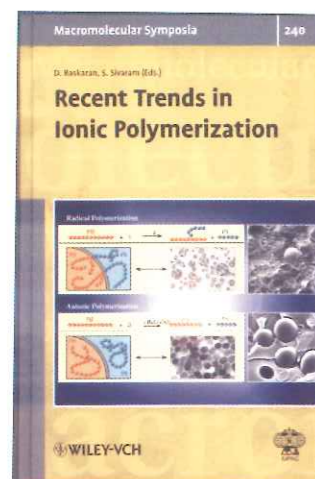
Title	Inventors	Patent No
An improved process for the hydrogenation of organic compounds	Upadhyaya, T.T., Katdare, S., Sabde, D.P., Daniel, T., Ramaswamy, V., Sudalai, A., Ravindranathan, T.	197236
An improved process for rapid deposition of conducting polymer films on insulating substrates	Radhakrishnan, S., Unde, S.G.	197239
An improved process for the preparation of 2,5-dihydrofuran	Panse, D.G., Deshmukh, A.R.A.S., Bhawal, B.M., Sarkar, A.	197276
A process for the preparation of 2-(4-[N-disubstituted] amino benzylidene) cycloalkanones	Raju, S.V.N., Subramaniam, S., Srinivasan, K.V., Rajan, C.R., Ponrathnam, S., Noel, C.	197322
A process for the preparation of 2-(4-methyl amino benzylidene) cycloalkanones	Raju, S.V.N., Mule, S.A., Srinivasan, K.V., Rajan, C.R., Ponrathnam, S., Noel, C.	197325
A process for the preparation of mesogens	Raju, S.V.N., Subramaniam, S., Srinivasan, K.V., Rajan, C.R., Ponrathnam, S., Noel, C.	197326
An improved process for the oxidation of cyclohexane to adipic acid	Saji, P.V., Ratnasamy, C., Gopinathan, S.	197329
A process for the separation of mono carboxylic and dicarboxylic acids from a mixture of mono and dicarboxylic acids	Patil, S.D., Sabne, M.B., Vernekar, S.P.	197341
An improved process for depositing conducting polymer films for use in electrochromic devices	Radhakrishnan, S., Unde, S.G.	197343
An improved process for the preparation of microporous crystalline titanium silicalite-1	Dongare, M.K., Sabde, D.P., Hegde, S.G.	197344
A process for the preparation of a novel titanium rich NU-1 zeolites	Kotasthane, A.N., Ahedi, R.K., Shevade, S.S., Ramaswamy, A.V.	197345
An improved process for the preparation of supported metallocene catalyst	Sensarma, S., Sivaram, S.	197346
An improved process for the polymerization and co-polymerization of olefins using supported metallocene catalyst	Sensarma, S., Sivaram, S.	197348
An improved process for the preparation of metallized polymer	Balamurugan, S., Patil, A.S., Vernekar, S.P.	197366
A process for the preparation of a polyurethane formulation useful for the manufacture of an artificial foot such as the Jaipur foot and an artificial foot made thereby	Nadkarni, V.M. (Ex.), Yemul, O.S., Sathe, S.N., Rajan, C.R.	197393
An improved process for the preparation of pillared interlayered clays	Katdare, S.P., Ramaswamy, A.V., Sivasanker, S., Ramaswamy, V.	199569
An improved process for the preparation of monocondensed benzylidene cycloalkanones	Raju, S.V.N., Sonpatki, V.M., Srinivasan, K.V., Rajan, C.R., Ponrathnam, S., Claudine, N.	199594



## BOOKS / CHAPTER IN BOOKS

## BOOKS

1. Baskaran and Sivaram S., Recent Trends in Ionic Polymerization, Macromolecular Symposia 240, Wiley VCH, Weinheim, Germany

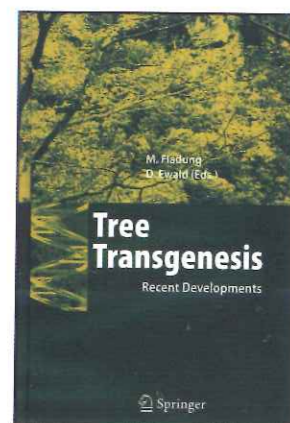


## CHAPTERS

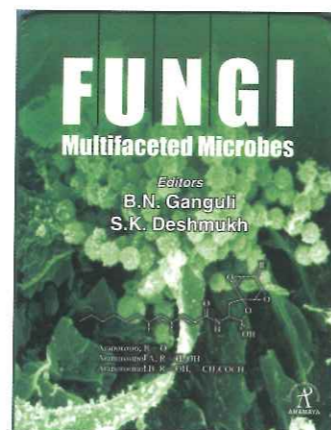
1. Halligudi S.B., Zirconia-supported heteropoly acid based catalysts for organic synthesis in Heterogeneous Catalysis in Organic Synthesis, Ed. Arpad Molnar, Bentham Science Publishers, Ltd., Sharjah, U.A.E.

2. Ms Ramaswamy Veda, Structural characterization of catalytic materials in Advanced X-ray Techniques in Research and Industry, Ed. A.K. Singh, Capital Publishing Company, New Delhi and IOC press, Amsterdam, The Netherlands, pp. 316-332.

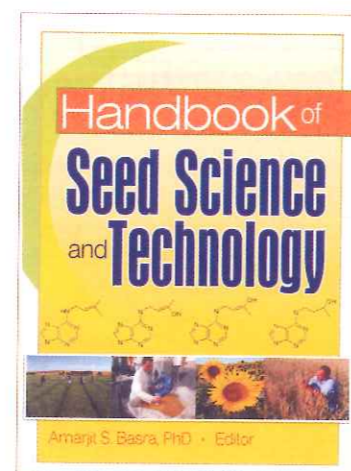
3. Ms Kendurkar Suchishweta V., (Mrs.) Nadgauda Rajani Satish, and Vaishali Naik, Genetic Transformation of tropical trees shrubs and tree like plants in Tree Transgenesis:Recent Developments, Ed. Mathias Fladung and D.Ewald, Springer, Berlin, Germany, pp 67-92.



4. A. Ahmad, S. Senapati, M.I. Khan, R. Kumar, and M. Sastry, Biosynthesis of Silver Nanoparticles Using Fungi, in Fungi: Multifaceted Microbes, Ed. B.N. Ganguli and S.K. Deshmukh, CRC Press.



5. Harsulkar A. M., Giri A. P., Deshpande V. V., Gupta V. S., Sainani M. N. and Ranjekar P. K., Seed protease inhibitors, in Handbook of seed science and technology, Ed. Amrjit Basara, The Howarth Press Inc. USA, pp 475 - 499.



## ACADEMIC COLLABORATIONS

NCL has collaborative projects with many leading national and international academic and scientific institutes. NCL scientists individually or as a team also have international collaborative programmes with leading research groups from abroad.

## Institute to Institute Collaborations

External Institute	Field(s) of Collaboration	NCL Nodal Scientist(s)
Bharati Vidyapeeth University Poona College of Pharmacy, Pune	Biotechnology, Polymer and Materials Science Engineering, Nanomaterials (Design and Development)	Dr. S. Sivaram
Center of Excellence in Polymer Science, Karnatak University, Dharwad	Polymer Science	Dr. M.G. Kulkarni
Centre for Development of Advanced Computing (C-DAC), Pune	Parallelisation of Coupled-Cluster Electronic Structure Theory, Parallelisation of Optimization Technique, and Biodiversity	Dr. Sourav Pal
Centre for Development of Advanced Computing (C-DAC), Pune and ERNET India	Promoting High Level Research with the help of GRID Technology and its Applications	Dr. Sourav Pal
Fuel Cell Materials Center, National Institute for Materials Science (NIMS), Tsukuba, Japan	Catalysis with Hierarchically Ordered Nanoporous Materials	Dr. Rajiv Kumar
Gwangju Institute of Science and Technology (GIST), Republic of Korea	Organic Materials, Photonic Polymers and Hybrid Materials	Dr. D. Baskaran
National Center for Cell Science, Pune	Exploitation of Biomedical Potentials of Fungal Extracts of Specific Tissues Related to Hitherto Unattained Aspects of Peptide/ Protein Fractionation, Purification and Bioactivity Testing from Fungi	Dr. Islam Khan
National Institute for Applied Sciences, Lyon (INSA, Lyon), France	Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Mr. Sanjay Nene
RMIT University, School of Applied Sciences, Melbourne, Australia	Catalysis, High Field Solid State NMR Studies and Nanoscience / Nanotechnology	Dr. S. Sivaram
The Ohio State University Research Foundation (OSURF), Columbus, Ohio, USA	Materials Science Engineering and Nanotechnology	Dr. K. Vijayamohan
University of Applied Sciences, Hochschule Anhalt HAS, Kothen, Germany	Biochemistry, Bioprocess Technology and Bioengineering (Design and Development)	Mr. Sanjay Nene
University of Kansas, Lawrence, USA	Environmentally Benign Catalysis, Oxidation and Hydroxy Formylation Reaction in Supercritical CO <sub>2</sub> Medium	Dr. R.V. Chaudhari
University of Science and Technology, Lille (USTL), France	High Field Solid State NMR Studies, Catalysis, Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Dr. Rajiv Kumar/ Dr S. Ganapathy



External Institute	Field(s) of Collaboration	NCL Nodal Scientist(s)
Vasantdada Sugar Institute, Pune	Zeolite assisted Ethanollic Fermentation	Dr. Archana Pundle
National Institute of Food and Agro Industries, Massy, France	Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Mr. Sanjay Nene

#### Scientist to scientist International Collaborations

Project Title	NCL Partner(s)	External Partner(s)
Synthesis of novel heterogeneous catalysts for asymmetric oxidation catalysis	Dr. A. P Singh	Dr. Stéphane Ménage DR CNRS Lab, Laboratoire de Chimie et Biochimie des Centres Redox Biologiques (CBCRB), 17 rue des Martyrs, CEA-Grenoble, 38054 Grenoble Cedex 9 France
Synthesis and surface modification of magnetic core-noble metal shell nanoparticles for biological applications	Dr. B.L.V. Prasad	Prof. Mathias. Brust University of Liverpool UK
Development of PP-clay nanocomposites and detailed investigations on the effect of drawing on the structure and morphology (Sponsored by DST)	Dr. C. Ramesh	Dr. Taweechai Amornsakchai, Mahidol University, Bangkok, Thailand
Study on crystalline transition in nylons using HTFTIR	Dr. C. Ramesh	Prof. K. Tashiro, Department of Macromolecular Science, Graduate School of Science, Osaka University, Japan
Design, synthesis and biological evaluation of cationised PNAs as antisense agents ex vivo and in vivo	Dr. K.N. Ganesh / Dr. V.A. Kumar	Prof. Bernard Lebleu Universite Montpellier 2 UMR-CNRS 5241 Montpellier
Developemnt of a mycoinsecticide against <i>Helicoverpa armigera</i> in pluses: from the laboratory to the market	Dr. M. V. Deshpande	Dr. J. Enkerli Swiss Federal Research Station for Agroecology and Agriculture, Zurich-Reckenholz, Switzerland
Polyamines, dimorphism in <i>Yarrowia lipolytica</i> and the petroleum oil degradation in marine environment	Dr. M. V. Deshpande	Prof. J.Ruiz-Herrera Unidad Irapuato, Apartado Irapuato, Guanajuato 36500 Mexico.
Interactions in nano-magnet arrays	Dr. Pankaj Poddar	Prof. W. Schwarzacher University of Bristol UK
Catalytic reaction engineering using ionic liquids	Dr. R. M. Deshpande	Prof. Henri Delmas ENSIACET, Toulouse, France



