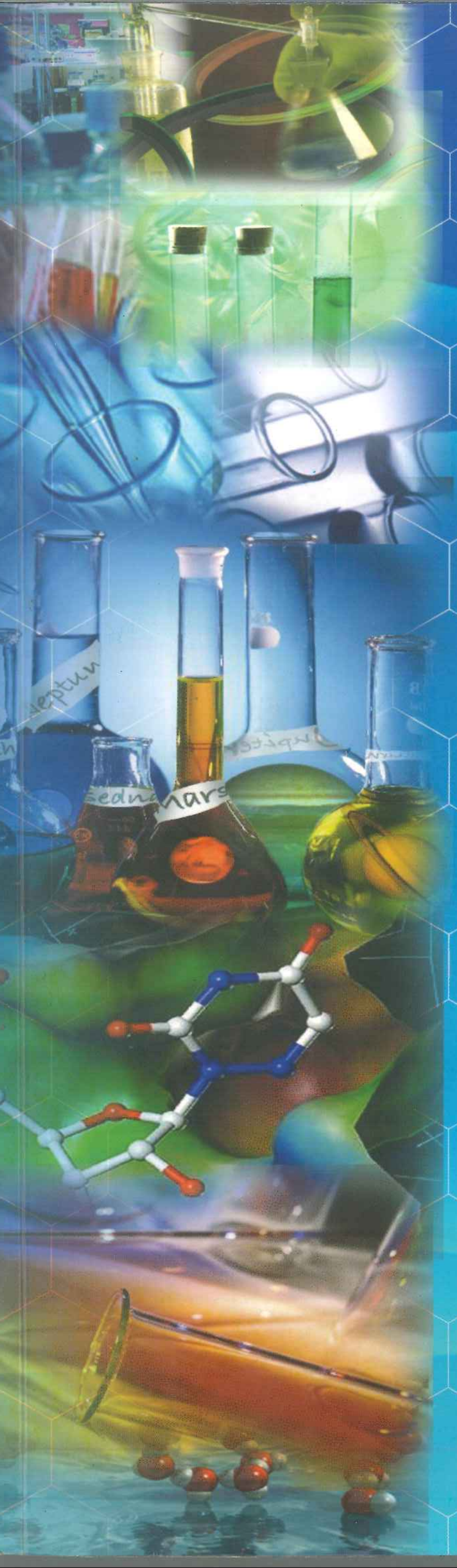

Annual Report
2005-2006

राष्ट्रीय रासायनिक प्रयोगशाला

वार्षिक प्रतिवेदन
२००५-२००६

NATIONAL CHEMICAL LABORATORY

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रासायनिक
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NATIONAL
CHEMICAL
LABORATORY

(Council of Scientific and Industrial Research, New Delhi)

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CONTENTS

PERFORMANCE INDICATORS

RESEARCH & DEVELOPMENT REPORTS

RESOURCE CENTERS

S&T SUPPORT SERVICES

ANNEXURES

निदेशक की कलम से

मुझे राष्ट्रीय रासायनिक प्रयोगशाला, पुणे की वर्ष 2005-06 की वार्षिक रिपोर्ट प्रस्तुत करते हुए प्रसन्नता हो रही है।

राष्ट्रीय रासायनिक प्रयोगशाला ने पिछले एक वर्ष के दौरान वैज्ञानिक अनुसंधान एवं विकास के सभी क्षेत्रों में महत्त्वपूर्ण प्रगति की है । इस अवधि में प्रयोगशाला को प्राप्त अनेक उपलब्धियों से रसायन विज्ञान एवं सम्बन्धित विज्ञान के प्रगत अनुसंधान केन्द्र के रूप में एनसीएल की प्रतिष्ठा सुदृढ़ हुई है।

एनसीएल विज्ञान में अनुसंधान के क्षेत्र में अग्रणी बनी हुई है । वर्ष 2005 के दौरान एनसीएल ने विश्व की प्रमुख पत्र-पत्रिकाओं में वैज्ञानिक लगभग 450 शोधपत्र प्रकाशित किए जिनका प्रति शोधपत्र औसत इम्पैक्ट फैक्टर 2.067 था। गत तीन वर्षों में एनसीएल के शोधपत्रों के इम्पैक्ट फैक्टर में लगातार वृद्धि हुई है । इम्पैक्ट फैक्टर प्रकाशनों की गुणवत्ता को परखने की विश्वस्तर पर मान्यताप्राप्त पद्धति है । एनसीएल में चार सौ बीस से अधिक शोधछात्र एवं डॉक्टरोत्तर शोध सहयोगी मौलिक अनुसंधान कार्यो में सहायता करते हैं ।

समीक्षाधीन अवधि में एनसीएल को 31 भारतीय पेटेण्ट और 30 अमरीकी पेटेण्ट स्वीकृत किए गए । इसी अवधि के दौरान एनसीएल ने भारत में 46 पेटेण्ट और विदेश में 28 पेटेण्ट फाइल किए । हमारे दो अमरीकी पेटेण्टों - पहला, प्रक्रिया संरक्षा नियंत्रण के क्षेत्र में (अमरीकी पेटेण्ट 6,826,513) और दूसरा, सम्मिश्र संकेतों के अवयवों में पृथक्करण के क्षेत्र में (अमरीकी पेटेण्ट 6,208,951) - का लाइसेंस एक अमरीकी कम्पनी को दिया गया है ।

प्रौद्योगिकी के मामले में भी एनसीएल ने अच्छी प्रगति की है । हमने छिद्रिल पॉली एथिलीन नामक एक नए उत्पाद का निर्माण किया है जिसका उपयोग चोटिल आँख के पुनर्निर्माण में होता है । इस नए उत्पाद को बाजार में व्यावसायिक रूप से लाने के लिए बायोपोर नामक एक नई कम्पनी स्थापित की गई है । इस कम्पनी की वेबसाइट है- www.bipore.in । एनसीएल ने एपीक्लोरोहाइड्रिन के उत्पादन हेतु आदित्य बिरला ग्रूप को एक उत्प्रेरकीय प्रक्रिया का लाइसेंस दिया है। हमने इस चुनौतीपूर्ण कार्य को स्वीकार करते हुए व्यावसायिक रूप से व्यवहार्य प्रक्रिया (अभिक्रिया एवं पृथक्करण) को विकसित करके उसे आदित्य बिरला ग्रूप को प्रदर्शित किया । यह उल्लेखनीय है कि आदित्य बिरला ग्रूप के साथ सम्पन्न हुई यह संविदा एनसीएल के प्रक्रिया लाइसेंस प्रदान करने के इतिहास में सबसे बड़ी है । यदि सब कुछ ठीक चलता रहा तो वर्ष 2007 के उत्तरार्ध में थाईलैण्ड में एपीक्लोरोहाइड्रिन के उत्पादन हेतु संयंत्र स्थापित हो जाएगा । हमने एक अभिनव रिएक्टर डिज़ायन और संचालन-प्रणाली का प्रयोग करते हुए सिलिकन टेट्रा क्लोराइड के उत्पादन हेतु एक समुन्नत प्रक्रिया विकसित की है । सतत तरल बेड रिएक्टर का प्रयोग करते हुए यह प्रक्रिया एक किलोग्राम प्रति घण्टा के मान पर ग्राहक को एक बार फिर से प्रदर्शित की गई है । ऐल्कीलफॉस्फीन ऑक्साइड समूह के उत्पादन हेतु प्रायोगिक संयंत्र स्तर पर एक प्रक्रिया विकसित करके उसे ग्राहक को प्रदर्शित किया गया है । यह पदार्थ देश के लिए अत्यन्त सामरिक महत्व का है । इस प्रक्रिया को उत्पादन हेतु विकसित करने के दौरान बड़े स्तर पर ग्रिगनार्ड अभिक्रियाएँ सम्पादित करते समय कुछ नए तथ्यों/कार्यविधियों का पता लगा । पेप्टिक व्रण के उपचार में प्रयोग में लायी जाने वाली किराल औषधि, एस (-) पैन्टोप्राज़ोल जो एक प्रोटॉन पम्प रोधक है, को व्यावसायिक रूप से बाजार में लाया गया ।

प्रयोगशाला ने कुल 110 ग्राहकों को ज्ञानाधारित सेवाएँ प्रदान कीं । इनमें से 18 ग्राहक भारत से बाहर अर्थात् विदेशों के थे ।

वित्त वर्ष की समाप्ति पर एनसीएल की बाहरी आय रु. 21.5 करोड़ रही जो वर्ष 2004-05 की रु.14.8 करोड़ की आय से अधिक है । महत्वपूर्ण बात यह है कि इस बाहरी आय में उद्योग जगत का योगदान रु. 11 करोड़ (51 प्रतिशत) है जो वर्ष 2004-05 के रु. 9.0 करोड़ से अधिक है । उद्योग जगत से प्राप्त आय के मामले में सी.एस.आई.आर. की प्रयोगशालाओं में हमारा प्रथम स्थान रहा है ।

रु. 21.5 करोड़ की बाहरी आय के अलावा एनसीएल को विभिन्न नेटवर्क और नई सहस्राब्दि भारतीय प्रौद्योगिकी एवं नेतृत्व पहल कार्यक्रमों के अन्तर्गत रु. 8.72 करोड़ की अतिरिक्त राशि प्राप्त हुई । हमने वर्ष 2005-06 के बजट के रूप में सीएसआईआर से भी रु. 45.1 करोड़ प्राप्त किए । इसे मिला कर हमारी कुल परिचालन आय रु. 75 करोड़ की हो गई । एनसीएल ने वर्ष 2005-06 में रु. 100 करोड़ का लेनदेन किया जो कि गत वर्ष से काफी अधिक है । लेनदेन में यह वृद्धि प्रति कर्मचारी उत्पादकता में हुई वृद्धि के कारण है न कि इन विभागों के कर्मचारियों की संख्या के कारण ।

एनसीएल ने वर्ष 2005-06 में रु. 11.5 करोड़ का पूंजीगत व्यय किया। इस व्यय से अनेक प्रमुख सुविधाएँ उपलब्ध कराई गईं । इन सुविधाओं में माल्डी टॉफ, एएफएम, 400 मेगाहर्ट्ज एनएमआर स्पेक्ट्रोमीटर, प्रोटीन शुद्धीकरण पद्धति, माइक्रो ऐरे स्पॉटर एवं स्कैनर, स्कैनिंग इलेक्ट्रोरसायन सूक्ष्मदर्शी, ईंधन सेल परीक्षण पद्धति, कार्बन नैनोट्यूबों हेतु सीवीडी यूनिट, स्मॉल ऐंगल एक्स-रे डिफ्रैक्टोमीटर, उच्च विभेदन संचारण इलेक्ट्रॉन सूक्ष्मदर्शी (एच.आर.टी.ई.एम.) तथा ड्यूएल बीम एन्वायरोन्मेण्टल एसईएम का समावेश है। हम भावी क्षमता के रूप में माइक्रो रिएक्शन इंजीनियरिंग हेतु सुविधाओं

का निर्माण कर रहे हैं । हमने अपनी अनुसंधान क्षमताओं को बढ़ाने के लिए अन्य अनेक निवेश किए हैं ।

सूचना एवं संचार प्रौद्योगिकी के क्षेत्र में हमारी क्षमताओं को बढ़ाने के लिए किए गए हमारे निवेश सही दिशा में चल रहे हैं । एनसीएल ने रु. 70 लाख की लागत से एक नई संचार प्रणाली स्थापित की है । हमने पिछले छह महीनों में एनसीएल के अन्दर टेलीफोन कनेक्शनों की संख्या दोगुनी कर दी है । हम अपने आन्तरिक प्रबन्धन के लिए जितना अधिक वेब आधारित प्रणालियों को अपनाते जाएँगे, सूचना की सुरक्षा का मुद्दा उतना ही महत्त्वपूर्ण होता जाएगा। सुरक्षा, नेटवर्क में प्रवेश का अधिकार, आपदा समुत्थान प्रबन्धन तथा अतिरेकता जैसे कुछ मुद्दे हैं जिन पर ध्यान दिया जा रहा है ।

हमने अपनी प्रयोगशालाओं तथा अन्य सम्बद्ध अवसंरचना को आधुनिक बनाने के लिए अनेक कदम उठाए हैं। पिछले वर्ष हमने इन कार्यों पर कुल रु. 3 करोड़ खर्च किए जिनमें से लगभग पचास प्रतिशत की राशि प्रयोगशाला की आन्तरिक आरक्षित निधि से खर्च की गई । रु. 1 करोड़ की अनुमानित लागत से 1000 किलो वोल्ट एम्पीयर की क्षमता का एक नया विद्युत उपकेन्द्र स्थापित किया गया है ।

सीएसआईआर का भूतपूर्व मेराडो परिसर अब एनसीएल प्रवर्तन पार्क के रूप में बदल दिया गया है । इसकी वेब साइट है (www.innovationpark.org)। यह प्रवर्तन पार्क एनसीएल के नए संसाधन केन्द्र के रूप में उभर रहा है । इस पार्क में वेंचर सेण्टर (www.venturecenter.co.in) नामक एक नई सेक्शन 25 कम्पनी एनसीएल द्वारा आगामी कुछ महीनों में स्थापित की जाएगी। यह कम्पनी दस हजार वर्ग फीट के स्थान में प्रारंभिक चरण के अन्वेषणों हेतु इन्क्यूबेटर के रूप में प्रयोगशाला का निर्माण करेगी जिसमें इन अन्वेषणों को व्यावसायिक उत्पादों या प्रक्रियाओं में रूपान्तरित करने की दिशा में कार्य किया जाएगा । इसके अलावा एनसीएल प्रवर्तन पार्क में अनेक व्यावसायिक कार्यकलापों के साथ-साथ उद्योग घरानों के स्वतंत्र अनुसंधान एवं विकास केन्द्र एकल रूप से अथवा एनसीएल के साथ संयुक्त उपक्रम के रूप में कार्यरत होंगे ।