Project Title	NCL Partner(s)	External Partner(s)
Evaluation and improvement of the durability in a composite insulator: study of the degradation/stabilization of epoxy fiber glass composites coated with elastomer	Dr. R. P. Singh	Prof. J.L. Gardette Laboratoire De PhotochimieMoleculaire et Macromoleculaire (LPMM) Universite Blaise Pascal, Cedex, France Prof. J.Lacoste, ENSCCF, France Dr. Emmanuel Brocard Sediver, St.Yorre, France
Synthesis of functionalized polyolefins and its durability improvements: Novel approach to stabilization against photochemical degradation	Dr. R. P. Singh	Dr. Maria das Mercedes Marques, Instituto Superior Technico, Centro de Qumica Estrutural II Lisboa Cedex, Portugal
Hydrogeneous for estimation of small organic molecules	Dr. Rajiv Kumar	Dr. G. Shankar Royal Society U.K.
Comparative study on the development of solid acid catalysts for alkylation of phenolics	Dr. S. B. Halligudi	Prof. Jack CQ Fletcher, Associate Professor Director, Catalysis Research Unit Department of Chemical Engineering University of Capetown, Rondebosch, South Africa
Modeling of zeolite framework relaxation	Dr. Sourav Pal	Dr. Francois Fajula (PI) Dr. Annick Goursot (Co-PI), ENSCM, Montpellier, France
Somatic hybridization of peanut ( <i>Arachis hypogaea</i> L) by protoplast fusion	Dr. Sulekha Hazra	Dr. Maria-Teresa Scarano, Istituto di Genetica Vegetale - Sezione di Palermo Consiglio Nazionale delle Ricerche, Palermo, Italy
Improved productivity, profitability and sustainability of sheep production in Maharashtra through genetically enhanced prolificacy, growth and parasite resistance	Dr. Vidya Gupta	Stephen Walkden-Brown, Associate Professor in Animal Health and Production Centre for Animal Health and Welfare W49 School of Rural Science and Agriculture University of New England, Armidale, NSW 2351 Australia  Dr. Jill Maddox Senior Research Fellow Centre for Animal Biotechnology School of Veterinary Science University of Melbourne, Victoria 3010 Australia



Project Title	NCL Partner(s)	External Partner(s)
Improving rust resistance in wheat suitable for marginal rain-fed and semi arid zone of central and peninsular India through molecular markers	Dr. Vidya Gupta	Prof. Beat Keller Institute of Plant Biology University of Zurich, Zollikerstr,107, CH-8008, Zurich Switzerland
Increasing the efficiency of production and nutritional value of chickpea	Dr. Vidya Gupta	Fred J. Muehlbauer USDA-ARS 303 Johnson Hall Washington State University Pullman, WA 99164-6434, USA  T.J. Higgins Deputy Chief CSIRO Plant Industry  John Gatehouse, Reader in Biological Sciences, School of Biological and Biomedical Sciences, University of Durham, South Road, Durham DH1 3LE, UK.



## DEPUTATION ABROAD

## Bilateral/ collaborative/ exchange programmes

**Dr. A.P. Singh,**

France, IFCPAR Project, 20 Apr 06 to 19 May 06

**Dr. P. Manikandan,**UK, Joint Scientific Project between NCL and Davy Faraday Research Laboratory UK,  
08 May 06 to 20 May 06**Dr. R.P. Singh,**

France, IFCPAR Project and Collaboration with French Universities, 24 Apr 06 to 27 May 06

**Dr.(Mrs.) Vijayanti Anil Kumar,**

France, IFCPAR Project, 24 May 06 to 20 Jun 06

**Dr. H.V. Pol,**

Japan, 22nd Annual Meeting of the Polymer Processing Society, 02 Jul 06 to 10 Jul 06

**Dr. M.V. Badiger,**

France, IFCPAR Project, 03 Jul 06 to 17 Jul 06

**Dr. P.C. Ghosh.,**

Germany, CSIR-DAAD Exchange of Scientist Programme, 26 June 06 to 25 Aug 06

**Dr. C. Ramesh,**Thailand, India-Thailand S&T Co-operation,  
10 Sep 06 to 17 Sep 06**Dr. D. Srinivas,**Germany, DST-DAAD and Conference,  
07 Sep 06 to 22 Sep 06**Dr. R.V. Chaudhari,**

France, IFCPAR Project, 11 Sep 06 to 22 Sep 06

**Dr. Sourav Pal,**

France, IFCPAR Project, 14 Sep 06 to 29 Sep 06

**Dr.(Mrs.) V.G. Puranik,**

Germany, DST-DAAD, 15 Sep 06 to 17 Oct 06

**Dr. S.B. Halligudi,**

Japan, Bilateral Programme, 18 Oct 06 to 02 Nov 06

**Dr. Sourav Pal,**Germany, Bilateral Programme,  
02 Nov 06 to 19 Nov 06**Dr. P. Manikandan,**U.K., Joint Scientific Programme,  
12 Nov 06 to 26 Nov 06**Dr. A.P. Singh,**

France, IFCPAR Project, 09 Nov 06 to 08 Dec 06

**Dr. Pankaj Poddar,**U.K., Study Magnetic Measurements,  
03 Dec 06 to 25 Dec 06**Dr. Sourav Pal,**Germany, Joint Project BASF Ludwigshafen,  
19 Mar 07 to 21 Mar 07**Dr. B.L.V. Prasad,**U.K., Collaborative Research Programme,  
13 Mar 07 to 24 Mar 07**Dr. P.G. Shukla,**

U.S.A., Collaborative Project, 12 Mar 07 to 29 Mar 07

## Business Development Activity

**Dr. P.G. Shukla,**

U.S.A., 31 May 06 to 13 Jun 06

**Dr. A.K. Lele,**

U.S.A., 06 Oct 06 to 15 Oct 06

**Mr. P.P. Barve,**

U.S.A., 31 Oct 06 to 08 Nov 06

**Dr. V.V. Ranade,**

Saudi Arabia, 11 Dec 06 to 13 Dec 06

## Conferences/ seminars/ symposia/workshops

**Dr. Sourav Pal,**Canada and Germany, 7th Annual deMon Developers Workshop and Visit Institutes for Future Co-operation,  
21 Apr 06 to 28 Apr 06





**Dr. C. Ramesh,**  
Japan, POLYCHAR-14 World Forum and Toyota  
Technological Institute, 16 Apr 06 to 29 Apr 06

**Dr. S. Ganapathy,**  
U.S.A., 47th ENC Conference and Business  
Development, 23 Apr 06 to 06 May 06

**Dr. B.L.V. Prasad,**  
Germany, Conference, 08 May 06 to 11 May 06

**Dr.S. Sivaram,**  
Thailand, to deliver an invited lecture in the conference  
titled "S&T Towards the Future" on the occasion of 43<sup>rd</sup>  
Anniversary of Thailand Institute of Scientific and  
Technological Research (TISTR), Bangkok, 25 May 06

**Dr. M.V. Deshpande,**  
Thailand, Preparatory Workshop on Persistent Organic  
Pollutants, 31 May 06 to 01 Jun 06

**Dr. Ganesh Pandey,**  
Japan, Conference, 24 May 06 to 05 Jun 06

**Dr. A.P. Singh,**  
Japan, 5th Tokyo Conference, 23 Jul 06 to 28 Jul 06

**Dr. M.K. Gurjar,**  
Japan, ICOB-5 and ISCNP-25 IUPAC,  
23 Jul 06 to 28 Jul 06

**Dr. P.G. Shukla,**  
Austria and Germany, 23rd Annual Conference of  
Controlled Release Society and Visiting Institutes of  
Technology and Biosystems, 22 Jul 06 to 28 Jul 06

**Mr. H.G. Joglekar,**  
Thailand, International Crop-Science Conference,  
27 Jul 06 to 28 Jul 06

**Dr. P.N. Joshi,**  
Japan, ZMPC Symposium 2006,  
30 Jul 06 to 02 Aug 06

**Dr. Rajiv Kumar,**  
Japan, 5th Tokyo Conference and International  
Symposium on Zeolites, 23<sup>rd</sup> Jul 06 to 02 Aug 06

**Mr. V.V. Bokade,**  
Japan, ZMPC Symposium 2006,  
30 Jul 06 to 02 Aug 06

**Dr.(Mrs.) A.A. Prabhune,**  
Iran, 10th Iranian Pharmaceutical Science Congress,  
22 Aug 06 to 24 Aug 06

**Dr. M.V. Deshpande,**  
China, 9th International Colloquium,  
27 Aug 06 to 01 Sep 06

**Dr.(Mrs.) Vidya Gupta,**  
U.S.A, International Workshop on Genomics Enabled  
Improvement of Legumes, 29 Aug 06 to 01 Sep 06

**Dr. M.K. Dongare,**  
Germany, IUPAC ICGC-1 Conference,  
10 Sep 06 to 15 Sep 06

**Dr. V.V. Ranade,**  
Germany, The Netherlands and U.S.A, 19th  
International symposium ISCRE-19, Visit to  
Universities and Business Development,  
03 Sep 06 to 16 Sep 06

**Dr. U.K. Kharul,**  
France, Seminar, 29 Nov 06 to 02 Dec 06

**Mr. Sanjay Nene,**  
France, Seminar, 29 Nov 06 to 02 Dec 06

**Dr. R.M. Deshpande,**  
Singapore, APCAT4, 06 Dec 06 to 08 Dec 06

**Dr. K. Guruswamy,**  
France, Rheology School (Flow in Glassy Systems),  
05 Feb 07 to 14 Feb 07

**Dr. (Mrs) Mala Rao,**  
Japan, IUMBM International Congress of Biochemistry  
and Molecular Biology, 18 Jun 06 to 23 Jun 06

**Dr. (Mrs.) Vidya Gupta,**  
USA, International Symposium, Discussion of  
Research Progress and Plan Future Implementation of  
Collaborative Project, 7 June 06 to 19 June 06