दीपक रिसर्च एण्ड डेवलपमेण्ट फाउण्डेशन (डीआरडीएफ) ने प्रवर्तन पार्क में पहले से ही 7500 वर्ग फीट स्थान में अपने कार्यकलाप शुरू कर दिए हैं। एनसीएल परिसर में यह पहला उद्योग घराना है जो अनुसंधान एवं विकास कार्यों में संलग्न है । एनसीएल तथा डीआरडीएफ ने एक समझौता-ज्ञापन पर हस्ताक्षर किए हैं जिसके अन्तर्गत दोनों एक दूसरे की गतिविधियों में सहयोगी बनकर परस्पर धनार्जन करेंगे ।

इस प्रकार एनसीएल प्रवर्तन पार्क एनसीएल के एक प्रमुख संसाधन केन्द्र के रूप में उभरेगा जो एनसीएल के सामर्थ्य की अभिवृद्धि करेगा और सार्वजनिक-निजी भागीदारी तथा उद्योग जगत के साथ मिलकर धनार्जन के नए प्रतिमानों की तलाश करेगा ।

किसी भी संगठन में युवा प्रतिभा एवं नए कौशल के बिना विज्ञान एवं प्रौद्योगिकी का विकास नहीं हो सकता । एनसीएल में अपनी रुचि के क्षेत्रों में अनुसंधान करने हेतु युवा वैज्ञानिकों को आमंत्रित करने का क्रम जारी है । एनसीएल में असाधारण शैक्षणिक योग्यता एवं विश्व की उत्कृष्ट शैक्षणिक प्रयोगशालाओं में उच्च प्रशिक्षण प्राप्त कई वैज्ञानिकों ने कार्यभार सम्हाला है ।

हमारे अनेक सहयोगियों ने अपने उत्कृष्ट कार्यों से हमें गौरवान्वित करने का क्रम जारी रखा है । डॉ. के.एन. गणेश को रसायनविज्ञान में प्रतिष्ठित थर्ड वर्ल्ड ऐकेडमी ऑफ साइंसेज पुरस्कार से सम्मानित किया गया है । श्री पी.पी. बर्वे के नेतृत्व वाले हमारे दल को एक्रीलामीडो टरसरी ब्यूटाइल सल्फोनिक अम्ल (एटीबीएस) की उत्पादन प्रक्रिया के विकास हेतु वर्ष 2005 का सीएसआईआर प्रौद्योगिकी पुरस्कार प्राप्त हुआ है । मेसर्स विनती ऑर्गैनिक्स लिमिटेड एटीबीएस का व्यावसायिक स्तर पर उत्पादन कर रहा है । डॉ. उपेन्द्र नटराजन को वर्ष 2006 का मैटेरियल रिसर्च सोसायटी ऑफ इण्डिया (एमआरएसआई) पुरस्कार दिया गया है तथा डॉ. गुरुस्वामी को अभियांत्रिकी विज्ञान में सीएसआईआर युवा वैज्ञानिक पुरस्कार से सम्मानित किया गया है । भारत के राष्ट्रपति ने दि.29 मार्च, 2006 को एनसीएल के निदेशक डॉ. एस.शिवराम को पद्मश्री अलंकरण से सम्मानित किया।

एस. शिवराम

(एस. शिवराम)

FROM THE DIRECTOR'S DESK

It is my great pleasure to present the Annual Report of National Chemical Laboratory, Pune for the period 2005-06.

NCL has made significant progress on all fronts during the past one year. NCL's reputation as a centre for advanced research in chemical and related sciences, pursuing knowledge based innovation, was reinforced by several accomplishments during this period.

NCL continues to maintain its lead in research in cutting edge science. During the year 2005 NCL published ~ 450 scientific papers in leading journals of the world. The average Impact Factor (IF) per paper from NCL was 2.067, which has been steadily increasing over the past three years. IF is a universally recognized metric for judging the quality of publications. NCL's basic research effort is supported by over four hundred and twenty research fellows and post doctoral research associates.

During the period 2005-06 NCL was granted thirty-one Indian patents and thirty US patents. NCL filed forty-six patents in India and twenty-eight patents abroad during 2005-06. Two of our US patents, one in the area of process safety control (U.S. Pat. 6,826,513) and the other in the area of separation of complex signals into components (U.S. Pat. 6,208,951) were licensed to a US company.

On the technology front, NCL made good strides. We introduced a new product, a porous PE for ocular reconstruction after trauma causing injuries. A new company, named Biopore (www.biopore.in) has been incorporated to introduce the product commercially. NCL licensed a catalytic process to produce epichlorohydrin to Aditya Birla Group (ABG). We met the challenge of developing as well as demonstrating a commercially viable process (reaction and separation) to ABG. It is worth stating that this contract with ABG is one of the largest in the history of process licensing at NCL. If all goes well, the plant for the production of epichlorohydrin will come up in Thailand in late 2007. We developed an improved process for the manufacture of silicon tetrachloride using an innovative reactor design and operations. Once again the process was demonstrated to the customer on a 1 kg/h scale using a continuous fluid bed reactor. A pilot plant process for the production of a family of alkylphosphine oxide was set up and the process demonstrated to the customer. This is a material of strategic relevance to the country. Innovations in performing Grignard reactions on a large scale were addressed in the course of developing this process. A chiral drug, S(-)-pantoprazole which is a proton pump inhibitor used in the treatment of peptic ulcer was commercially introduced in the market.

The laboratory rendered knowledge-base services to a total of one hundred and ten customers including eighteen from outside India.

NCL closed the financial year with an external cash flow (ECF) of Rs 21.5 crore, an increase from Rs 14.8 crore in 2004-05. More importantly, the contribution from industry to ECF was Rs 11 crore (51%), up from Rs 9.0 crore in 2004-05. NCL was ranked first in ECF from industry.

Over and above the ECF of Rs. 21.5 crore, NCL received, as grants, an additional sum of Rs 8.72 crore under various Network and NMITLI programmes. We also received from CSIR a sum of Rs 45.1 crore as budgetary support for the year 2005-06. This takes the total value of our operating income to Rs 75 crore. NCL transacted funds to the extent of Rs 100 crore in 2005-06, a substantial increase over the last year. This increase in transactions has come from productivity increase per employee, not the number of employees in these functions.

FROM THE DIRECTOR'S DESK

NCL expended a sum of Rs 11.5 crore towards capital expenditure in the year 2005-06. Several major facilities were added. These include, MALDI ToF, AFM, 400 MHz NMR spectrometer, protein purification system, micro array spotter and scanner, scanning electrochemical microscope, fuel cell test system, CVD unit for carbon nanotubes, small angle X-Ray diffractometer, high resolution transmission electron microscope and dual beam environmental SEM. We are in the process of building facilities for micro reaction engineering as a capability for the future. Several other investments towards enhancing our research capabilities were undertaken.

Our investments in augmenting our capabilities in Information and Communication Technology are proceeding on track. NCL commissioned a new communication system at a cost of Rs 70.00 lakhs. We have doubled the telephone connections within NCL during the past six months. As we move to more and more web based systems for our internal management, security of information is of paramount importance. Security, access rights, disaster recovery management and redundancy are all issues that are being looked into.

We continue with several initiatives to modernize our laboratories and other associated infrastructure. Last year we spent a total of Rs 3.00 crore on works and services, of which, approximately 50% was spent from our internal Laboratory Reserves. A new 1000 KVA substation was commissioned at an estimated cost of Rs 1.00 crore.

The erstwhile MERADO campus of CSIR was rechristened as NCL Innovation Park (www.innovationpark.org). NCL Innovation Park is emerging as one of the new Resource Centers of NCL, which will house the Venture Center (www.venturecenter.co.in), a new Section 25 Company that NCL will float in the next few months. The Venture Center will provide 10, 000 sq feet fully built up laboratory space as incubators for early stage discoveries to be converted to marketable products or processes. In addition NCL Innovation Park will house several business facilitation functions as well as independent R&D centers of corporate entities, either as stand alone facilities or as joint ventures with NCL.

Deepak Research and Development Foundation (DRDF) have already occupied a 7500 sq feet facility at the Innovation Park. This is the first corporate R&D facility within NCL campus. NCL and DRDF have signed an MOU to synergize their activities and create mutual value.

NCL Innovation Park is thus poised to emerge as a key Resource Center of NCL that will leverage the strengths of NCL and explore new models of public – private partnerships and wealth creation with industry.

Science and technology in an organization cannot flourish without the infusion of young talent with new skills. NCL continues to attract young scientists in areas of its interest. Several scientists joined NCL with exceptional academic credentials and sound training in some of the best academic laboratories around the world.

Several of our colleagues continue to do us proud. Dr. K.N. Ganesh won the prestigious TWAS Award in chemistry. Our team led by Mr. P.P. Barve won the CSIR Technology Award for the year 2005, for their contributions to the development of a manufacturing process for ATBS, commercialized by M/s. Vinati Organics Ltd. Dr. U. Natarajan won the MRSI Award for 2006 and Dr. Guruswamy was awarded the CSIR Young Scientist Award in Engineering Sciences. Dr. S. Sivaram was awarded Padma Shri by the honorable President of India on March 29, 2006

S. Sivaram

(S. Sivaram)

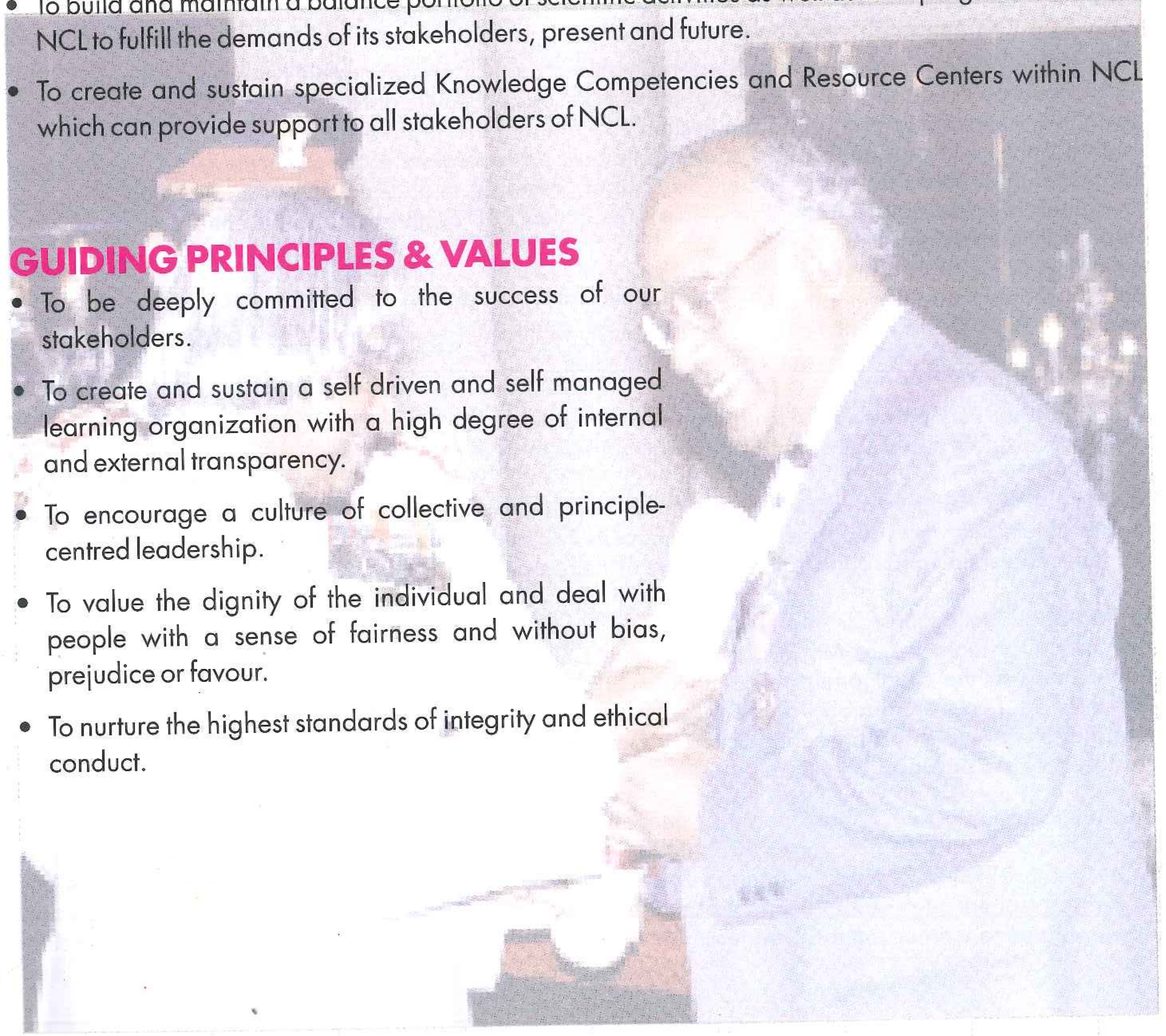
VISION, MISSION, AND GUIDING PRINCIPLES & VALUES

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

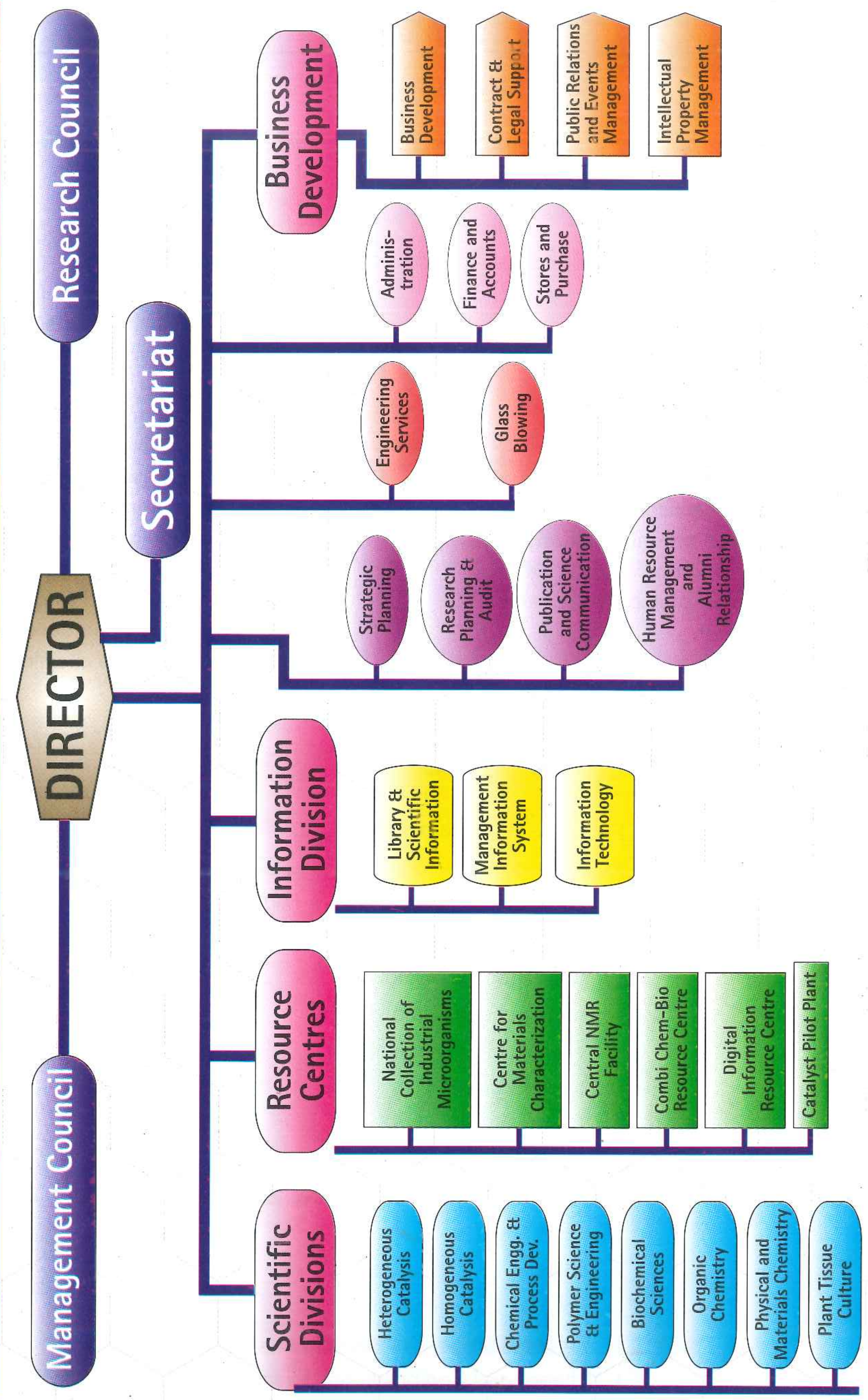
- To carry out R&D in chemical and related sciences with a view to eventually deliver a product, process, intellectual property, tacit knowledge or service that can create wealth and provide other benefits to NCL's stake holders.
- To build and maintain a balance portfolio of scientific activities as 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