**Dr. R.V. Chaudhari,**  
USA, Symposium 2006 and Business Development,  
11 Jun 06 to 24 Jun 06

**Extra Ordinary Leave / Fellowship / Sabbatical  
Leave/ Visiting Professor**

**Dr. M.K. Dongare,**  
France, Visiting Professor, 1 Jun 06 to 21 Jul 06

**Dr. M. Karthikeyan,**  
U.S.A, Visiting Scholar, 14 Aug 06 to 14 Nov 06

**Dr. Pradeep Kumar,**  
Germany, Alexander Von Humboldt Fellowship,  
01 Sep 06 to 30 Nov 06

**Dr. C.V. Rode,**  
Japan, Guest Researcher, 11 Oct 06 to 08 Dec 06

**Dr.(Ms) Sapna Ravindranathan,**  
Switzerland, Fellowship, 15 Nov 06 to 15 Jan 07

**Dr. A.P. Giri,**  
Germany, Fellowship Extension,  
09 Dec 06 to 28 Feb 07

**Dr. V.R. Pedireddi,**  
Germany, Raman Research Fellowship,  
01 Oct 06 to 31 Mar 07

**Dr. R.A. Shaikh,**  
South Korea, EOL to work as a Research Associate,  
01 May 06 to 30 Apr 07

**Dr. B.B. Idage,**  
South Korea, EOL Extension,  
06 Jun 06 to 06 Jun 07

**Dr. A.K. Lele,**  
France, UK and The Netherlands, Visiting Professor,  
27 Jun 06 to 24 Jul 06

**Dr. S. Sivaram,**  
USA, Professor H.A. Morton Distinguished Visiting  
Professor at the University of Akron, College of Polymer  
Science and Polymer Engineering, Akron, USA  
1 Sept 06 to 30 Nov 06



**Dr. M.K. Dongare,**  
France, Sabbatical Leave, 01 Feb 07 to 31 Jul 07

**Dr. V.H. Rane,**  
South Korea, KOFST Fellowship,  
01 Nov 06 to 31 Oct 07

**Dr. R.P. Singh,**  
South Korea, EOL - Brain Pool Fellowship,  
30 Dec 06 to 29 Dec 07

**Dr. A.S. Mamman,**  
Korea, EOL Extension, 10 Jan 07 to 09 Jan 08

**Dr.(Ms) S.V. Awate,**  
South Korea, EOL, 26 Feb 07 to 25 Feb 08

**Dr.(Mrs) S.B. Idage,**  
South Korea, EOL, 01 Mar 07 to 28 Feb 08

**Meetings**

**Dr. S. Sivaram,**  
Russia, to participate on behalf of INSA, New Delhi in a  
meeting at Russian Academy of Sciences, Moscow.  
Preparatory to G-8 Summit in St. Petersburg,  
19 April 06 to 20 April 06

**Dr. S. Krishnan,**  
Thailand, SCOPUS Content Selection and Advisory  
Board Meeting, 27 Apr 06 to 28 Apr 06

**Mr. V.S. Chavan,**  
Denmark, CBIF Science Committee Meeting,  
13 Jul 06 to 14 Jul 06

**Mr. V.S. Chavan,**  
Philippines, OBIS, 20 May 06 to 27 May 06

**Dr. C.V. Ramana,**  
Canada, ICO and ICS-2006 Symposium,  
21 Jul 06 to 28 Jul 06

**Dr.S. Sivaram,**  
USA, to attend Board Meeting of Procter & Gamble,  
Cincinnati, USA and to develop collaborative R&D  
relationship as a part of Master Collaboration Agreement  
with CSIR, 27 Aug 06 to 30 Aug 06



**Pradeep Kumar,**  
Taiwan, Member of Indian Delegation,  
08 Jan 07 to 11 Jan 07

**Dr.S. Sivaram,**  
Hongkong, to act as a Member of the jury for the 2007  
DuPont Plunkett Awards, Asia Pacific, DuPont China  
Limited, Kowloon, 13 Feb 07 to 15 Feb 07

#### Training

**Mrs. U.D. Phalgune, Mr. V.T. Sathe,**  
**Mr. K.D. Deshpande and Mr. P.M. Suryavanshi,**  
Switzerland, Training Course on Advance NMR  
Methods, 11 Mar 07 to 19 Mar 07

#### Students' participation in conference/research projects

**Ms. Sophy Bhasi K.,**  
Canada, 7<sup>th</sup> DeMon Developer's Annual Workshop,  
Alberta, 21 Apr 06 to 25 Apr 06

**Ms. Sneha Kulkarni,**  
Singapore, International MEMS conference,  
09 May 06 to 12 May 06

**Mr. Diganta Sarma,**  
Japan, 7<sup>th</sup> Tetrahedron Symposium,  
25 May 06 to 26 May 06

**Mr. Ambarish Sanyal,**  
Japan, 3rd IUPAC International Symposium on Macro  
and Supra-molecular Architectures and Materials  
(MAM-06), 28 May 06 to 01 Jun 06

**Ms. Tanushree Bala,**  
Japan, 3rd IUPAC International Symposium on Macro  
and Supra-molecular Architectures and Materials  
(MAM-06), 28 May 06 to 01 Jun 06

**Mr. Vinod V.P.,**  
Japan, Young Scientist Program, 20<sup>th</sup> IUBMB  
International Conference of Biochemistry and  
Molecular Biology and 11<sup>th</sup> FAOBMB Congress,  
16 Jun 06 to 24 Jun 06

**Mr. Sarvesh Kumar Soni,**  
Turkey, 31st FEBS Congress on Molecules in Health  
Diseases, 24 Jun 06 to 29 Jun 06

**Mr. M. Sankar,**  
Germany, 1st International IUPAC Conference on  
Green Sustainable Chemistry,  
10 Sept 06 to 15 Sept 06

**Mr. K. Manoj,**  
Japan, Joint conference of Asian Crystallographic  
Association and Crystallographic Society of Japan,  
19 Nov 06 to 24 Nov 06

**Mr. Ankush Biradar,**  
Germany, to work at Leibniz-Institut fur Katalyse,  
Rostock, 1 Sep 06 to 15 Dec 06

**Mr. Santosh Chavan,**  
Germany, to work at Biological Control Laboratory,  
Darmstad, 1 Nov 06 to 15 Dec 06

**Mr. Raj Sankar C,**  
Singapore, to work at National University of Singapore,  
04 Dec 06 to 10 Jan 07

**Mr. Sagar Pandit,**  
Germany, to work at Max-Planck Institute,  
15 Aug 06 to 16 Jan 07

**Mr. A.S. Bairagi,**  
Germany, to work at Kiel University,  
01 Dec 06 to 24 Feb 07

**Ms. Aarti Shedge,**  
France, "Sandwich" thesis program at Universite Du  
Maine, 15 Sept 06 to 15 Mar 07

**Mr. Deepak Salunke,**  
France, "Sandwich" thesis program at Institut de  
Chimie et des Substances Naturelles, Center for  
National Scientific Research 91198 GIF ON YVETTE  
Cedex, 15 Sept 06 to 15 Mar 07

**Mr. S. Tamang,**  
UK, to work at University of Liverpool,  
23 Feb 06 to 23 Mar 07

**Mr. M. Shabab,**  
Germany, to work at Max-Planck Institute,  
12 Mar 07 to 11 Mar 08



#### LECTURES / SEMINARS DELIVERED BY VISITORS

Date	Topic	Speaker
1-5-2006	Environment Friendly Organic Synthesis Using Bismuth Compounds	<b>Prof. Ram S. Mohan,</b> Illinois Wesleyan University, Bloomington, Illinois., USA
2-5-2006	Controlling the structure of complex nanocrystals; from chemistry to magnetism	<b>Prof. Gil Markovich,</b> School of Chemistry, Tel Aviv University, Israel
11-5-2006	Cationic polymerization kinetics of styrene and ring-substituted styrene derivatives	<b>Dr. Priyadarsi De,</b> Department of Chemistry, University of Massachusetts, Lowell, USA
12-5-2006	Research Activity of Nano-ionic group in fuel cell materials center and Outline of Fuel Cell Project at NIMS	<b>Dr. T. Mori,</b> Group Leader, National Institute of Materials Science, Tsukuba, Japan
16-5-2006	Alternatives to Animals in Research	<b>Dr. Alok Dhawan,</b> Scientist, Industrial Toxicology Research Centre, Lucknow
17-5-2006	Potential Glycosidase Inhibitors, Amino Acids and Peptides : A brief Insight	<b>Dr. R. G. Bhat,</b> Simon Fraser University, Canada
24-5-2006	Diluted Magnetic Oxides and Multiferroic thin films	<b>Dr. Darshan Kundaliya,</b> University of Maryland, College Park, USA
29-5-2006	Organometallics, Asymmetric Catalysis, Total Synthesis, and Medicinal Chemistry: Never Ending Journey of a Chemist	<b>Dr. Sunil K. Mandal,</b> Senior Chemist, Acenta Discovery Inc., Tucson, Arizona, USA
31-5-2006	Breast Cancer--Causes, Risk factors, Symptoms, Prevention, Detection and Treatment	<b>Dr. CB Koppiker and Dr. Rama Sivaram,</b> Director Ruby Hall Cancer Center and Head, Jehangir, Dept of Oncology, Managing Trustee, Prashanti, Ruby Hall Cancer Center, Pune
28-6-2006	Greenchem Program- Environment friendly enzyme technologies	<b>Prof. Rajni Hatti-Kaul,</b> Department of Biotechnology, University of Lund, Sweden
3-7-2006	The three dimensional structure of proteins from leucine biosynthetic pathway of Mycobacterium tuberculosis	<b>Rajesh Kumar Singh,</b> Visiting Scientist, European Molecular Biology Laboratory, Hamburg, Germany
11-7-2006	New Trends in Pd Catalyzed Coupling	<b>Dr. Thomas J. Colacot,</b> Development Manager, Homogeneous Catalysis, Catalysis & Chiral Technologies, Johnson Matthey, New Jersey, USA.
3-8-2006	Influence of Kinetic and Spatial Segregation on Fate of Commensalistic Cultures	<b>Prof. Satish Parulekar,</b> Illinois Institute of Technology, USA
7-8-2006	Engineering Carbon Nanotube Structures	<b>Prof. P.M. Ajayan, Henry Burlage</b> Professor of Engg., Dept. Materials Science & Engg., Rensselaer Polytechnic Inst., Troy, USA
8-8-2006	Semi-fluorinated thiol monolayers on gold surface, Organic and Bio-organic monolayers on Single crystal Semiconductor surfaces and Nanocrystals	<b>Dr. Samson Patole,</b> Postdoctoral Research Fellow, University of St Andrews and University of Newcastle, UK
9-8-2006	Development of nanomaterials, surface engineering and their applications in biosciences	<b>Dr. Tapas Sen,</b> Department of Biosciences, University of Kent, Canterbury, UK