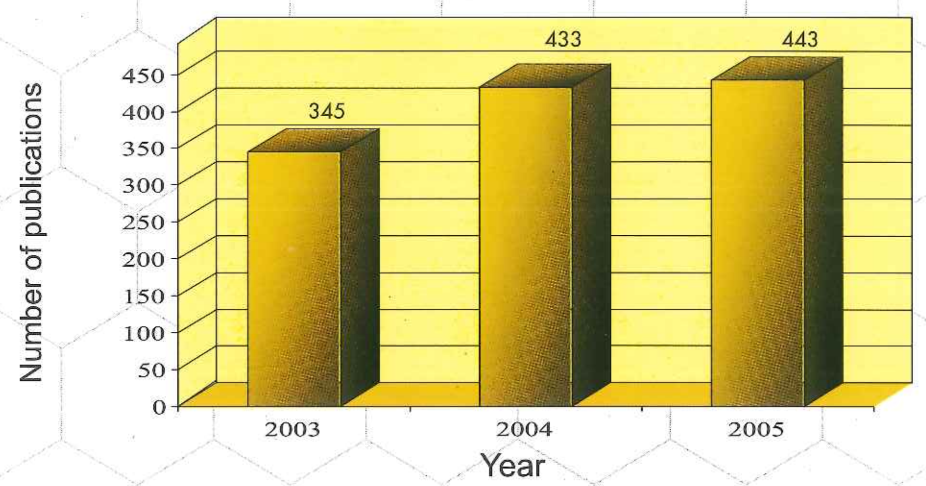
Knowledge Competencies

- ☐ 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

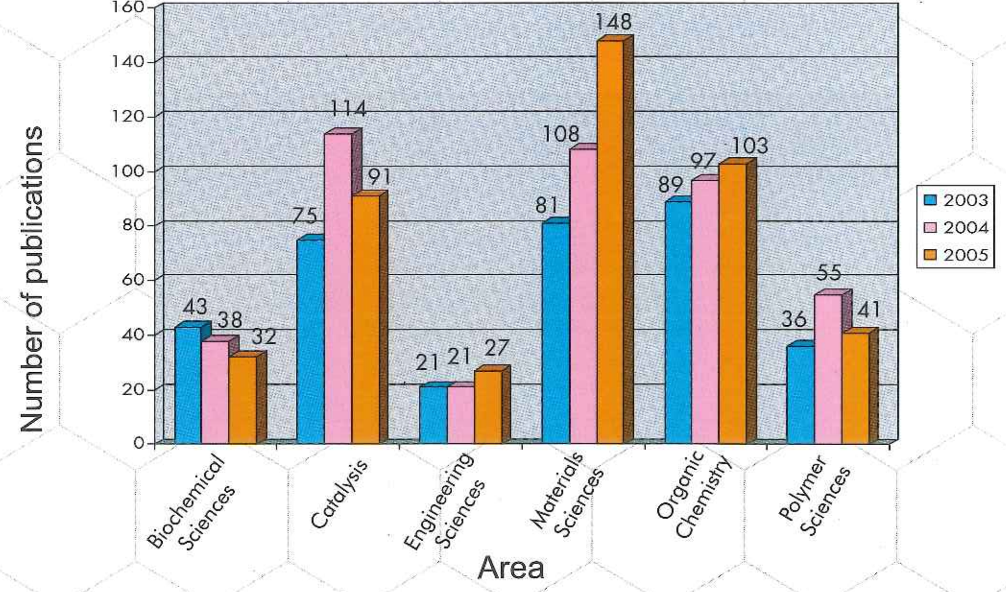
PERFORMANCE INDICATORS

Science Performance Indicators

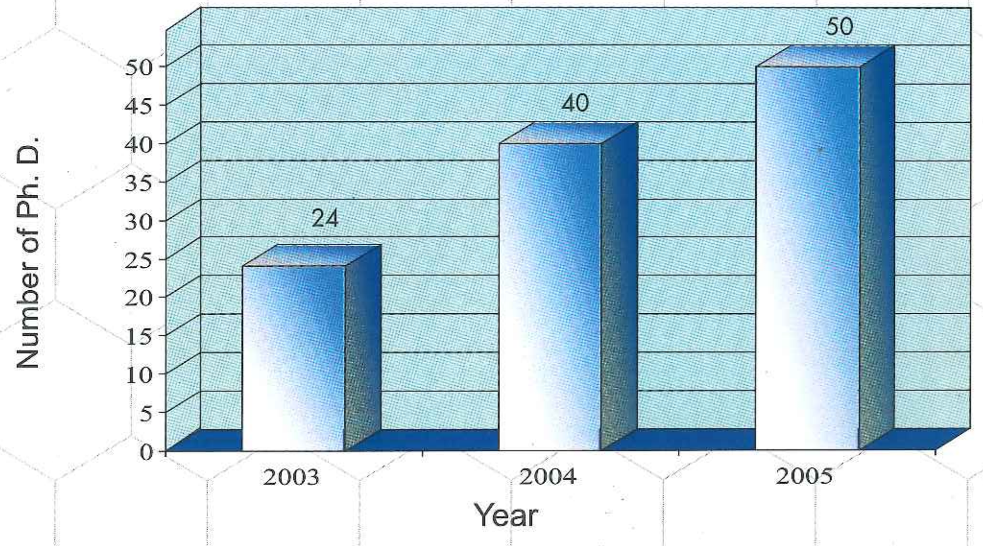
Research output: Publications



Area wise publications

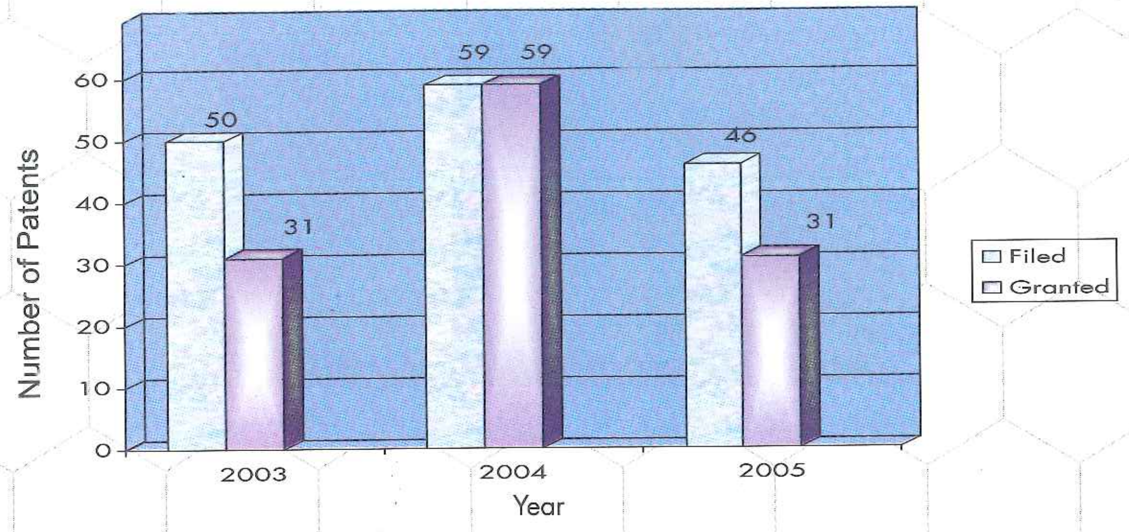


Ph.D. Awarded

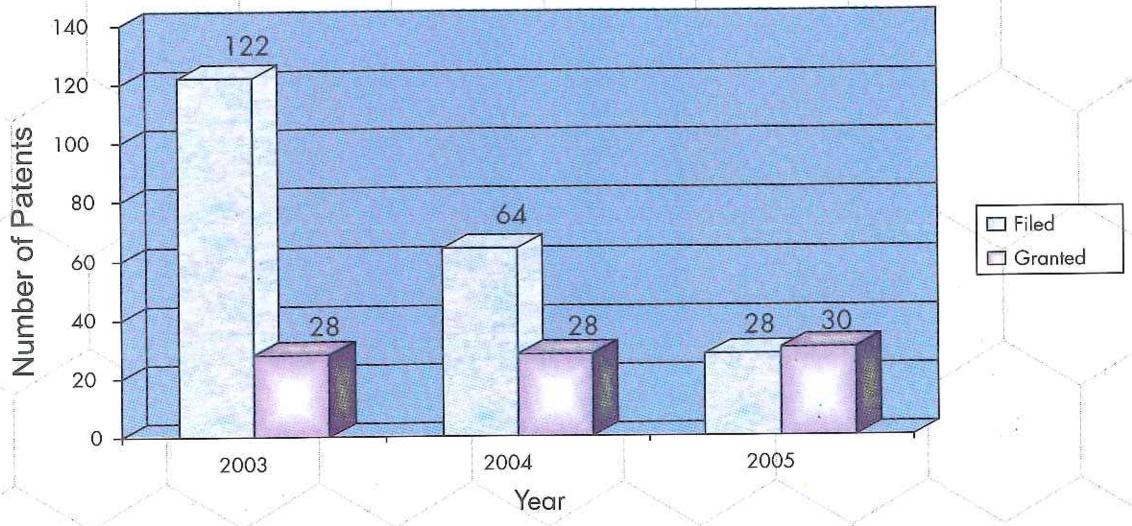


Technology Performance Indicators

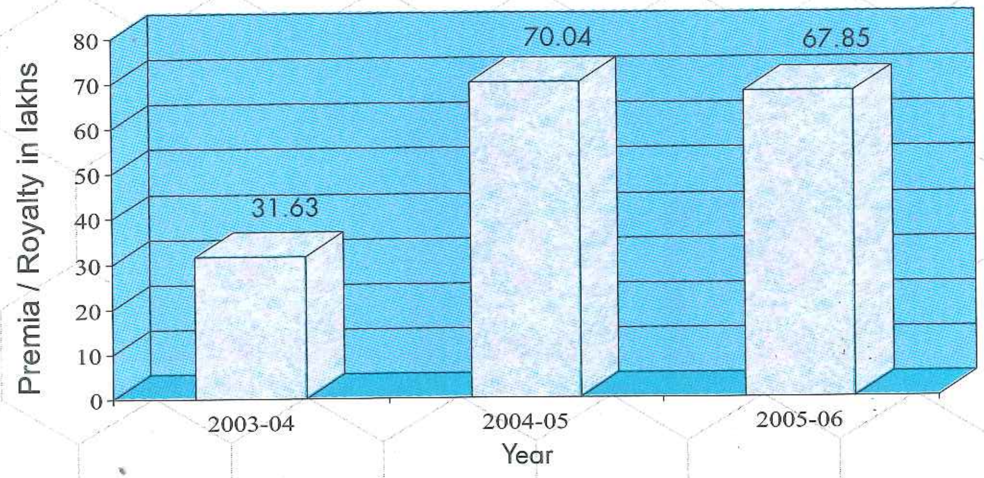
Indian Patents: Filed and Granted



Foreign Patents: Filed and Granted

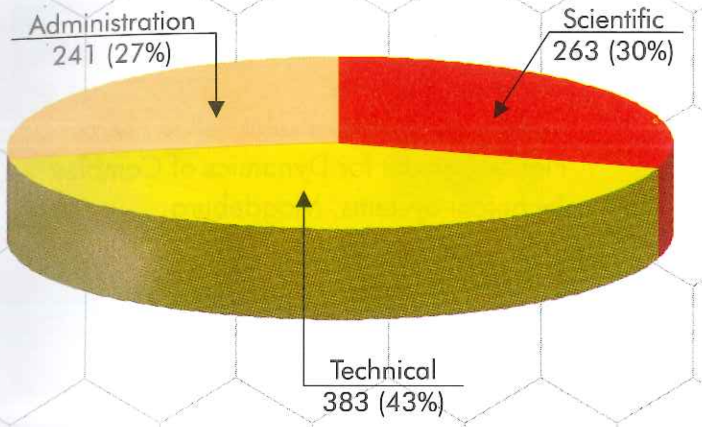


Premia / Royalty Earnings

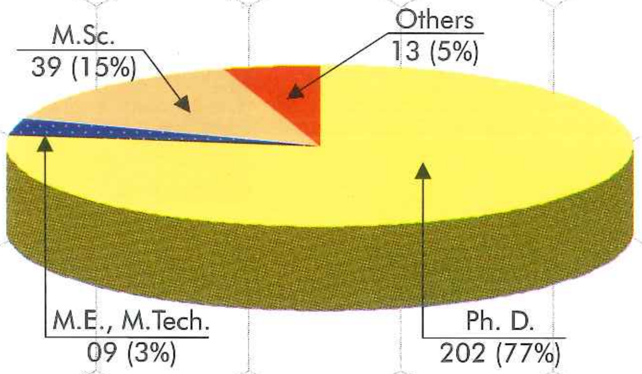


Human Resource Indicators

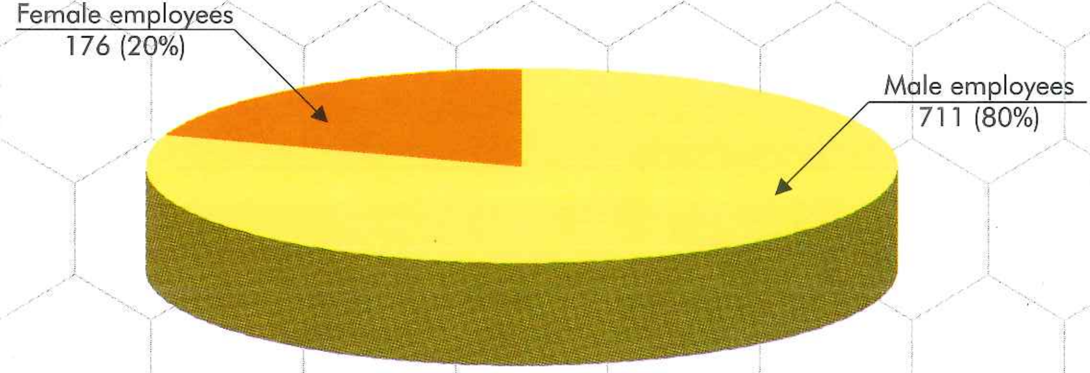
Total Staff : 887



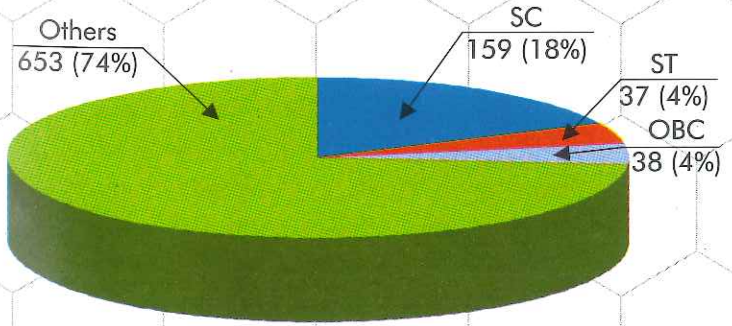
Scientific Staff : 263



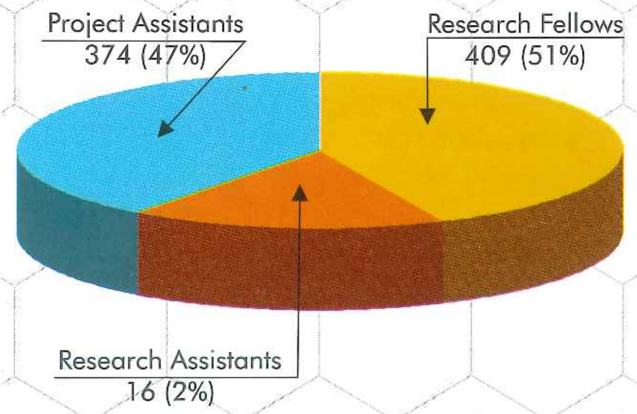
Male : Female ratio



SC, ST and OBC employees



Number of Students and Project Staff: 799



Human Resource Indicators

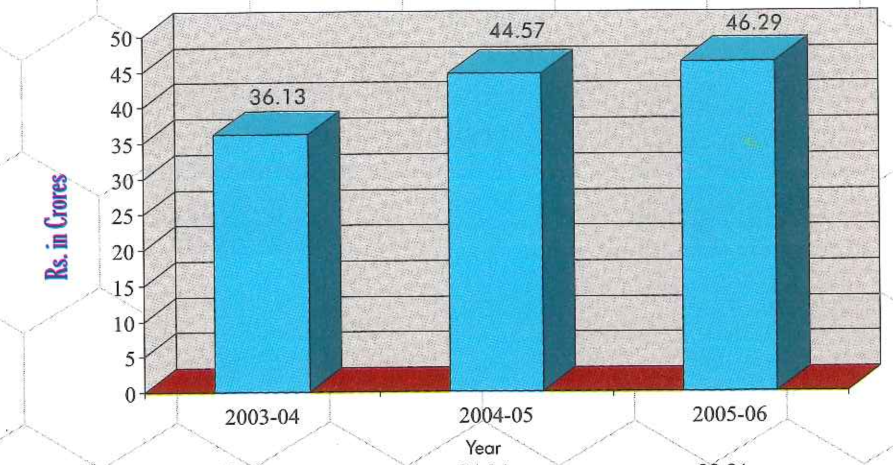
Name and date of joining		Subject	Qualifications
Dr. Amol A. Kulkarni (4 April 2005)		Chemical engineering	Ph.D. (Tech.) Chemical Engineering, UICT, Mumbai University; Post Doctorate (Humboldt Fellow) Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany.
Dr. Pankaj Poddar (4 April 2005		Structural and electronic properties	Ph.D. (Physical Sciences) ; Research Associate: Tel Aviv University, Israel, University of South Florida, Tampa-Materials Modifications Inc., Fairfax, VA, USA.
Dr. D. Baskaran (27 May 2005)		Polymer science & engineering	Ph.D., Polymer Chemistry, Pune University; Director, Polymer Characterization Laboratory, University of Tennessee, Knoxville, USA, Senior Research Associate, University of Tennessee, Knoxville, USA.
Dr. Anil Kisan Kinage (31 May 2005)		Chemistry	Ph. D. (Chemistry), Pune University, Visiting Research Scientist, (Center of Excellence, Hokkido University, Sapporo, Japan), Research Associate (Technical University of Munich, Germany), Post-Doc, (The University of Tokyo, Japan).

Human Resource Indicators

Name and date of joining		Subject	Qualifications
Mr. B. Senthilkumar (9 June 2005)		Organic chemistry	M.Phil., Organic Chemistry, University of Madras Research Associate, Shasun Research Centre, Chennai.
Dr. A. Bhattacharya (14 June 2005)		Organic chemistry	Ph.D., CIMAP, Lucknow, DAAD Post-Doctoral Research Fellow, Universitaet Konstanz, Germany.
Mr. Nikhilesh Yadav (25 July 2005)		Computer science	MCA (Computer Science).
Dr. Parag Kinge (2 January 2006)		Intellectual property management and business development	D.Sc. (Molecular Biology and Genetics), Max Plank Institute for Medical Research and University of Heidelberg, Germany; LL.M. (Master of Laws: Intellectual Property Law), Munich Intellectual Property Law Centre, Munich, Germany.

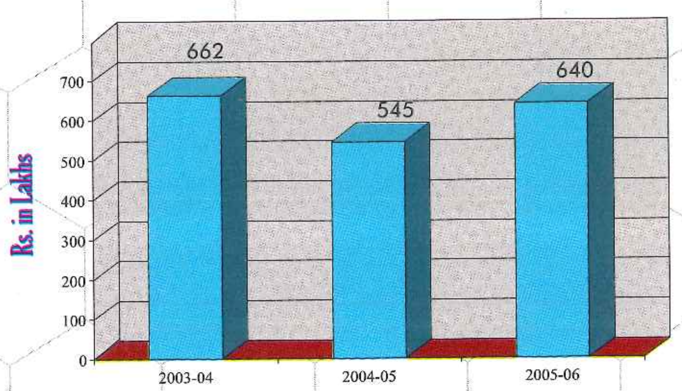
Financial Performance Indicators

CSIR budget

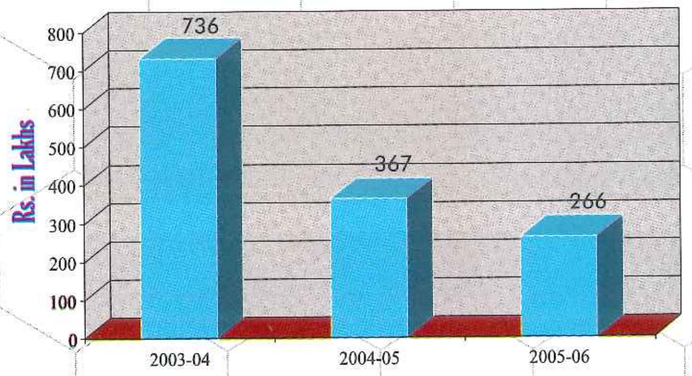


	2003-04	2004-05	2005-06
CSIR Budget	29.39	34.04	39.96
Network Project :	06.74	10.53	06.32