## ANNEXURES

11-8-2006	Application of thermal analysis for polymer reasearch	<b>Mr. Louis Waguespack</b> , Specialist in Thermal Analysis, TA Instruments, USA
14-8-2006	Nanostructured Materials: Emerging Technologies for Energy Storage Applications	<b>Prof. Prashant N. Kumta</b> , Department of Materials Science and Engineering, Biomedical Engineering, Carnegie Mellon University, Pittsburgh, USA
17-8-2006	Gold nanoparticles in cancer treatment : mechanistic and Preclinical studies	<b>Prof. Devbrata Mukhopadhy</b> a, Professor and Consultant, Mayo Cancer Research Center, Rochester USA
17-8-2006	Hydrogen Energy	<b>Prof. A. K. Shukla</b> , Director, CECRI, Karaikudi
25-8-2006	Towards SiC based Ceramic Microfluidics with Inorganic Polymers	Materials Lab., Fine Chemicals Eng. & Chemistry, Chungnam National University, Daejeon, Korea
1-9-2006	Health and Mental Fitness Through Self Observation	<b>Dr. Hamir Ganla</b> , Paediatrician, Pune
4-9-2006	Resonant tunnelling and fast switching in amorphous carbon quantum wells	<b>Dr. Somnath Bhattacharyya</b> , Post-doctoral Fellow, School of Electronics and Physical Sciences, University of Surrey, UK
7-9-2006	Microwave Assisted Organic Synthesis	<b>Dr. Alexander Stadler</b> , Application Specialist, Anton Paar, Graz, Austria
12-9-2006	Stock Investment Decisions and Risk Analysis	<b>Dr. Vasant Patwardhan</b> , Ex-Chairman Mahabank, Pune, India
31-10-2006	Self-Assembled Peptide Fibrils-based Nanocomposite: Using Peptides as both the Matrix and Reinforcement	<b>Rohan Hule</b> , University of Delaware, Newark, USA
6-11-2006	Hiyama Cross-Coupling Reactions using Tetraorganosilicon Reagents for Biaryl Synthesis; Efforts to find novel and useful reactions on Porphyrin Periphery	<b>Dr. Akhila K. Sahoo</b> , Kyoto University, Japan
8-11-2006	Natural product-like probes - Small molecule microchips: Emerging tools aimed at dissecting signaling networks using small molecules	<b>Prof. Prabhat Arya</b> , Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada
9-11-2006	Fuel Cells activities at Juelich	<b>Dr. Holger Janssen</b> , Scientist, FZJ, IWV-3, Juelich, Germany Research Centre
15-11-2006	Heterocalixarene based Synthetic Receptors	<b>Dr. Harjit Singh</b> , Professor Emeritus & INSA Sr. Scientist, Guru Nanak Dev University, Amritsar (10th Prof. Sukh Dev Endowment Lecture)
21-11-2006	The origins of specificity in polyketide synthase protein interactions	<b>Dr. Mukund Thattai</b> , Scientist, Biophysics and Bioinformatics Group, National Centre for Biological Sciences, Bangalore
22-11-2006	Engineered Nanoparticles: Scaled-Down Chemical Engineering	<b>Prof. Sheryl Ehrman</b> , University of Maryland, College Park, USA
22-11-2006	Nanoparticles to Bionanoparticles: From synthesis to Assembly to materials	<b>Dr. Antonios G. Kanaras</b> , Department of Chemistry, Liverpool University, UK
22-11-2006	Therapeutic Transport Devices: A Supramolecular Approaches	<b>Dr. Gareth W.V. Cave</b> , Senior Lecturer, Nottingham Trent University, UK



## ANNEXURES

24-11-2006	Coinage Metal Particles in Nanometer Length Scale	<b>Prof. Tarashankar Pal</b> , Indian Institute of Technology, Kharagpur
28-11-2006	New Materials	<b>Dr. Marc Drillon</b> , Director, Institute of Physics and Chemistry of Materials, University of Louis Pasteur, Strasbourg, France
29-11-2006	New Titanium Reagents for Applications in Organic Synthesis	<b>Prof. M. Periasamy</b> , Central University, Hyderabad
5-12-2006	Polypropylene	<b>Dr. Markus Gahleitner</b> , Scientist, Borealis, Linz, Austria
6-12-2006	Slow dynamics in liquids and critical arrest in gels	<b>Sujin Babu</b> , Polymers Colloids Interfaces UMR6120 CNRS, University du Maine, Le Mans, France
7-12-2006	Conversion of Cellulose to Sugar Alcohols over Supported Metal Catalysts	<b>Dr. Paresh L. Dhepe</b> , Research Associate, Catalysis Research Center, Hokkaido University, Sapporo, Japan
8-12-2006	Surface-grafted molecular and macromolecular gradients for studying adsorption of synthetic nanoparticles and biological species	<b>Dr. Rajendra R Bhat</b> , Scientist, BD Technologies, RTP, NC, USA
13-12-2006	Using transformed plants to study ecological interactions	<b>Dr. Ian Baldwin</b> , Director, MPI, Jena, Germany
14-12-2006	Microreactor Technology for Chemical Synthesis	<b>Dr. Thomas Schwalbe</b> , CEO and Founder, Micro-Reactor Systems Provider, Inc., Brookline, USA
14-12-2006	Organic Synthesis in Pheromone Science	<b>Professor Kenji Mori</b> , The University of Tokyo, Japan
26-12-2006	Advanced Applications of Catalysts for Future Energy Requirements	<b>Dr. Sreekumar Kurungot</b> , Scientist, Production Engineering Development Division, Toyota Motor Corporation, Toyota City, Aichi, Japan
27-12-2006	Modular Approaches to the Functional Dendrimers: Synthesis and Prospective	<b>Dr. Amaresh Mishra</b> , Scientist, University of Ulm, Germany
28-12-2006	Synthesis of CdS nanoparticle and its application in photogeneration of hydrogen	<b>Prof. R.P. Viswanath</b> , IIT-Madras, Chennai
4-1-2007	CFD simulation of droplet impact	<b>Dr. Vinayak Khatavkar</b> , Post-Doctoral Fellow, Technical University of Eindhoven, The Netherlands
4-1-2007	Structure Property Relationships in Rubber Modified Polymers: ABS and Blends Containing ABS	<b>Dr. Satish Gagar</b> , Research Scientist, GE Plastics, USA
5-1-2007	Synthesis and Characterization of Hydrophilic Polymer Brushes via Surface Initiated Aqueous RAFT Polymerization from Azo Initiator Incorporated Surface	<b>Dr. Krishnan Ranganathan</b> , Post-Doctoral Associate, The University of British Columbia, Vancouver, Canada
8-1-2007	Molecules that don't exist but should	<b>Prof. Rodney J. Bartlett</b> , Graduate Research Professor of Chemistry and Physics, Quantum Theory Project, Department of Chemistry, University of Florida, Gainesville, USA
18-1-2007	Towards a Molecular Level Understanding of Biomolecule-Mineral Interactions	<b>Dr. Siddharth Patwardhan</b> , Research Scientist, Nottingham Trent University, Nottingham, UK



23-1-2007	Seminar/Presentation on New Technologies in Microwave Digestion System	<b>Dr. Dieter Gutwerk</b> , Technical Manager, M/s Berghof Products GmbH, Germany
25-1-2007	Thermoplastic Elastomers for Consumer Applications	<b>Dr. Krishna Venkataswamy</b> , Director of Research and Development, GLS Corporation, McHenry, IL, USA
27-1-2007	Nanoscale Characterization of Catalytic Materials	<b>Prof. Douglas Buttrey</b> , Dept. of Chemical Engineering, University of Delaware, Newark, USA
13-2-2007	Peptide based delivery of nucleic acids for therapeutic applications	<b>Prof. B. Lebleu</b> , University of Montpellier II, France
14-2-2007	Unusual cation distribution and magnetic anisotropy in bulk and nano-spinel ferrites	<b>Prof. S.K. Date</b> , Department of Physics, University of Pune
23-2-2007	Phase transitions and elasticity in liquid crystals	<b>Prof. Sri Singh</b> , Department of Physics, Banaras Hindu University, Varanasi
26-2-2007	Structural insights into post-transcriptional regulation from the NMR structures of protein-RNA complexes	<b>Prof. Frederic Allain</b> , Institute for Molecular Biology and Biophysics, ETH, Zurich, Switzerland
27-2-2007	Neutralization kinetics of charged surface : A percolation of surface domains	<b>Dr. Manabendra Mukherjee</b> , Saha Inst of Nuclear Physics, Kolkata
27-2-2007	Organometallic Synthesis and Pharmacological Activity of Carbazoles	<b>Prof. Hans-Joachim Knäcker</b> , Department Chemie Technische Universität Dresden Bergstrasse, Germany
2-3-2007	Nano Architected Electrodes for Lithium-ion Battery Application	<b>Dr. Sagar Mitra</b> , Principal Electrochemist, Replisaurus Technologies AB, Isafjordsgatan, Kista, Sweden
6-3-2007	Life on the edge: surface science studies of reactions and islands at a Cu(110) surface	<b>Prof. Phil Davies</b> , Cardiff University, UK
21-3-2007	Synthesis of Allelopathic Natural Products: The Heliannuols	<b>Prof. R. V. Venkateswaran</b> , Department of Organic Chemistry, Indian Association for the Cultivation of Science, Kolkata
23-3-2007	AutoBrane- High Temperature Automotive Fuel Cell Membrane	<b>Dr. Arun K. Salunke</b> , Scientist, Laboratoire des Agrégats Moléculaires et Matériaux Inorganiques, Université Montpellier II Franc



## INVITED TALKS / LECTURES DELIVERED BY NCL SCIENTISTS

**Dr. Ahmad, Absar**

- Bioinspired nanomaterials synthesis and its application in drug delivery, National Seminar on Prospecting Fungal Diversity in Tropical India, Its Conservation and Applications in Biotechnology, Agharkar Research Institute, Pune, 28 April 2006
- Synthesis of inorganic nanoparticles using enzymes and proteins from microbes., National Workshop on Fungal Bioremediation, S.I.E.S College, Sion, Mumbai, 14 Oct. 2006
- Biological Synthesis of inorganic nanoparticles and their applications in hyperthermia and drug delivery, Workshop on Nanotechnology with ion beams and possible applications, Inter University Accelerator Centre (Nuclear Science Centre), New Delhi, 1 Nov. 2006

**Dr. Bhat, Suresh Kumar**

- Structure, Dynamics and Rheology of Soft Materials using Laser Light Scattering Techniques, National Laser Symposium 2006, Raja Ramanna Centre for Advanced Technology, Indore, 6 Dec. 2006

**Dr. Chavan, S. P.**

- A quest for a practical synthesis of commercially important molecules, National Seminar on Process chemistry in pharmaceutical industry, Saswad College for Pharmacy, Saswad (Pune), 20 Feb. 2007

**Dr. Gupta, Vidya**

- Proteinase inhibitor: A strategy to control *Helicoverpa armigera* in crop plants, International Symposium in Plant Cell: Structure Function Relationship, Washington State University, Pullman, USA. 8 June 2006.
- Efforts towards chickpea productivity improvement through biotic stress control, International workshop on Genomics enabled improvement in legumes at Asilomer Conference Centre, Pacific Grove, California, USA, 29 Aug. 2006
- Role of biotechnology in agriculture, National seminar on Innovations in agricultural education at

Agriculture College, Pune, 31 Dec. 2006.

- Recent applications of plant biotechnology, Symposium on Recent trends in life sciences, Modern College, Pune, 8 Jan. 2007.