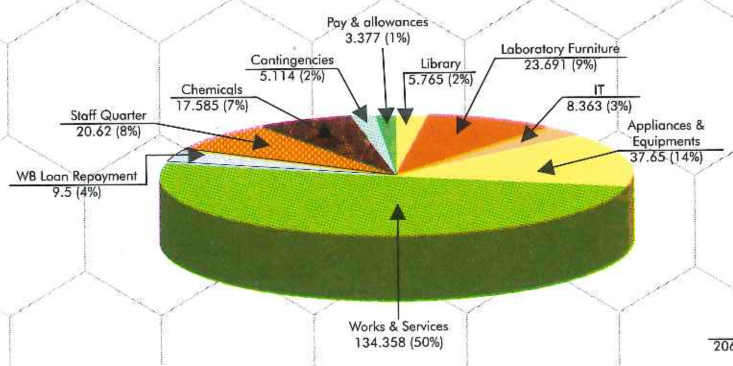
Laboratory reserve: Receipts



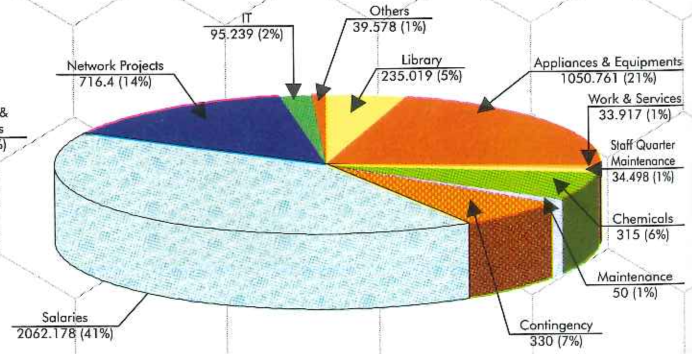
Laboratory reserve: Expenditure



Expenditure: Laboratory reserve (Rs. 266 lakhs) 2005-06



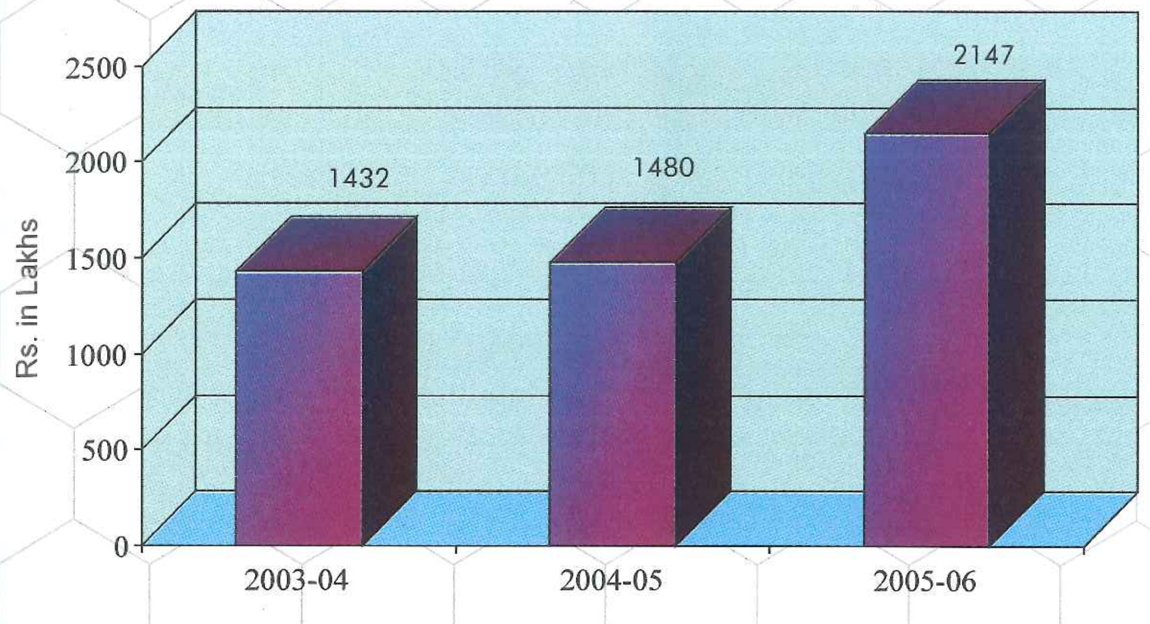
Expenditure: CSIR and Network Projects 2005-06 (Rs. 4629 lakhs)



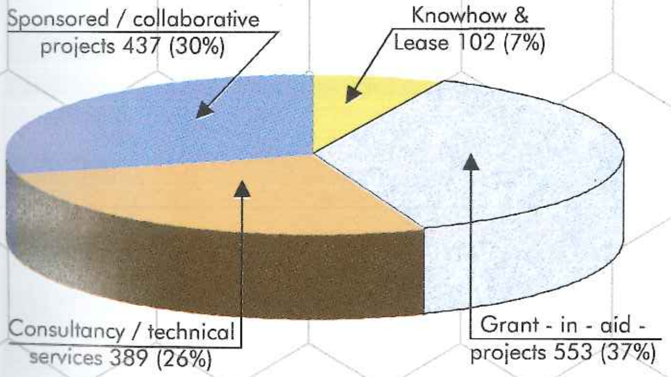
1 Lakh = 0.10 Million

Financial Performance Indicators

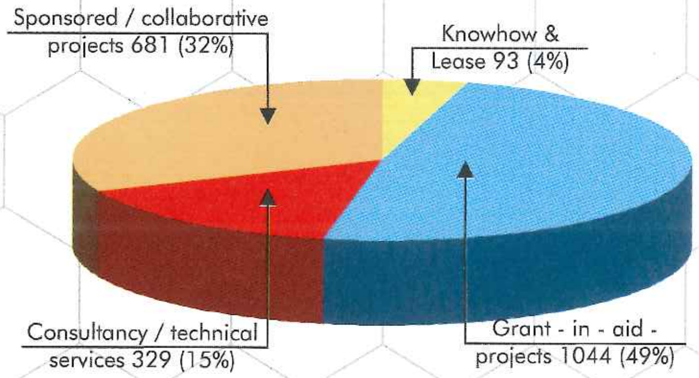
External Income



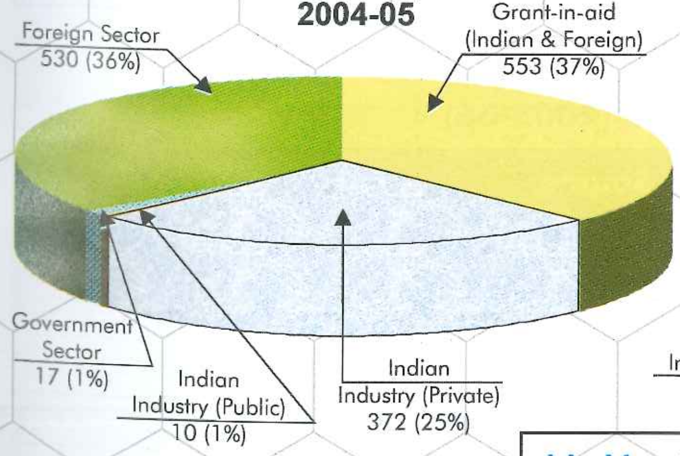
ECF : Project wise break-up Rs. 1480 lakhs (2004-05)



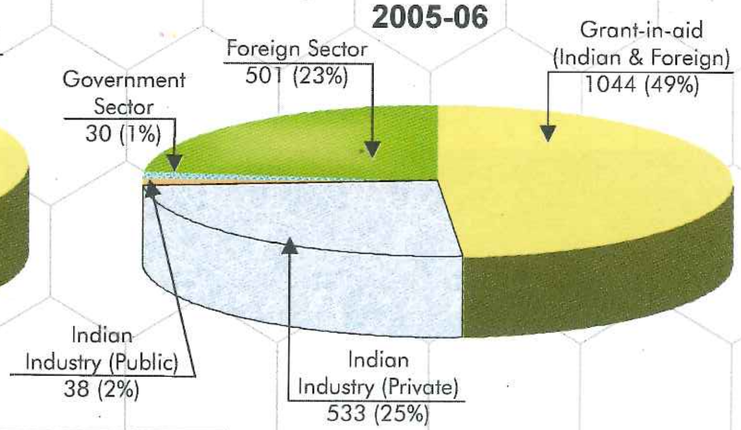
ECF : Project wise break-up Rs. 2147 lakhs (2005-06)



ECF :by source Rs. 1480 lakhs 2004-05



ECF :by source Rs. 2147 lakhs 2005-06



1 Lakh = 0.10 Million

Financial Performance Indicators

Capital and Recurring Expenditure on R&D (2004-2006)

Rs. in lakhs

Source	Capital		Recurring	
	2004-05	2005-06	2004-05	2005-06
CSIR	601	1254	546	2743
Lab Reserves	105	255	9	11
Projects *	336	720	1071	1330
Network Projects	615	290	576	301
Total	1657	2519	2202	4385
Percent (%)	43	36	57	64

*- Excluding NMITLI projects

Ongoing Publicly Funded Mission Mode and Internal Projects (2005-06)

Sr. No.	Description	Amount in Lakhs
1	CSIR NMITLI	472.42
2	Major publicly funded projects (DST / DBT / NPSM/ SDC / McNIGHT etc.)	1044.36
3	X Five year plan network projects	632
4	Internal projects *	89.00
	Grand Total	**2237.78**

* - Funded from Internal resources of NCL.

Scientific Budget (2005-06)

Funding Source			
			Rs. in Lakhs
	Recurring	**Capital**	**Total**
CSIR	200	200	400
LR	413	371	784
Total	613	571	1184

1 lakh = 0.1 million

Outputs & Outcomes

Select Outputs and Outcomes of NCL during 2003-2006

Category of Benefits	Benefit	Indicators	Performance		
			03-04	04-05	05-06
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in international peer-reviewed journals/ publications(Calendar year)	356	404	426
		Number of papers published in Indian journals(Calendar year)	26	29	17
		Normalized Impact Factor (if latest NIF is not available, previous value may be used)	1.73	1.83	2.07
		Number of patents filed in India (Calendar year)	50	58	46
		Number of patents filed outside India (Calendar year)	119	63	28
		Number of patents commercialized	1	4	2
		Number of major national/ regional collections, compilations, databases	2	3	3
	Highly trained man-power	Number of PhDs produced (Calendar year)	24	40	50
		Number of NET/GATE qualified students joined	70	35	30
	Science awareness, popularization etc;	Number of popular S&T articles published (in all languages)	12	8	4
		Number of national and regional workshops, seminars organized	9	12	12
	Pride and standing among nations; National image	Number of international awards won (Give titles/details on separate sheet)	NIL	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)	23	26	30
		Number of papers in international peer-reviewed journals	356	404	426
		Number of IF research papers	346	381	420
		Number of foreign patents granted (Calendar year)	28	28	30
	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	6
Private goods	Research, consulting, teaching and analytical services	Total earnings from projects done for Indian & Foreign businesses/ industry (Rs Crore) (Industrial ECF, excluding Grant-in-Aid)	8.15	9.28	11.02
	Continuing education	Total earnings from continuing education/ training programs (Rs Crore)	NA	NA	0.17
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (Rs Crore)	0.32	0.70	0.68

* - Dr. Paul Ratnasamy was awarded the International Zeolite Award

** - Dr. K.N. Ganesh was awarded the Chemistry Prize of The Third World Academy of Sciences

PERFORMANCE INDICATORS

Outputs & Outcomes

Select Outputs and Outcomes of NCL during 2003-2006

Category of Benefits	Benefit	Indicators	Performance		
			03-04	04-05	05-06
Strategic goods and options	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (Rs Lakhs)	400	568	470
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (Rs Lakhs)	617	533	1044
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	Number of papers in international peer-reviewed journals	356	408	426
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	9	10	17
		Number of PhDs granted where lab scientists were research guides	24	40	49
		Number of staff who are members of National academies (Cumulative) *	23	27	27
		Number of Bhatnagar awardees (Cumulative)	12	13	13
		Number of Padma awardees (Cumulative)	4	4	5
	Lab's standing with industry	Total worth of projects with industry (only industry: both Indian & foreign) (excluding Grant-in-Aid) – Industrial ECF (Rs Lakhs)	783	928	1102

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

Research & Development Reports

Annual Report
2005-06

1. BIOCHEMICAL SCIENCES

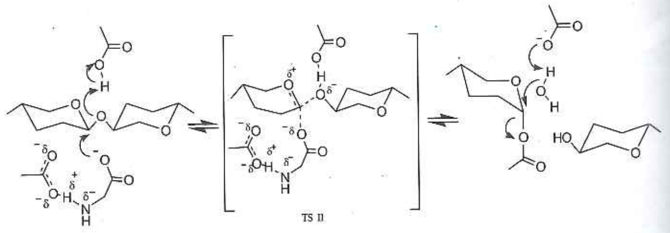
1. 1. Basic biochemical sciences

1.1.1. Enzymology

Structure-function studies
Cellulase / Xylanase

A low molecular weight (14.2 kDa) 1,4 β D–glucan glucanohydrolase was purified from *Thermomonospora* sp. The secondary structure of the enzyme is made up of α helix regular 0.588, α helix distorted 0.226, β sheet regular 0.001, β sheet distorted 0.002, β turn 0.062 and unordered structure 1.04. The importance of various functional groups for the activity of 1,4 β D–glucan glucanohydrolase was investigated using chemical modifiers with restricted amino acid specificity, under the conditions which did not alter the enzyme conformation. Modification of enzyme by 2,4,6-trinitrobenzene sulfonic acid (TNBS), a lysine–specific modifier resulted in inactivation of the enzyme. Kinetic analysis of TNBS modified enzyme implicated the presence of an essential lysine residue at the active site of enzyme. The inhibition of enzyme by p-hydroxymercury benzoate (PHMB) indicated the presence of an essential Cys residue at the active site of the enzyme. The substrate protection studies confirmed the presence of these residues in the active site.

Xylanases have potential applications in a wide range of industrial processes. To make the application of xylanases realistic the improvement of enzyme properties is of utmost importance. Hence attention is focused on the discovery of new xylanases or improvement of existing ones in order to meet the requirements of industry such as stability and activity at high temperature and pH. Enhancement of xylanase activity in alkaline pH by the addition of a neutral amino acid glycine into the reaction mixture was demonstrated. The xylanase activity increased seven-fold at alkaline pH in presence of glycine and its pH optimum shifted from 7 to 8 without applying protein engineering techniques. The steady state kinetics revealed that glycine in the reaction mixture increases the K_m and K_{cat} values of the enzyme. The mechanism of enhancement of xylanase activity by glycine was deciphered by monitoring the isoindole fluorescence of the o-phthalaldehyde labeled enzyme and studies using glycine analogs. Based on the observed experimental evidences, a novel possible mechanism of glycine assisted catalytic action of xylanase has been proposed.



Glycine assisted catalytic mechanism of xylanase through a transient glycosyl-enzyme-glycine intermediate (TS II)

Ntn Hydrolases
Penicillin G acylase

This pharmaceutically important enzyme from *Kluyvera citrophila* was cloned and overexpressed in *E. coli*. However, due to possible discrepancy in intracellular processing of precursor protein a degraded inactive protein was produced by the recombinant. To overcome this problem the said gene was cloned and expressed as an active secretary protein. Further studies are underway. Novel marine bacterial source has been identified for clinically important enzyme, bile salt hydrolase. The fermentation parameters are being studied for optimum production of enzyme. Studies on inhibition kinetics were performed on bile salt hydrolase (BSH) from *Bifidobacterium longum* using various ligands of penicillin V acylase and BSH to trace the possible evolutionary relationship between the two enzymes.

Cephalosporin C acylase

Novel isolate was studied for production of 7-ACA from cephalosporin C. This culture showed both cephalosporin C acylase and glutaryl 7-ACA activity. The fermentation parameters for optimum production of enzyme were standardized. This enzyme was purified to homogeneity. For continuous production of 7-ACA immobilization of whole cells/ enzyme were used. Effect of different matrices, crosslinking agents and their studies are under progress.

Monolignol polymerization to lignin by covalently bound peroxidases

Polymerization of monolignols to lignins involves cell wall bound peroxidases. These class III peroxidases (EC number 1.11.1.7) are monomeric, heme-containing glycoproteins found exclusively in the plant secretory pathways. These dehydrogenate cinnamyl alcohols and other phenolic substrates, at the expense of hydrogen peroxide. Two cell wall bound peroxidases, a ~150kD cationic peroxidase and a ~66 kD anionic peroxidase, were purified from the leguminous tree *Leucaena leucocephala*. The former is present only in highly differentiated tissues and the latter is of ubiquitous presence. Both, however, catalyse monolignol polymerization to lignin. The genes for these in sense as well antisense orientation are to be used to study the down regulation of the lignin polymerization.

1.1.2 Glycobiology

A lectin from the mycelial extract of an endophytic strain of *Fusarium solani* was purified. Its hemagglutinating activity is inhibited by glycoproteins possessing N-linked as well as O-linked glycans. The thermodynamics and kinetics of binding of glycans and glycoproteins to *F. solani* lectin was studied using surface plasmon resonance. The lectin showed very high affinity for asialo-bovine submaxillary mucin. The affinity for various glycoproteins were in the order of asialo-BSM>>BSM ≈ asialofetuin > fetuin ≈ asialofibrinoger > fibrinogen. Compared to glycans, their corresponding glycoproteins showed several fold higher affinity with significant contribution from enthalpy and positive entropy, suggesting the involvement of non-polar protein-protein interaction. Moreover, the higher affinity of the glycoproteins was due to their faster association rates and low activation energy.

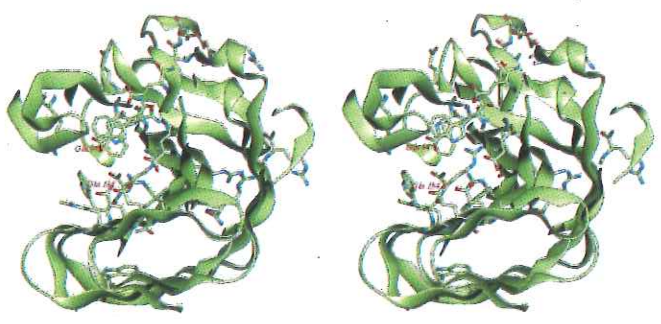
1.1.3 Structural biology Cellulase

A low molecular weight (14.2 kDa) cellulase from *Thermomonospora* sp. was crystallized by hanging drop vapour diffusion method using commercial crystallization kits. Good quality crystals, were obtained using 0.2M sodium acetate, 0.1M

sodium cacodylate pH 6.5, 18% PEG 8000. The crystals were diffracted at 2.3 Å resolution. The crystals belonged to the orthorhombic space group $P2_12_12_1$, with unit cell parameters a = 49.9, b = 79.5, c = 99.7Å. The Matthew's coefficient VM was calculated to be 2.7 $Å^3Da^{-1}$. The amino acid sequence analysis of the peptides obtained after tryptic digestion of the enzyme was carried out. The C-terminal sequence is ASHMDQTYYLCSDVNFV. The other five peptides sequenced are NYGCWLR, SMDAVGPWK, HVVFTIWK, LPDGQLCSGGLAEGGR, PLTWGSLDLVHR. Of these, ASHMDQTYYLCSDVNFV and LPDGQLCSGGLAEGGR showed sequence homology with the cellulase binding domain of other enzymes from *Themobifida fusca* and *Streptomyces coelicolor*. The conserved residues found in the multiple sequence alignment of these peptides, were cysteine, serine, phenylalanine, and glycine.

Xylanase

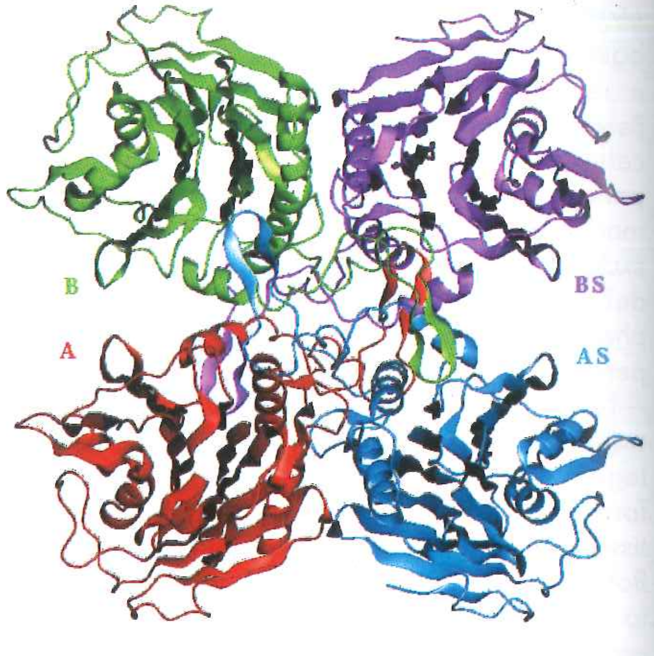
An alkaline xylanase from an alkalophilic *Bacillus* sp. (NCL 87-6-10) has been crystallized, its three-dimensional structure was determined and refined using X-ray diffraction data at 2.8 Å resolution. Active site characterization and mechanism of substrate binding were explored. Binding studies including growing of crystals of complexes of the enzyme with xylobiose and xylotriose were tried.



Stereo picture of the structure of alkaline xylanase showing the active site

Conjugated bile salt hydrolases and penicillin V acylases

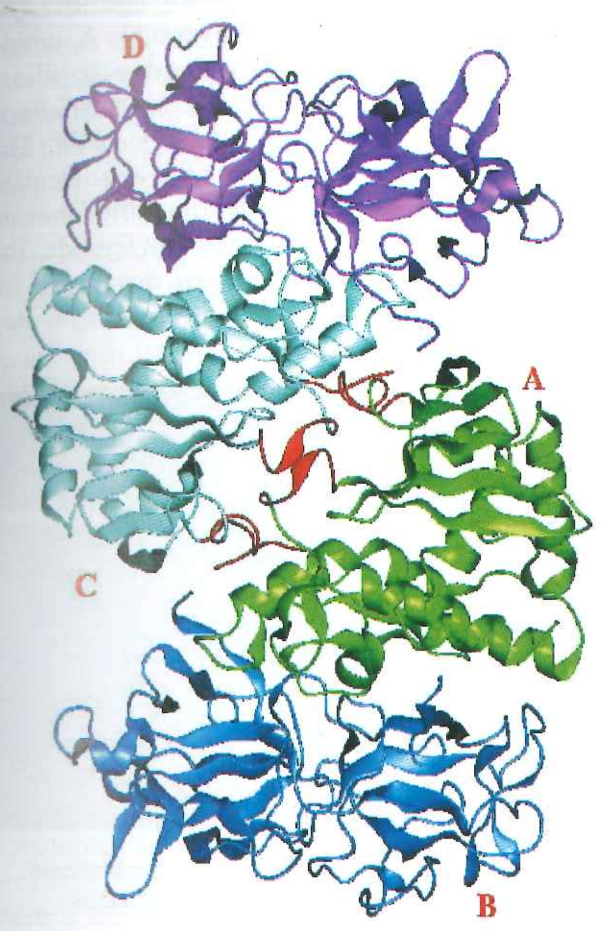
The processing mechanism and substrate binding of penicillin V acylase from *Bacillus sphaericus* (*Bsp*PVA) were thoroughly studied using crystal structures of several mutants. A mechanism could be proposed for the processing of penicillin V acylase based on these studies. Some of the crystals of PVA mutants happened to be twinned. The twinning could be correctly interpreted. Biophysical and kinetic studies to understand the substrate specificity of *Bsp*PVA and to assess its stability to denaturation conditions are also being carried out. The structure was determined and refined of the un-annotated protein from *B.subtilis* cloned in *E.coli.* and characterized as penicillin V acylase. The structure turned out to be very similar to that of *Bsp*PVA. Kinetic studies were carried out to understand its specificity and to compare with other penicillin acylases. The stability of this PVA under denaturing conditions and its folding pathways were explored. The structural analysis was carried out, of a conjugated bile salt hydrolase from *Bifidobacterium longum* (*Bl*BSH) cloned in *E. coli*. purified and crystallized. The structure was solved in two crystal forms and refined using data at resolution up to 2.5 and 2.3 Å, respectively. Biophysical and kinetic studies were carried out to understand the specificity of the enzyme and its stability. Molecular modeling and docking studies were also carried out to understand the interactions involved in substrate binding of the enzyme.



Tetramer structure of conjugated bile salt hydrolase from *B. longum*

Lectins

The lectin from chickpea (*Cicer arietinum*) was found to have no structural analog available in the protein data bank, by the determination and comparison of N-terminal sequence. Hence, multiple isomorphous replacement method has to be tried for solving its crystal structure. Initial data collected on a crystal belonging to space group R3 was found to be twinned data. Subsequently, data on crystals belonging to P3 space group was collected. On screening for heavy atom derivative we got crystals of lead and mercury. However, no successful Patterson solution could be obtained using either of the derivatives. A third prospective heavy atom derivative of iodine could be obtained in $P2_12_12$. After several trials native crystals also could be grown in the same space group. The data could be collected on crystals in the same space group grown each with platinum and gold present in the crystallization solution. The diffraction data on gold derivative turned out to be not good. Efforts to establish the formation of heavy atom derivative in the crystals by calculating Patterson function are in progress. Better crystals were grown and higher resolution data could be collected on two galactose specific lectins from *Trichosanthes dioica* and *Erythrina indica*. We could locate the covalently linked sugar chain in the latter. Further refinement of these structures is in progress.



Dimer-dimer association of two heterodimer molecules of *T.dioica* lectin in their crystals

1.1.4 Molecular biology

Human mitochondrial DNA studies

The study on the presence and the extent of spread of M haplogroup characterized by the AluI/DdeI sites at 10924/10927 in the Indian population was completed. These findings through the analysis of nearly 200 Indian samples are compiled. Analysis by sequencing the hypervariable segment of mtDNA samples collected from tribal and caste populations of Maharashtra to infer their relationships was completed. Samples of around forty patients diagnosed as having mitochondrial genetic disorder were collected. Sequencing and analysis for deleterious mutations of a part of the samples was carried out. Biochemical assays for detecting some of these disorders were also standardized.

1.2. Biotechnology

1.2.1 Development of novel bioconjugates

Preparation and characterization of urea-formaldehyde-pepsin bioconjugate

The synthesis of urea formaldehyde microspheres by dispersion polycondensation polymerization method was studied. These microspheres with proper F/U molar ratio can provide highly reactive groups, capable of further condensation with the amino acid residues of enzyme/ proteins. Presence of methylols groups in UF microspheres was confirmed by ^{13}C NMR study. Pepsin, a proteolytic enzyme, was immobilized on the UF microspheres to form bioconjugate system. As compared to the free enzyme in solution, the pepsin in the bioconjugate system exhibited significantly enhanced pH and temperature stability. The urea-formaldehyde-pepsin bioconjugate system also exhibited excellent proteolytic activity over eight successive reuse cycles with more than 50 % of initial activity. A highlight of this new biocatalyst is the ease with which separation of this biocatalyst from the reaction medium achieved by mild centrifugation.

Encapsulation of cellulase for detergent application

The enzyme was encapsulated in a natural polymer for its commercial application in detergent industry. The modified enzyme was found to retain complete biocatalytic activity with a shift in the optimum temperature (50 - 55°C) and considerable increase in the pH and temperature stabilities as compared to the free enzyme. Encapsulation of the enzyme also protected the activity in presence of detergents and enhanced the shelf life. A three-fold decrease in the initial rate of reaction indicated a controlled release of the enzyme conferring properties preferred for its potential application in the manufacture of detergents.