**Dr. Kulkarni, B. D.**

- On sustainable development, Technology Day celebration, High Energy Materials Research Institute, Pune, 11 May 2006
- Emerging trends in environmental engineering, Environmental Day celebrations, Indian Institute of Petroleum, Dehradun, 5 June 2006
- Emerging Trends in Separation Sciences and Technology, Conference in separation sciences and technology, Bhabha Atomic Research Centre, Mumbai, 29 Sept. 2006

**Dr. Mohapatra, D. K.**

- Route selection and process development for a magnetic resonance imaging contrast agent, Invited Lecture, Indian Institute of Chemical Technology, Hyderabad, 2 Feb. 2007

**Dr. Poddar, Pankaj**

- Study of ferroelectric and ferromagnetic properties of nanoparticles, Indo-Israel Workshop From Molecules to Composites: Interdisciplinary approaches to Materials Research, JNCASR, Bangalore, 5 May 2006

**Dr. Pradeep Kumar**

- Enantioselective total synthesis of biologically active natural products, Invited talk during visit to the institute as visiting scientist, Institute of Molecular Pharmacology, Campus Berlin-Buch, 13125, Berlin, Germany, 14 Sept. 2006
- Enantioselective total synthesis of biologically active natural products, During visit to Berlin as visiting Scientist, Chemistry Department, Frei University, Berlin, Germany, 31 Oct. 2006 Frei University, Berlin, Germany, 31 Oct. 2006
- Synthesis and application of Yttria Zirconia based strong Lewis acid catalyst, During visit to Berlin as



- visiting Scientist, Chemistry Department, Humboldt University, Berlin, Germany, 31 Oct. 2006
- Carbohydrate-derived chiral building blocks: application to the synthesis of biologically useful compounds, Carbo XXI conference, Department of chemistry, Delhi University, Delhi, 29 Nov. 2006
- Enantioselective total synthesis of biologically active natural products, 1st India-Taiwan Conference on Frontiers of Organic Chemistry,, National Tsing Hua University, HFINGHU, Taiwan, 7 Jan. 2007
- Enantioselective total synthesis of biologically active natural products, 1st India- Taiwan conference on Frontiers of organic Chemistry, National Tsing Hua University, Hsinchu, Taiwan, Hsinchu, Taiwan, 9 Jan. 2007
- Total synthesis of compounds of pharmaceutical importance, Current trends in drug discovery research (CTDDR), Central Drug Research Institute, Lucknow, 17 Feb. 2007
- Enantioselective synthesis of compounds of pharmaceutical importance, CTDDR conference, Central Drug Research Institute, Lucknow, 19 Feb. 2007

**Dr. Prasad, B. L. V.**

- Nanomaterials: New Synthetic Methods, Nanotrends 2006: 4th MSTI Nanotechnology and Business Congress and Exhibition, MSTI, Berlin-potsdam, Germany, 10 May 2006

**Dr. Radhakrishnan, S.**

- Applications of Conducting Polymers for Piezo-sensors and Actuators, Work shop cum Symposium on Conducting Polymers, CECRI, Karaikudi, 30 June 2006

**Dr. Suresh, C. G.**

- The structural similarity, stability, substrate diversity and evolution of some NTN hydrolase enzymes, 75th Annual meeting of the Society of Biological Chemists, Jawaharlal Nehru University, New Delhi, 11 Dec. 2006

- Pharmaceutical Applications to Therapeutics The Evolution of an Enzyme, Bioinformatics center, Pune University, 12 Feb. 2007

**Dr. Sivaram, S.**

- Fuelling One Billion Plus: Energy Technologies And Sustainable Development, Meeting of the Russian Academy of Sciences, Russian Academy of Sciences, Moscow, Russia, 19 April 2006
- Leveraging Science and Technology for Promoting Competitiveness : The Indian Experience, Conference on S&T Towards the Future, Thailand Institute of Scientific and Technological Research, Bangkok, Thailand, 25 May 2006

**Dr. Vijaymohan, K.**

- Application of Hybrid Nanomaterials Electrochemical Energy Storage, Nano Trends 2006 : 4th MSTI Nanotechnology and Business Congress and Exhibition, MSTI, Berlin-Potsdam, Germany, 10 May 2006

**CONFERENCES / SEMINARS / WORKSHOPS ORGANISED**

- (30 May 2006): Bruker-AXS Single Crystal X-ray Diffractometer User's Workshop 2006
- (12 - 15 Dec. 2006): Workshop on "Proteomic insights into plant-insect interactions under the Max Planck Society-India partnership program
- (13 - 14 Dec. 2006): International conference on "Developing chemical processes for active pharmaceutical ingredients" organised by Scientific Update, UK
- (14 - 16 Dec. 2006): Workshop on "Sustainable plastics in India and Asian Countries"
- (15 - 17 Dec. 2006): Training workshop on "Combinatorial chemistry and technologies, molecular design and their applications to exploit biodiversity"
- (17 - 20 Dec. 2006): Macro-2006 - 9th National conference on "Polymers for advanced technologies"
- (14 - 17 Jan. 2007): 6th International Symposium on Catalysis in multiphase reactors (CAMURE-6) and 5th International Symposium on multifunctional reactors (ISMR-5)
- (22 - 24 Jan. 2007): International Conference on Chemoinformatics
- (5 - 8 Feb. 2007): 13th National Magnetic Resonance Society of India (NMRS) symposium
- (16 - 17 Feb. 2007): International Conference on "Biology of yeasts and filamentous fungi:
- (24 - 28 Feb. 2007): DST-JSPS Asia Academic Seminar on "Molecular and supramolecular materials with designed functions".





## AWARDS / RECOGNITIONS (2006-07)

• Vice president Indian Academy of Sciences	Dr S Sivaram
• J C Bose National Fellowship DST	Dr S Sivaram Dr K N Ganesh Dr Ganesh Pandey
• Dr Jagdish Shankar Memorial Lecture award by the Indian National Science Academy INSA	Dr Sourav Pal
• Fellow of Zoological Society Kolkata	Dr S N Mukherjee
• INSA Medal for Young Scientist in Chemical Sciences • CSIR Young Scientist Award in Chemical Sciences	Dr Srinivas Hotha
• Fellow Maharashtra Academy of Sciences	Dr. M. V. Badiger Dr. M. N. Deshmukh Dr. S. N. Mukherjee Dr. V. R. Pedireddi Dr. C. V. Rode Mr. V. S. Chavan
• Distinguished Alumni Award of IIT Madras	Dr Murali Sastry
• Manthan AIF Award	Mr V S Chavan
• Shanti Swarup Bhatnagar SSB prize in Engineering Sciences	Dr Ashish Lele
• Young Scientist Award of Catalysis Society of India	Dr P Manikandan
• Professor M Santappa Silver Jubilee Award in Polymer Science by the Society for Polymer Science	Dr P P Wadgaonkar
• Ramanna Fellowship by Department of Science and Technology (DST) New Delhi • FICCI Award in the category of Outstanding Contribution to Knowledge Based Industries • Vice President of the National Academy of Sciences India (Allahabad) • Chemito 2006 award	Dr Anil Kumar
• 20 <sup>th</sup> Khwarizmi International Award	Dr R P Singh
• CDRI Award for excellence in Drug Research • Young Associate Maharashtra Academy of Sciences	Dr D K Mohapatra



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**Dr. (Mrs.) R D Wakharkar**

- Bakul Finechem Research Centre, Mumbai



## EDITOR/EDITORIAL BOARD MEMBERS OF JOURNALS

**Dr. Anil Kumar**

- Indian Journal of Chemistry Section A, NISCAIR (CSIR), New Delhi
- Editor (Chemistry), Proceedings of The National Academy of Sciences (India), Allahabad

**Dr. V. R. Choudhary**

- Catalysis Communications, Elsevier, The Netherlands

**Dr. M.V. Deshpande**

- Indian Journal of Mycology and Plant Pathology, Indian Society of Mycology and Plant Pathology, Udaipur

**Dr. K.N. Ganesh**

- Chemistry An Asian Journal, Wiley-VCH
- Indian Journal of Chemistry Section B, NISCAIR (CSIR), New Delhi

**Dr. (Mrs) Vidya Gupta**

- BMC Plant Biology, BioMed Central
- Plant Cell Biotechnology & Molecular Biology, Society for Biology and Biotechnology, Salem

**Dr. M.K. Gurjar**

- Associate Editor, Synthetic Communications, Marcel Dekker, USA
- Carbohydrate Letters, Harwood Academic Publishers, Paris, France
- Organic Process Research & Development, American Chemical Society, USA

**Dr. B.D. Kulkarni**

- Chemical Engineering Science, Pergamon/Elsevier, UK
- Industrial and Engineering Chemical Research, American Chemical Society, USA

**Dr. Sourav Pal**

- Board of Advisors, Springboard, Inc. (Engineering education), USA
- International Journal of Molecular Sciences, MDP International, Switzerland
- International Journal of Applied Chemistry, Research India Publications, Delhi.
- Journal of Chemical Sciences, The Indian Academy of Sciences, Bangalore
- Proceedings of the Indian National Science Academy, New Delhi

**Dr. Rajiv Kumar**

- Applied Catalysis A: General, Elsevier, The Netherlands
- Bulletin of Catalysis Society of India, Chennai
- Advances in Nanoporous Materials, Elsevier Publishers, Amsterdam.

**Dr. V. V. Ranade**

- Associate Editor, Asia-pacific Journal of Chemical Engineering, Wiley InterScience

**Dr. Paul Ratnasamy**

- Applied Catalysis, Elsevier, The Netherlands
- Catalysis letters, Kluwer, USA
- Catalysis Surveys from Asia, Kluwer, USA
- CATTECH, Kluwer/ Plenum, USA
- Journal of Catalysis, Elsevier, The Netherlands
- Microporous and Mesoporous Materials, Elsevier, The Netherlands
- Topics in Catalysis, Kluwer, USA

**Dr. S. Sivaram**

- Bulletin of Materials Science, The Indian Academy of Sciences, Bangalore
- Designed Monomers and Polymers, VSP International Science Publishers, The Netherlands

- Indian Journal of Chemical Technology, NISCAIR (CSIR), New Delhi
- Journal of Scientific and Industrial Research, NISCAIR (CSIR), New Delhi
- International Journal of Polymeric Materials, Gordon and Breach Publishers, New York, USA
- Journal of Polymer Materials, Oxford and IBH Publishers, New Delhi
- Journal of Chemical Sciences, The Indian Academy of Sciences, Bangalore
- Regional Editor for India, Polymer International, Society of Chemical Industry, UK

**Dr S. Sivasanker**

- Catalysis Surveys from Asia, Kluwer, USA

**Dr. (Mrs) V.S. Tare**

- Journal of Environmental Biology, Triveni Publishers, Lucknow

**Dr. Anjani Varma**

- Carbohydrate Polymers, Elsevier, The Netherlands

**Dr. K. Vijayamohan**

- Bulletin of Materials Science, Indian Academy of Sciences, Bangalore





## NCL RESEARCH FOUNDATION

The National Chemical Laboratory Research Foundation (NCL RF), a not for profit organization, was established in 1991 with a mission to promote excellence in science and technology and create an environment in which creative and innovative endeavours in scientific, technical and R&D support areas are recognised and rewarded. It aims to bring creative research, novel technologies and organisational innovations into clear focus and encourages those core values which NCL considers important for the well being of the organisation.