1.2.2 Microbial biotechnology

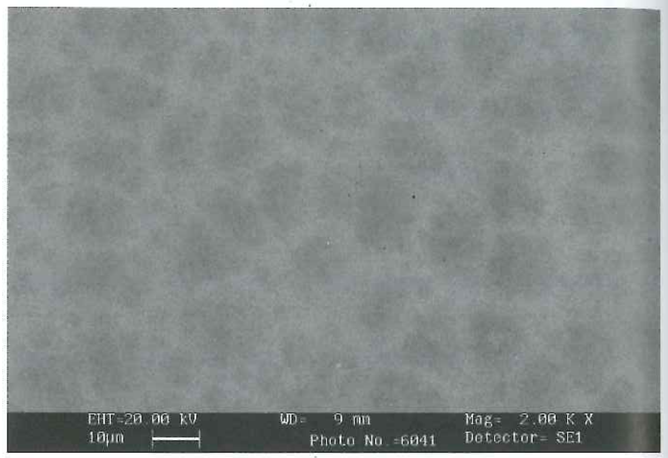
Production of chitosan using fungi

The fungi are gaining lot of importance in the modern biotechnology for applications such as biomedical applications, paper production, textile finishes, photographic products, cements, heavy metal chelating agents, biocontrol and waste removal. Chitin comprises 22-44% of cell walls of fungi. Various fungi were collected from NCIM for the estimation of chitin- chitosan contents in their cell walls. Number of non-zygomyceous fungi also showed increased percentage of chitosan in their cell walls for the self –defence. Among the studied organisms, namely *Benjaminiella, Rhizopus* and *Absidia* the cell walls of *Benjaminiella* and *Rhizopus* showed higher amounts of chitosan contents. The solid state NMR studies showed that the chitosan of *B. poitrasii* was 90% deacetylated. Further large scale chitosan production is being studied.

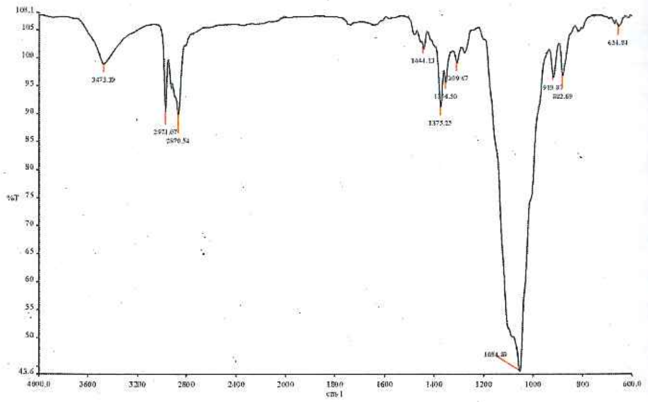
Bioseparation

The work on developing affinity membranes for purifying therapeutically and diagnostically useful proteins sponsored by Department of Biotechnology (DBT), New Delhi was undertaken. Separation and purification of biomolecules from large volumes of biologically derived fluids is both difficult and expensive. Therefore, downstream processing remains a critical factor for a commercial application. Usually, purification of a biomolecule requires four to five independent steps and accounts 50% of the total cost of a biomolecule production process. Affinity separation, which is based on specific interaction between the biomolecules and ligand can significantly help in optimization of the process. In the search for superior affinity substrates it was inevitable that membranes would emerge as an alternative to packed columns. An advantage of affinity membrane filtration is that the high flow rates at low pressure drop can be achieved, thereby greatly improving the washing, elution, and regeneration processes. Decreasing the probability of deactivation of the biomolecules by shortening their exposure to an unfavorable medium is an attractive feature.

Experiments were carried out to prepare cellulose based affinity membranes. The developed membrane was found suitable to carry out necessary modifications and couple different ligands. The coupling of ligand groups such as protein A, amino acids, DEAE, CM, polyethyleneimine, brilliant green, reactive orange, procion red and their effects on blood protein adsorption were studied. The methodology was developed for the modification of commercially available nylon membranes to make it suitable for binding of different ligands. The process of selective desorption was developed for the purification of blood protein in a single step operation.



SEM of a novel cellulose based porous membrane suitable for the separation of biomolecules



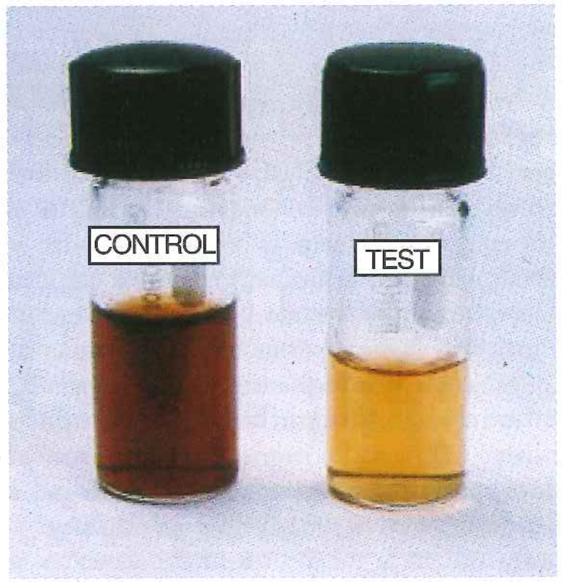
Attenuated total reflectance Fourier Transform Infrared (ATR/FT-IR) spectrometry of the prepared novel cellulose based porous membrane suitable for the separation of biomolecules

Biodegradation

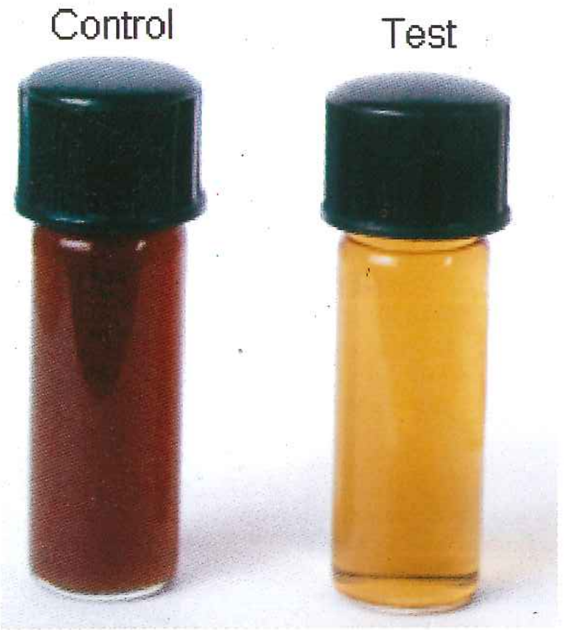
Developing a process for the biodegradation of pollutants present in the distillery effluent using membrane reactor sponsored by Ministry of Environment & Forest, New Delhi is underway.

Most of the distillery industries are based on molasses as the principal raw material due to its low cost and availability. Molasses contains numbers of organic as well as inorganic materials that find way in the effluent resulting high biological oxygen demand (BOD) and chemical oxygen demand (COD). These organic and inorganic materials have very high nutritive value and can therefore be used for irrigation purposes. The major problem in effluent treatment of molasses spent wash (MSW) is the presence of a dark brown natural polymer, melanoidin. It has antioxidant properties and is toxic to many microorganisms used in wastewater treatment. Due to its recalcitrant nature it can not be removed by conventional wastewater treatment. It has also the potential of preventing oxygenation by blocking light from contaminated waterways. Other than being a potential water pollutant, it removes manganese from the soil resulting loss of fertility. The removal of pollutants by physical or chemical means or dilution to meet legal obligations is not enough for a pollutant free environment. There is a need to develop a process, which will degrade these pollutants and make them suitable for other natural processes. To develop a biodegradation process, there is need to isolate a highly specific microbe(s) that has high pollutant degrading activity and a reactor system where these type of reactions will be carried out effectively.

Under this project, thirty-eight soil samples from various locations where MSW was exposed to the soil were collected. The soil sample, which showed higher decolorization and decrease in COD was selected for the culture isolation. In selected soil sample 81% decolorization on 18th day, in absence of any additional carbon source, was observed, while in the presence of additional carbon source, 96% decolorization was observed on 7th day itself. The biomass generated using soil as inoculum showed significant MSW degradation in batch/ continuous mode of operation using a stirred reactor coupled with microporous membrane in a flat sheet module configuration. Twelve bacterial strains and three fungal strains were isolated from selected soil. The culture identification was carried out where higher decolorization was observed. Two bacterial and two fungal strains, *Bacillus subtilis, B.sphaericus, Aspergillus nidulans*, and *A.terreus* were identified. *A.nidulans* showed significant decolorization and decrease in COD. Particularly, a fungal strain *A.nidulans* AA which showed significant decolorization and decrease in COD, appears to be naturally developed mutant as the morphology of the isolated strain was significantly different from the conventional strain. MSW decolorization activity by *A.nidulans* is a novel finding. The significant decolorization and decrease in COD was obtained using intracellular enzyme preparation and fungal strains.



Decolorization of molasses spent wash obtained in the absence of any additional nutrient



Decolorization of molasses spent wash obtained in the presence of glucose as additional nutrient

1.2.3 Nano-biotechnology

Fabrication, characterization and enzymatic activity of fungal protease – nanogold membrane bioconjugate

The synthesis of a free-standing nanogold membrane by the spontaneous reduction of aqueous chloroaurate ions by the diamine molecule DAEE at a liquid-liquid interface was studied. The free standing nanogold membrane provides a biocompatible surface for the immobilization of proteins. F-Protease (F-Prot) was then bound to the nanogold membrane via interaction with the gold nanoparticles leading to a new class of biocatalyst. A highlight of the new biocatalyst wherein the enzyme is bound to the nanogold membrane is the ease with which separation from the reaction medium achieved by simple filtration. In relation to the free enzyme in solution, the F-Prot in the bioconjugate material exhibited a slightly higher biocatalytic activity and significantly enhanced pH and temperature stability. The F-Prot nanogold membrane bioconjugate material also exhibited excellent biocatalytic activity over ten successive reuse cycles.

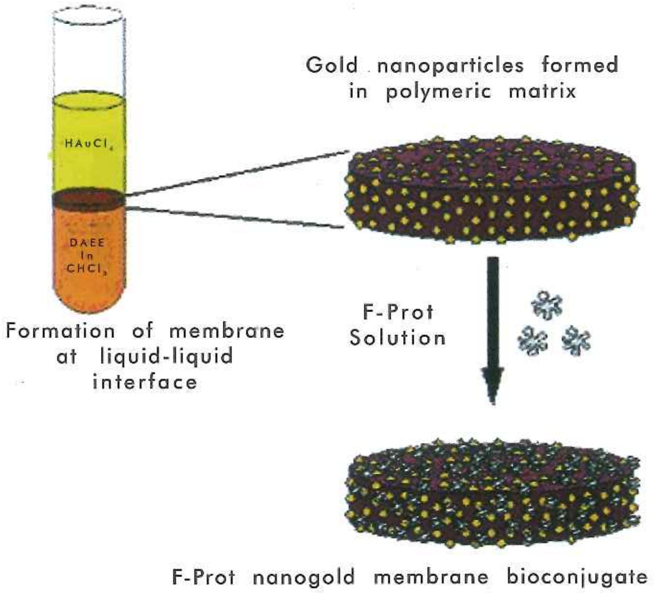
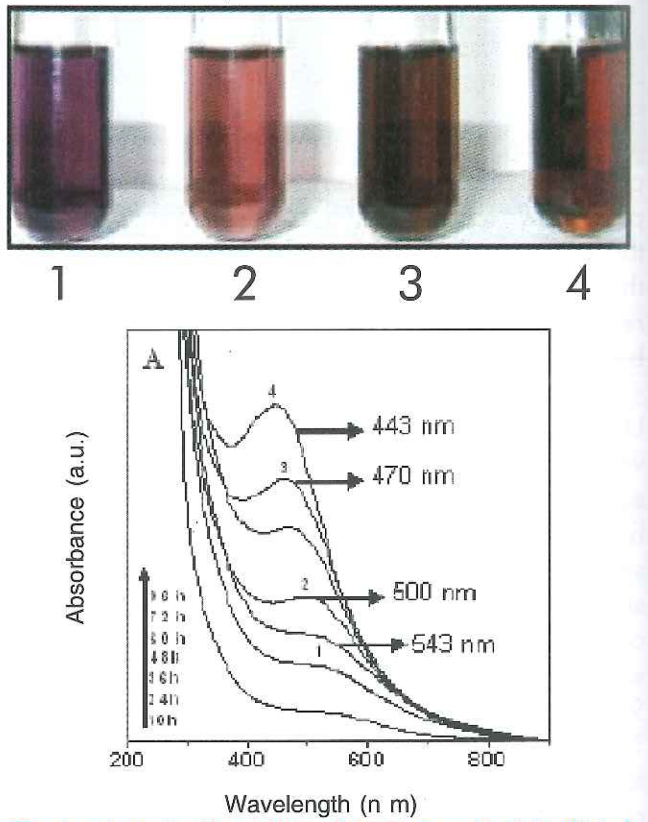


Illustration of the formation of enzyme nanogold membrane bioconjugate

Extracellular biosynthesis of bimetallic Au–Ag alloy nanoparticles

Highly stable bimetallic Au-Ag alloy nanoparticles were synthesized using fungus *Fusarium oxysporum* when incubated with equimolar solutions of $HAuCl_4$ and $AgNO_3$ for 96 hr at 25-28 °C. It has been found that initially gold is reduced followed by silver leading to nanoparticles of Au-Ag alloy. Depending on the amount of fungal biomass, the different composition of alloy nanoparticles can be synthesized. Exactly the same effect can be achieved using lower fungal biomass concentration by adding extraneous NADPH to the solution containing the biomass and the salts.