## Board of Trustees :

Position	Present board	By virtue of
Chairman	Dr. S. Sivaram	Director, NCL
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## Awards and Lectures

NCL RF gives various awards on NCL Foundation Day and National Science Day. Besides organizing invited lectures on the occasion of NCL Foundation Day, National Science Day and National Technology Day, NCL RF organizes several special lectures in memory/ honour of former NCL Directors such as:

- Prof. B.D. Tilak Memorial Lecture
- Prof. J.W. McBain Memorial Lecture
- Prof. K. Venkataraman Memorial Lecture
- Dr. R.A. Mashelkar Endowment Lecture
- Dow Endowment Lecture in honour of Dr. Paul Ratnasamy

Award of merit based scholarships to the children of NCL employees: NCL RF awards merit based scholarships for the children, studying in IX to XII Standards, of NCL employees in group D (non-tech) and support staff in group I. The scholarship amount for the students who stood first is Rs.4000/- and for those who stood second is Rs.3500/- from each class. Sixteen meritorious children, including nine girls were awarded the scholarships to facilitate the students to defray the fees, including computer fee, science fee, etc.



## ANNUAL AWARDS - NCL FOUNDATION DAY : 2007

Name of Award	Award	Award winner	Awarded for
NCL RF Technology Award (Sponsored by ICICI Ltd.)	Rs.30,000/- +Citation	Dr. U. K. Kharul Dr. S. S. Kulkarni Mr. M. D. Jagtap Mr. A. S. Phadke	For development & successful transfer of technology of a unique ultrafiltration membrane suitable for excluding bacteria and viruses in water.
NCL RF-Cipla Hamied Award for the Best Process/ Product Development (sponsored by Cipla Ltd.)	Rs.20,000 +Citation	Dr. V. Premnath Dr. A. K. Lele & team	For development & successful transfer of technology for the manufacturing of porous polyethylene ocular implants.
Highest Industrial Earning Award	Rotating Shield & Trophy	Homogeneous Catalysis Division	Highest per capita (net) industrial earning during 2005-06.
Award for "New Initiative taken by the R&D Support System"	Rs.20,000/- + Certificate of Merit	Mrs. Neelima S. Iyer Mrs. Rupali Waichal Mr. B. K. Ghodke Mr. P. B. Kokney Mr. S. S. Yerande	For installation and commissioning of efficient and expeditious campus wide communication systems.
Director's Commendation Award	Rs. 5,000/- + Certificate of Commendation	Dr. G. J. Sanjayan Dr. P. R. Rajamohanar Mr. Rajesh Gonnade Mr. Amol Kendhale	For enhancing the prestige of NCL through a paper "Isotactic N-alkyl acrylamide oligomers assume self-assembled sheet structure: first unequivocal evidence from crystal structures" a cover page article in "Chemical Communications"
	Rs. 5,000/- + Certificate of Commendation	Dr. V. R. Pedireddi Mr. Sunil Varughese	For enhancing the prestige of NCL through a paper "A Competitive Molecular Recognition Study: Syntheses and Analysis of Supramolecular Assemblies of 3,5 Dihydroxybenzoic Acid and Its Bromo Derivative with Some N-Donor Compounds" a cover page article in "Chemistry A European Journal".
	Rs. 5,000/- + Certificate of Commendation	Dr. (Mrs.) Vidya Gupta Ms. Varsha Pardeshi	For enhancing the prestige of NCL through a paper "Mitochondrial Sequence Reveals High Levels of Gene Flow Between Breeds of Domestic Sheep from Asia and Europe" a cover page article in "Journal of Heredity".
	Rs. 2,000/- each + Certificate of Commendation	Mr. D. K. Gade Mr. M. B. Choudhari Mr. S. Tipugade	For exhibiting exemplary courage and high sense of duty in apprehending sandalwood thieves in the colony and, thereby, deterring future thefts.
	Rs. 5,000/- + Certificate of Commendation	Mrs. V. R. Khedekar	For efficient and conscientious service rendered towards management of performance appraisal record of staff and scientists of NCL.





Name of Award	Award	Award winner	Awarded for
	Rs. 2000/- each + Certificate of Commendation	<p>Administrative Services - Mr. M. S. Vidyathanan Mr. B. B. Kasture Mr. R. S. Malge Mrs. Balakrishnan Prema Mrs. Vishwambharan S. Mrs. A. A. Kulkarni Mrs. S. S. Deshpande Mr. N. H. Maidargi Mr. M. B. Vadnere</p> <p>Engineering Services - Mr. D. B. Pradhan Mr. R. P. Purandare Mr. A. V. Mahajan Mr. S. M. Mane Mr. Jaipal Singh Mr. S. R. Jogdand Mr. D. P. Jadhav Mr. A. S. Phadke</p> <p>Finance &amp; Accounts Services - Mr. S. Chandras Mrs. M. John Mr. U. A. Thakre Mrs. A. G. Badar Mr. Rao N. N. B. Mrs. S. A. Bhondve Mr. S. S. Khan Mr. S. B. Giri</p> <p>Stores &amp; Purchase Services - Mr. P. Chiranjeevi Mr. V. K. Zunjarrao Mr. S. P. Koli Mrs. M. M. Kenkre Mr. S. H. Jadhav Mrs. Nair Lalitha G. Mr. Sachin Gawali</p> <p>Web Designing &amp; Communication Services - Dr. P. K. Ingle Mr. Nikhilesh Yadav Mr. C. J. Jagtap Mr. K. D. Deshpande Mr. P. K. Mane Mr. Sanjay Patil</p>	For efficient and timely completion of all activities related to physical infrastructure leading to the commencement of programme at the Indian Institute of Science Education & Research, Pune in August 2006.



Name of Award	Award	Award winner	Awarded for
Individual Merit Award	Rs. 5,000/- Certificate of Merit	Mr. S. R. Narwade & (Homogeneous Catalysis Division)	For investing extra efforts in repairing a hydrogen gas under supercritical water conditions. Timely completion of this intricate job ensured successful completion of a high visibility research project in Mr. S. H. Durethe Homogeneous Catalysis Division.
	Rs. 5,000/- + Certificate of Merit	Mr. R. M. Murkute (Chemical Engineering and Process Development Division)	For excellence in designing and executing comprehensive plumbing and fitting jobs in the microreactor and Industrial Flow Modeling laboratory.
	Rs. 5,000/- + Certificate of Merit	Mr. L. Mayavan & Mr. S. S. Palande (Civil Engineering Section)	For exemplary efforts in maintaining water pipelines and thereby ensuring regular water supply to the laboratory and colony; and for putting together a network of pipelines to provide water supply to NCL Innovation Park.

## ANNUAL AWARDS - NATIONAL SCIENCE DAY : 2007

Name of Award	Award	Award winner	Awarded for
NCL RF Scientist of the Year Award (Sponsored by Maneckji & Shirinbai Neterwala Foundation)	Rs. 20,000/- + Citation	Dr. V. K. Jayaraman (Chemical Engineering & Process Development Division)	Outstanding contributions to the development of methodologies and design procedures like Ant colony optimization, taboo search, multicanonical jump walk annealing and other evolutionary algorithms leading to wide spectrum of applications in Process Engineering.
NCL RF Scientist of the Year Award (Sponsored by Dr. R. A. Mashelkar Endowment Fund)	Rs. 20,000/- + Citation	Dr. C. S. Gopinath (Catalysis Division)	Outstanding contributions to the studies in surface reaction kinetics, understanding the correlation of electronic structure and activity of catalysts through surface science studies and thereby providing a molecular level understanding of catalytic reactions and catalysts.
Keerti Sangoram Memorial Endowment Award for Research Students	Rs. 2,500/- + Certificate of Merit	Mr. Balachandra Kakade (Guide : Dr. K. Vijayamohan)	Physical / Material Sciences (shared)
		Mr. Akhilesh Tanwar (Guide : Dr. S. Pai)	
		Ms. Manasi Telang [Guide : Dr. (Mrs.) Vidya Gupta]	Biological Sciences (shared)
		Mr. Atul Bharde [Guide : Dr. (Mrs.) A. Prabhune]	



Name of Award	Award	Award winner	Awarded for
		Mr. N. S. Pujari (Guide : Dr. S. Ponarathnam)	Engineering Sciences
		Mr. Kapil Dev Arora (Guide : Dr. V. R. Pedireddi) Ms. Anupa R. Menjoge (Guide : Dr. M. G. Kulkarni)	Chemical Sciences (shared)
Dr. Rajappa Prize for the research paper in Organic	Rs. 1,000/- + Citation	Mr. Sudhir Kashyap, (Guide : Dr. Srinivas Hotha)	Propargyl glycosides as stable glyco syl donors : Anomeric activation and glycoside syntheses

**VENTURE CENTER**

The Venture Center is a technology business incubator specializing in technology enterprises offering products and services exploiting scientific expertise in the areas of materials, chemicals and biological sciences and engineering. The Venture Center is an independent not-for-profit company.

**Core purpose**

To nucleate and nurture technology and knowledge-based enterprises for India by leveraging the scientific and engineering competencies of the institutions in the region.

**Envisioned future**

To be the organisation that will be credited with creating, shaping and sustaining a "Pune cluster" of innovative technology businesses with a significant economic impact regionally, nationally and globally within the next twenty years.

**Focus areas**

Focus areas by know-how:

- Material science
- Chemical synthesis
- Biomedical sciences and technology
- Chemical and process engineering
- Research, technology and knowledge management

Focus areas by markets/ sectors served:

- Health care
- Specialty chemicals and nano-materials
- Energy and environment
- Specialty packaging
- Process design and simulation
- Research

**Core activities**

The core activities of the Venture Center shall be

- To nucleate new business by creating the environment and opportunities for know-how providers, entrepreneurs and financiers to meet each other and form business teams
- To nurture businesses through their start-up phase by creating and running an efficient business incubator offering not only space but

also access to technology support, business mentoring, networks, scientific and information resources, and a generally conducive and supportive environment.

- To promote and run an active program for identification, creation, acceleration and translation (into practice) of technology ideas suitable for new venture creation.
- To run an active program in building and sharing resources, networks, competencies and special expertise in select areas at the interfaces of technology and innovation, business and entrepreneurship, and government and policy.

**Company structure and major partners**

Venture Center (trademark) is registered as "Entrepreneurship Development Center" under the Companies Act, 1956 as a Section 25 (not for profit) company. The Venture Center is an initiative of the NCL under CSIR's scheme titled "Scheme for setting up incubation centers in CSIR laboratories". It was formally incorporated as a Section 25 (not-for-profit) company under the Companies Act, 1956 on 10 January 2007. NCL registered the company after securing necessary approvals from CSIR (3 August 2006) and assurance of funding support from DST-NSTEDB (19 Sep 2005).

A Board of Directors governs the company. The board currently consists of:

- Dr. S Sivaram, Chairman and Founding Director
- Dr. Premnath V, Secretary and Founding Director

Venture Center shall be building an Advisory Board while also expanding its Board of Directors during the course of 2007-2008.

The Venture Center is currently engaged in discussions with other potential partners. The National Science and Technology Entrepreneurship Development Board (NSTEDB) of the Department of Science and Technology (DST), Government of India is expected to begin funding support for the Venture Center in the near future.

**Inauguration of venture center**

The Venture Center was inaugurated by Prof. Sir Richard Friend (Cavendish Professor at the University of Cambridge, UK and Founder of Cambridge Display Technology Ltd and Plastic Logic Ltd.) on 18 December 2006 at NCL Innovation Park in the presence of Dr. R.A. Mashelkar, the then DG-CSIR, Dr. S. Sivaram, Director, NCL, Prof. Ashok Mishra, Director, Indian Institute of Technology, Mumbai and Prof. K.N. Ganesh, Director, Indian Institute of Science Education and Research, Pune. The Venture Center is the trademark of Entrepreneurship Development Center, a not-for-profit company located at 100, NCL Innovation Park. Dr R.A. Mashelkar, the then DG-CSIR, launched the website ([www.venturecenter.co.in](http://www.venturecenter.co.in)) of the Venture Center.


**राजभाषा का कार्यान्वयन**

राष्ट्रीय रासायनिक प्रयोगशाला रसायनविज्ञान एवं रासायनिक अभियांत्रिकी के अंतर्राष्ट्रीय शोध केन्द्र के रूप में विख्यात है। यह प्रयोगशाला अपने वैज्ञानिक कार्यकलापों के साथ-साथ राजभाषा कार्यान्वयन की दिशा में भी तत्पर है। अतः इस प्रयोगशाला में राजभाषा के कार्यान्वयन तथा उसके प्रगामी प्रयोग हेतु अनेक प्रकार से हर स्तर पर प्रयास किए जाते हैं। इस प्रयोगशाला के दैनिक कामकाज में वैज्ञानिक अनुसंधान कार्यों के अलावा अन्य क्षेत्रों में राजभाषा के प्रयोग को भी प्रोत्साहित किया जाता है। चूँकि यह एक अनुसंधान प्रयोगशाला है, अतः यहाँ 75 प्रतिशत कार्य वैज्ञानिक एवं तकनीकी स्वरूप का एवं शेष 25 प्रतिशत कार्य प्रशासनिक स्वरूप का होता है। प्रशासनिक स्वरूप के कार्य का अधिकांश भाग हिन्दी में संपादित किया जाता है। राजभाषा अधिनियम की धारा 3 (3) के अन्तर्गत जारी होने वाले सभी दस्तावेज अनिवार्य रूप से हिन्दी तथा अंग्रेजी दोनों में साथ-साथ जारी किए जाते हैं। हिन्दी में प्राप्त पत्रों के उत्तर हिन्दी में ही दिए जाते हैं। राजभाषा कार्यान्वयन समिति की बैठकें निदेशक की अध्यक्षता में प्रत्येक तिमाही में नियमित रूप से होती हैं, जिनमें हिन्दी के प्रगामी प्रयोग की समीक्षा की जाती है। सभी रबड़ की मोहरें, पत्र-शीर्ष, फॉर्म तथा मानक मसौदे द्विभाषी बना लिए गए हैं। सभी साइनबोर्ड एवं नामपट्ट द्विभाषी बने हुए हैं। प्रयोगशाला के मुख्य कम्प्यूटर सर्वर में द्विभाषी सॉफ्टवेयर "लीप ऑफिस-नेटवर्क वर्ज़न" स्थापित करके कम्प्यूटरों को द्विभाषी बना दिया गया है।



प्रयोगशाला के स्वागत कक्ष में ब्लैकबोर्ड पर प्रतिदिन एक सुविचार लिखा जाता है। इससे कर्मचारियों के हिन्दी के ज्ञान में वृद्धि होती है और वे अपना दैनिक सरकारी कामकाज हिन्दी में करने में अधिक रुचि लेते हैं। प्रयोगशाला के तीन अनुभाग अपना सारा सरकारी कार्य हिन्दी में ही करते हैं। राजभाषा विभाग के वार्षिक कार्यक्रम में दिए गए निर्देशानुसार प्रयोगशाला के पुस्तकालय हेतु खरीदी जाने वाली पुस्तकों के कुल मूल्य के 50 प्रतिशत राशि की हिन्दी पुस्तकें प्रतिवर्ष खरीदी जाती हैं। निदेशक महोदय का स्टाफ को सम्बोधित पत्र प्रत्येक तिमाही में अंग्रेजी के साथ-साथ हिन्दी तथा मराठी में भी जारी किया जाता है। प्रयोगशाला से जारी होने वाली सभी निविदा सूचनाएँ हिन्दी में भी प्रकाशित की जाती हैं।

प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानो एवं आयोजनों की रिपोर्ट "सीएसआईआर न्यूज" एवं "सीएसआईआर समाचार" में प्रकाशनार्थ हिन्दी और अंग्रेजी दोनों में राष्ट्रीय विज्ञान संचार एवं सूचना स्रोत संस्थान (निस्केयर), नई दिल्ली को नियमित रूप से भेजी जाती हैं। राष्ट्रीय रासायनिक प्रयोगशाला पुणे नगर राजभाषा कार्यान्वयन समिति के कार्यकलापों को भी गत 7 वर्षों से सम्पादित कर रही है। इसकी छमाही बैठकों का भी आयोजन नियमित रूप से किया जाता है तथा प्रयोगशाला के निदेशक इन बैठकों में उपाध्यक्ष के रूप में भाग लेते हैं। प्रयोगशाला में कर्मचारियों एवं अधिकारियों के लिए टिप्पण एवं आलेखन सम्बन्धी प्रोत्साहन योजना तथा अन्य प्रोत्साहन योजनाएँ भी लागू हैं। 'क' तथा 'ख' क्षेत्रों को जाने वाले अधिकांश पत्रों के लिफाफों पर पते हिन्दी में ही लिखे जाते हैं। हिन्दी का कार्यसाधक ज्ञान रखने वाले कर्मचारियों के लिए नियमानुसार हिन्दी कार्यशालाओं का आयोजन किया जाता है। 'एनसीएल आलोक' नामक वार्षिक राजभाषा पत्रिका का प्रकाशन नियमित रूप से किया जाता है। प्रयोगशाला की शीर्ष स्तर की प्रबन्ध परिषद की बैठकों में हिन्दी में भी चर्चा होती है। भारत सरकार के जैवप्रौद्योगिकी विभाग के सौजन्य से प्रयोगशाला ने हिन्दी में 'वसुन्धरा का हरित परिधान' नामक एक वृत्त चित्र (डॉकुमेंटरी फिल्म) का भी निर्माण किया है। प्रयोगशाला में प्रतिवर्ष हिन्दी सप्ताह का भव्य आयोजन किया जाता है। इस उपलक्ष्य में विभिन्न प्रतियोगिताएँ एवं सांस्कृतिक कार्यक्रम आयोजित किए जाते हैं। इसके अलावा सी.एस.आई.आर. मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिन्तन लेखमाला आदि योजनाओं में प्रयोगशाला के वैज्ञानिक एवं कर्मचारी भाग लेते हैं। इन योजनाओं में वैज्ञानिकों एवं कर्मचारियों को पुरस्कार भी प्राप्त हुए हैं। प्रयोगशाला के लगभग 90 प्रतिशत कर्मचारियों को हिन्दी का प्रशिक्षण दिया जा चुका है। शेष कर्मचारियों को भी प्रशिक्षित करने की प्रक्रिया जारी है। चूँकि प्रयोगशाला के 80 प्रतिशत कर्मचारियों को हिन्दी का कार्यसाधक ज्ञान प्राप्त है, अतः इसे राजभाषा नियम, 1976 के नियम 10 (4) के अधीन राजपत्र में अधिसूचित किया जा चुका है। प्रयोगशाला की वेबसाइट हिन्दी में भी तैयार की गई है।

यह प्रयोगशाला वैज्ञानिक अनुसंधान के क्षेत्र में राजभाषा के प्रगामी प्रयोग की दिशा में पूर्ण रूप से सजग है। यहाँ के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाले राष्ट्रीय विज्ञान सम्मेलनों/संगोष्ठियों में भाग लेकर हिन्दी में अपना शोधपत्र प्रस्तुत करते हैं। प्रयोगशाला में भी राजभाषा के प्रयोग को बढ़ावा देने के लिए समय-समय पर हिन्दी माध्यम से विज्ञान संगोष्ठियों एवं सम्मेलनों का आयोजन किया जाता है। वैज्ञानिक कार्यकलापों में हिन्दी का प्रयोग और अधिक करने के लिए यथासंभव प्रयास किए जा रहे हैं।



## हिन्दी सप्ताह समारोह का आयोजन

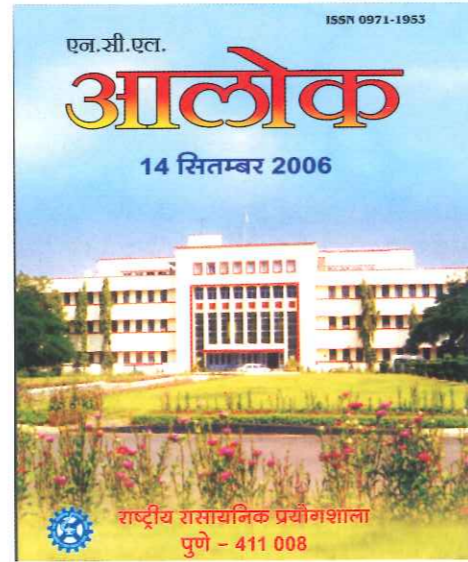
राष्ट्रीय रासायनिक प्रयोगशाला, पुणे तथा भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान, पुणे के संयुक्त तत्वावधान में दि. 14 सितम्बर से 21 सितम्बर, 2006 की अवधि में हिन्दी सप्ताह समारोह का आयोजन किया गया। इस अवधि में प्रयोगशाला के स्टाफ हेतु चार प्रतियोगिताएँ तथा भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान के छात्रों के लिए दो प्रतियोगिताएँ आयोजित की गईं। समारोह के प्रथम दिन 14 सितम्बर, 2006 को हिन्दी दिवस के अवसर पर प्रयोगशाला की वार्षिक राजभाषा पत्रिका 'एनसीएल आलोक' का लोकार्पण सम्पन्न हुआ। इस पत्रिका का विमोचन मुख्य अतिथि के रूप में उपस्थित पुणे विमानपत्तन प्राधिकरण के निदेशक कैप्टन दीपक शास्त्री एवं प्रयोगशाला के कार्यवाहक निदेशक डॉ. भास्कर कुलकर्णी के द्वारा संयुक्त रूप से सम्पन्न हुआ। इसी दिन भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान, पुणे के छात्रों के लिए हिन्दी शब्दज्ञान प्रतियोगिता आयोजित की गई जिसमें 33 छात्र/छात्राओं ने भाग लिया। दिनांक 15 सितम्बर, 2006 को प्रयोगशाला के स्टाफ के लिए हिन्दी निबन्ध प्रतियोगिता आयोजित की गई।



इस प्रतियोगिता में प्रयोगशाला के 12 स्टाफ सदस्यों ने भाग लिया। दिनांक 18 सितम्बर, 2006 को प्रयोगशाला के स्टाफ के लिए हिन्दी टिप्पण एवं प्रारूपण प्रतियोगिता आयोजित की गई जिसमें 12 स्टाफ सदस्यों ने भाग लिया। उसी दिन अपराह्न में प्रयोगशाला की राजभाषा कार्यान्वयन समिति की तिमाही बैठक भी अध्यक्ष महोदय की अध्यक्षता में आयोजित की गई। इसके बाद दिनांक 19 सितम्बर, 2006 को भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान के छात्रों के लिए हिन्दी निबन्ध प्रतियोगिता आयोजित की गई। इस प्रतियोगिता में भी 34 छात्र/छात्राओं ने भाग लिया दिनांक 20 सितम्बर, 2006 को प्रयोगशाला के चतुर्थ श्रेणी कर्मचारियों के लिए हिन्दी सुलेख एवं शुद्धलेखन प्रतियोगिता आयोजित की गई। विशेष रूप से चतुर्थ श्रेणी कर्मचारियों के लिए पहली बार आयोजित इस प्रतियोगिता में 22 कर्मचारियों ने भाग लिया।

हिन्दी सप्ताह समापन समारोह का आयोजन दिनांक 21 सितम्बर, 2006 को अपराह्न 3.00 बजे प्रयोगशाला के व्याख्यान-कक्ष में किया गया। समापन समारोह का प्रारम्भ दीप प्रज्वलन एवं

सरस्वती वन्दना से शुरू हुआ। इस अवसर पर हिन्दी विभाग, पुणे विश्वविद्यालय के प्रमुख प्रो. (डॉ.) तुकाराम पाटील मुख्य अतिथि के रूप में उपस्थित थे। भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान के निदेशक, डॉ. के.एन. गणेश भी विशेष अतिथि के रूप में इस समारोह में शामिल हुए। मुख्य अतिथि डॉ. तुकाराम पाटील, विशेष अतिथि डॉ. के.एन. गणेश एवं प्रयोगशाला के कार्यवाहक निदेशक डॉ. भास्कर कुलकर्णी ने संयुक्त रूप से सभी विजेता स्टाफ सदस्यों एवं छात्र-छात्राओं को नकद पुरस्कार एवं प्रमाण-पत्र प्रदान किए।



पुरस्कार वितरण के बाद मुख्य अतिथि के रूप में संबोधित करते हुए डॉ. पाटील ने राजभाषा और राष्ट्रभाषा हिन्दी की व्यापकता और उसके महत्त्व पर प्रकाश डाला। उन्होंने कहा कि आज हिन्दी केवल भारत में ही नहीं अपितु अंतर्राष्ट्रीय स्तर पर भी अपनी अपरिहार्यता का अहसास करा चुकी है। उन्होंने आगे कहा कि हिन्दी एक सशक्त और समृद्ध सम्पर्क भाषा के रूप में पूरे हिन्दुस्तान को एकता के सूत्र में बांधे हुए है। यही एक भाषा है जिससे सभी देशवासी परस्पर सम्पर्क कर सकते हैं। डॉ. तुकाराम पाटील ने कहा कि वर्तमान में 135 विदेशी विश्वविद्यालयों में हिन्दी के



अध्ययन-अध्यापन का कार्य चल रहा है इस प्रकार हिन्दी विदेशों में भारत की पहचान बना चुकी है और हिन्दी के माध्यम से ही विश्व के लोगों ने भारतीय संस्कृति, दर्शन और सभ्यता को जाना है। भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान के निदेशक, डॉ. के.एन. गणेश ने अपने सम्बोधन में कहा कि हमारे संस्थान के लिए यह एक अच्छा अवसर उपलब्ध हुआ है जब हमारे छात्रों को हिन्दी में अपनी प्रतिभा प्रदर्शित करने का अवसर मिला। हम चाहते हैं कि इस देश में विज्ञान और हिन्दी साथ-साथ चले और हमें आशा है कि हमारा यह संस्थान इस दिशा में अग्रणी रहेगा। समापन समारोह के अन्त में कार्यवाहक निदेशक, डॉ. भास्कर कुलकर्णी ने अपने अध्यक्षीय भाषण में हिन्दी सहित सभी भारतीय भाषाओं के प्रति अपना गहन समर्पण भाव प्रदर्शित करते हुए कहा

कि हमें आज इस अवसर पर हिन्दी को अधिक से अधिक अपने प्रयोग में लाने के लिए एक कार्य योजना बनानी चाहिए। उन्होंने कहा कि हिन्दी एक विशिष्ट वैज्ञानिक भाषा है। इसका व्याकरण और इसके शब्दों की व्युत्पत्ति तथा अर्थ में एक सुन्दर व्यवस्था झलकती है। उनका विचार था कि हमें हिन्दी के विकास के लिए हरसंभव प्रयत्न करना चाहिए। समारोह के अंत में हिन्दी अधिकारी, श्री उमेश गुप्ता ने धन्यवाद ज्ञापन किया। हिन्दी सप्ताह समापन समारोह के प्रारंभ में डॉ. रमाशंकर व्यास, वरिष्ठ हिन्दी अधिकारी ने सभी का स्वागत किया और हिन्दी सप्ताह समापन समारोह की प्रासंगिकता को रेखांकित करते हुए हिन्दी तथा अन्य सभी भारतीय भाषाओं के महत्त्व और उनकी उपयोगिता पर प्रकाश डाला। इस समारोह में पुणे शहर के हिन्दी के कुछ विद्वान भी अतिथि के रूप में सम्मिलित हुए।





## DATELINE NCL

**(8 May 2006)** : Orientation Programme for newly joined staff members and research fellows

**(11 May 2006)** : 4th Prof. B. D. Tilak Memorial Lecture on "Biomass based fuels and improved cookstoves" by Dr. A.D. Karve, Founder President, Appropriate Rural Technology Institute (ARTI), Phaltan (Maharashtra)

**(30 May 2006)** : Bruker-AXS Single Crystal X-ray Diffractometer User's Workshop 2006

**(7 June 2006)** : 5th Prof. K. Venkataraman Memorial Lecture on "Total synthesis of natural products using cyclohexadienes" by Prof. G S R Subba Rao, Indian Institute of Science, Bangalore

**(30 June 2006)** : Awareness programme on "Chemical weapons convention"

**(17 Aug. 2006)** : 6th Prof. J.W. McBain Memorial Lecture on "Arresting change and decay by continuous observation: The quantum zeno effect" by Prof. Narendra Kumar, Homi Bhabha Distinguished Professor (DAE Chair), Raman Research Institute, Bangalore

**(30 Aug. 2006)** : Fire safety: demonstration and training

**(5 Sept. 2006)** : Sterling Group 2006 lecture on "Tangling with long molecules" by Prof. Julia S. Higgins, Faculty of Engineering, Department of Chemical Engineering, Imperial College, London

**(9 Sept. 2006)** : A conference on "Horizons of Science Research" by Sakal group of publications

**(13 Sept. 2006)** : Users training workshop-CSIR e-journals consortium

**(14 Sept. 2006)** : Hindi week celebration and NCL Alok, an annual Hindi Magazine of NCL was released by the chief guest Capt. Deepak Shastri, Airport Director, Pune Airport

**(26 Sept. 2006)** : CSIR Foundation Day Function and Lecture on "A boom in aeronautics must match the boom in aviation" by Professor R. Narasimha, Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore

**(6 - 10 Nov. 2006)** : Observance of "Vigilance awareness week"

**(15 Nov. 2006)** : 10th Prof Sukh Dev Endowment Lecture Heterocalixarene based synthetic receptors by Prof. Harjit Singh, Prof Emeritus and INSA senior scientist, Department of Chemistry, Guru Nanak Dev University, Amritsar

**(12 - 15 Dec. 2006)** : Workshop on "Proteomic insights into plant-insect interactions under the Max Planck Society-India partnership program"

**(13 - 14 Dec. 2006)** : International conference on "Developing chemical processes for active pharmaceutical ingredients" organised by Scientific Update, UK

**(14 - 16 Dec. 2006)** : Workshop on "Sustainable plastics in India and Asian Countries"

**(15 - 17 Dec. 2006)** : Training workshop on "Combinatorial chemistry and technologies, molecular design and their applications to exploit biodiversity"

**(17 Dec. 2006)** : Third Dr. R.A. Mashelkar Endowment Lecture (Sponsored by Dorabji Tata Trust) on "Organic electronics: interfaces, heterojunctions and semiconductor device engineering": by Professor Richard Friend, FRS, FREng, Cavendish Professor, University of Cambridge, UK

**(17 - 20 Dec. 2006)** : Macro-2006 - 9th National conference on "Polymers for advanced technologies"

**(18 Dec. 2006)** : Inaugural lecture of the innovation and technology enterprise lecture series on "Company start-up in Cambridge: From science to technology to products" by Prof Sir Richard Friend, FRS, FREng Cavendish Professor, University of Cambridge, UK

**(27 - 28 Dec. 2006)** : CSIR programme on "Youth for leadership in science" (CPYLS), and two-day counseling session for Std X meritorious students

**(29 Dec. 2006)** : NCL Foundation Day lecture on "Reinventing Chemistry" by Prof. George M. Whitesides, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, USA

**(29 Dec. 2006)** : Public Lecture on "The future of science and technology: Assumptions" by Prof. George M. Whitesides Department of Chemistry and Chemical Biology, Harvard University, Cambridge

**(14 - 17 Jan. 2007)**: 6th International Symposium on Catalysis in multiphase reactors (CAMURE-6) and 5th International Symposium on multifunctional reactors (ISMR-5)

**(22 - 24 Jan. 2007)** : International Conference on Chemoinformatics



**(5 - 8 Feb. 2007)** : 13th National Magnetic Resonance Society of India (NMRS) symposium

**(8 - 9 Feb. 2007)** : Orientation course for newly joined staff members and Ph. D. students

**(16 - 17 Feb. 2007)** : International Conference on "Biology of yeasts and filamentous fungi:"

**(24 - 28 Feb. 2007)** : DST-JSPS Asia Academic Seminar on "Molecular and supramolecular materials with designed functions"

**(27 - 28 Feb. 2007)** : National Science day



## COMMITTEES

Scientists, in addition to their research and development functions, also give their valuable time for effectively managing various activities in the laboratory. The committees are charged with the responsibility of effective utilization and management of available resources and to ensure wider participation of scientists and staff in decision making in the laboratory.

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Committee to safeguard the welfare of Women Employees	Dr. (Mrs.) Vidya Gupta
Canteen Management Committee	Dr. C.R. Rajan
Official Language Implementation Committee	Dr. S. Sivaram
Investigation team for write-off	Dr. R.A. Joshi
Standing Committee for recommending distribution of income from intellectual property, fee for contract R&D & S&T	Dr. B.D. Kulkarni
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Coordinating Committee for Central NMR facility	Dr. M.K. Gurjar
Human resource development and management committee	Dr. S. Sivaram
Monitoring Committee on Stores Management	Dr. M.G. Kulkarni
Students Academic Committee	Dr. Sourav Pal
Financial assistance to students to participate in International Conferences	Dr. Sourav Pal



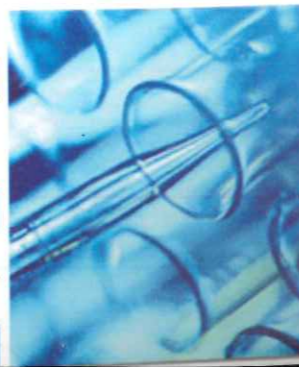
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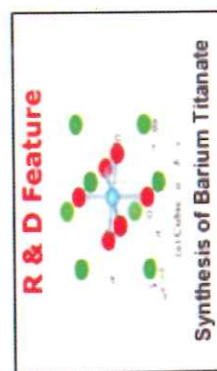
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