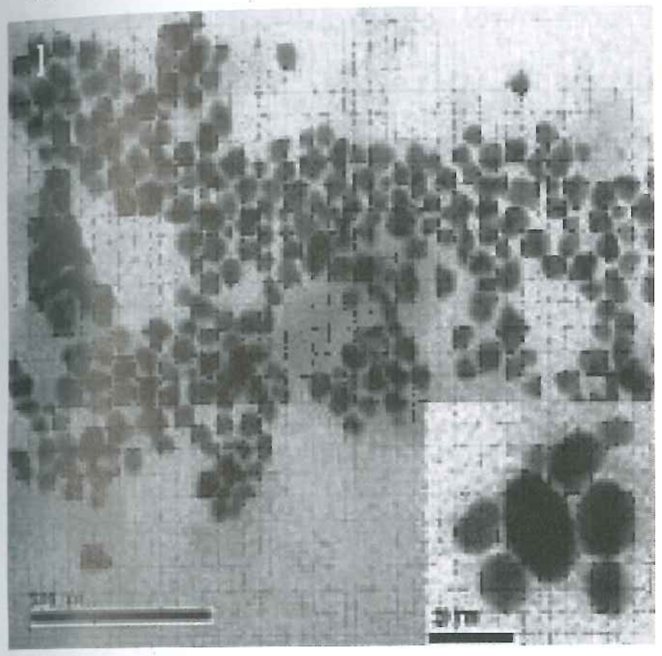
$$1\ \text{mM}\ HAuCl_4 + 1\ \text{mM}\ AgNO_3 \xrightarrow[\text{60 g, 96 h}]{\textit{F. oxysporum}}$$



The inset shows the picture of test tubes (1-4) of diluted colloidal solution and the corresponding UV-Vis spectra of Au-Ag alloy nanoparticle with respect to time

The gradual change of color from purple (tube 1) to deep brown (tube 4) as well as the surface plasmon resonance (543 to 443 nm) is the clear indicative of the formation of bimetallic Au-Ag alloy nanoparticles.

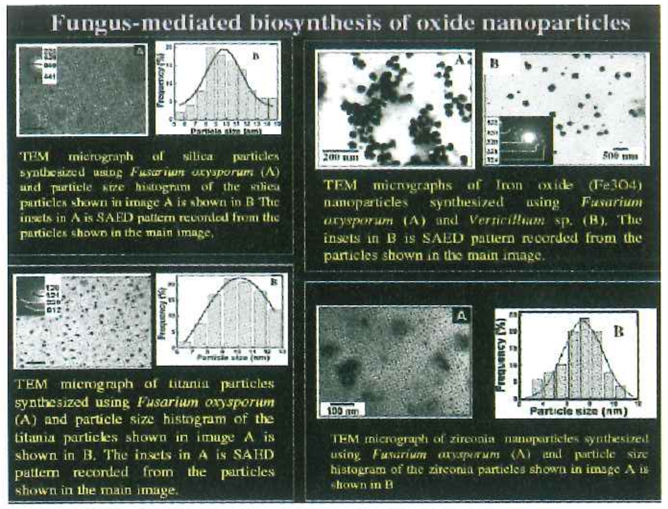
The figure below shows TEM images of well-separated nanoparticles with occasional aggregation in the size range 8–14 nm.



TEM images of Au-Ag alloy nanoparticles for 96 h

Fungus-mediated biosynthesis of oxide nanoparticles

Chemical methods for synthesis of oxide nanomaterials are 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 neutral pH. We have shown that nanoparticulate magnetite (Fe_3O_4) 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 fungus results in the room-temperature synthesis of crystalline magnetite particles that exhibit a signature of a ferromagnetic transition with a negligible amount of spontaneous magnetization at low temperature. SiO_2, TiO_2 and ZrO_2 nanoparticles were also synthesized at room temperature extracellularly by challenging the fungus *F. oxysporum*, to an aqueous solution of K_2SiF_6, K_2TiF_6 and K_2ZrF_6, respectively.



Fungus-mediated biosynthesis of oxide nanoparticles

TEM micrograph of silica particles synthesized using *Fusarium oxysporum* (A) and particle size histogram of the silica particles shown in image A is shown in B The insets in A is SAED pattern recorded from the particles shown in the main image.

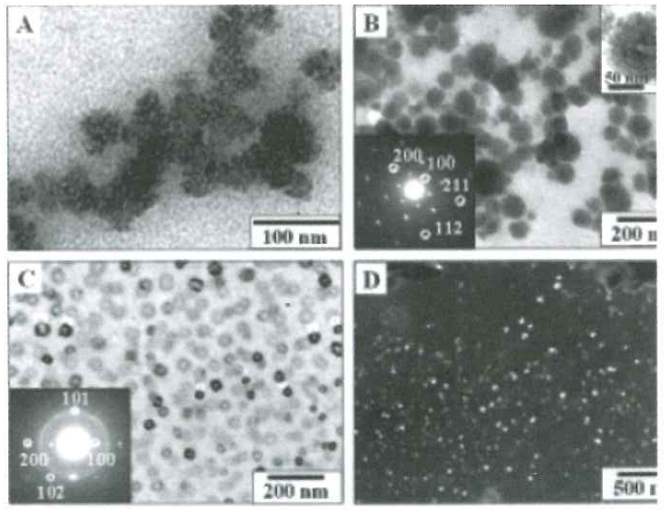
TEM micrographs of Iron oxide (Fe3O4) nanoparticles synthesized using *Fusarium oxysporum* (A) and *Verticillium* sp. (B). The insets in B is SAED pattern recorded from the particles shown in the main image.

TEM micrograph of titania particles synthesized using *Fusarium oxysporum* (A) and particle size histogram of the titania particles shown in image A is shown in B. The insets in A is SAED pattern recorded from the particles shown in the main image.

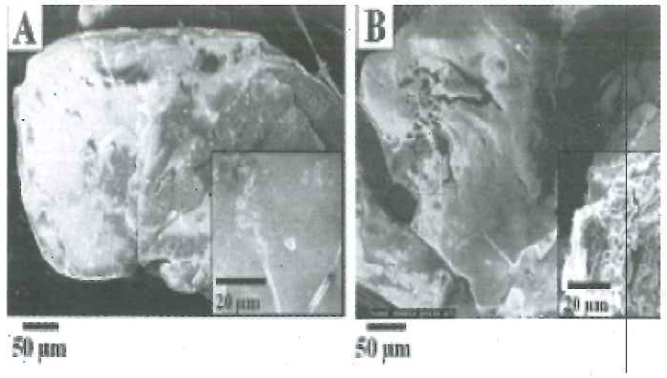
TEM micrograph of zirconia nanoparticles synthesized using *Fusarium oxysporum* (A) and particle size histogram of the zirconia particles shown in image A is shown in B

Bioleaching of sand by a fungus for producing extracellular silica nanoparticles

The concept of biosynthesis of oxide nanoparticles was extended and tried to make the process fully biogenic and eco-friendly by substituting the chemical precursors with naturally-available raw materials. White sand consisting of complex silicates was exposed to the fungus, *F. oxysporum*. The reaction results in room temperature synthesis of spherical, porous silica nanoparticles, which on further calcinations at 400°C for 2 hr form hollow silica nanoparticles. These porous and hollow nanoparticles have great potential applications as catalyst supports because of the larger surface area as compared to solid silica nanoparticles.



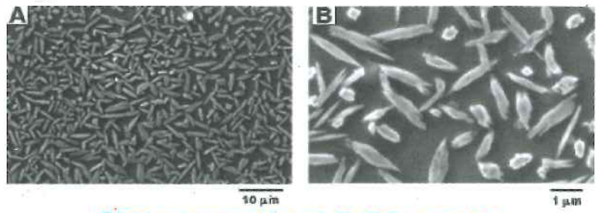
TEM micrographs at different magnifications of silica nanoparticles synthesized by the exposure of sand to the fungus, Fusarium oxysporum before (A and B) and after calcination at 400 °C for 2hrs (C and D)



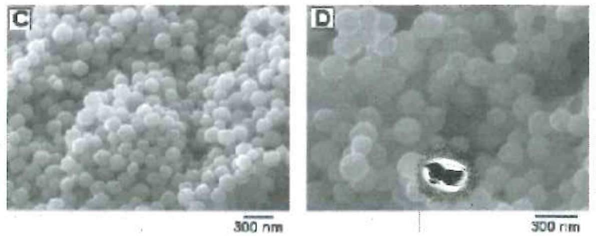
SEM micrograph of a single grain of sand before (A) and after (B) exposure to the fungus, *Fusarium oxysporum* for 24 h. The insets in A and B show magnified views of a selected area from the respective grains

Heavy-metal remediation by a fungus for production of lead and cadmium carbonate crystals

The reaction of the fungus, *F. oxysporum*, with the aqueous heavy-metal ions Pb^{2+} and Cd^{2+} resulted in one-step formation of the corresponding metal carbonates. The metal carbonates are formed by reaction of the heavy-metal ions with CO_2 produced by the fungus during metabolism and thus provided a completely biological method for production of crystals of metal carbonates. The $PbCO_3$ and $CdCO_3$ crystals thus produced have interesting morphologies because of interaction of the growing crystals with specific proteins secreted by the fungus during reaction. An additional advantage of this approach is that the reaction leads to detoxification of the aqueous solution and could have immense potential for bioremediation of heavy metals. The metal ions were not found toxic to the fungus.



SEM micrographs of $CdCO_3$ crystals



SEM micrographs of $PbCO_3$ crystals

1.2.4 Secondary metabolites, inhibitors and drugs

Biochemical characterization of a low molecular weight API from thermo-tolerant *Bacillus licheniformis*

The aspartic proteases of pharmaceutical importance such as pepsin, plasma renin, HIV-1 protease, plasmepsin and lysosomal cathepsin D have evoked considerable interest for investigating the kinetic role of their inhibitors. Pepsin is a major aggressive factor in the gastro-easophgeal reflux diseases (GERD). Alginate containing products are currently used in the treatment of GERD (e.g., gavicon advance) that interact with pepsin in vitro, in a non-competitive manner. Considering the physiological importance of the aspartic proteases and their role in various diseases, there is a lacuna in the studies of the mechanism of inhibition by slow-binding inhibitors. The known slow-binding inhibitors of pepsin are pepstatin, its analogous and a low molecular weight (1147Da) inhibitor. A low molecular weight aspartic protease inhibitor (API) was purified and characterised from a newly isolated moderately thermo-tolerant *Bacillus licheniformis*. The evaluation of the kinetic parameters showed that API is a slow-tight binding competitive inhibitor of pepsin. Being a low molecular weight hydrophilic compound, and produced from a bacterial source, API possesses tremendous potential for the economical and effective production. The inhibitor was purified to homogeneity as shown by rp-HPLC and SDS-PAGE. API is found to be stable over a broad pH range of 2-11 and at temperature 90°C for 2½ h. It has a molecular weight of 1363 Da as shown by MALDI-TOF spectra and 1358 Da as analyzed by SDS-PAGE. The amino acid analysis of the peptide shows the presence of 12 amino acid residues having molecular weight of 1425 Da. The secondary structure of API as analyzed by the CD spectra showed 11% α-helix, 39% β sheet, and 50% aperiodic structure. The kinetic studies of pepsin-API interactions revealed that API is a slow-tight binding competitive inhibitor with the IC_{50} and K_i values 4.0nM and 3.83nM-5.31nM, respectively. The overall inhibition constant K_i^* value is 0.107±0.015 nM. The rate constants from the intrinsic tryptophanyl fluorescence data is in agreement with those obtained from the kinetic analysis; therefore, the induced conformational changes were correlated to the isomerization of EI to EI*.

ATBI against human pathogenic fungi and yeast

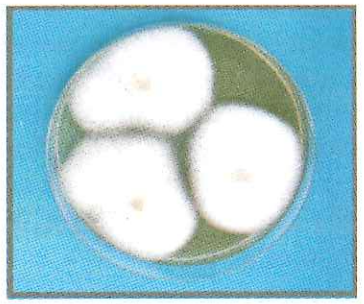
Human pathogenic yeast and fungi are studied due to their emerging resistance and significance in nosocomial infections. In the present study the control of opportunistic pathogens with an alkalothermophilic *Bacillus* inhibitor (ATBI) isolated from an alkalothermophilic *Bacillus* sp. was analyzed providing a new direction in the search for new potential lead molecule. The low molecular peptidic aspartic protease inhibitor has been demonstrated to be active against various human pathogenic yeast and fungi. The in vitro studies demonstrated that the growth of various human pathogens including yeasts such as *Candida albicans, C. krusei, C. parapsilosis, C. tropicalis, C. kefyr* and fungi such as *Aspergillus oryzae* and *A. flavus* is inhibited by ATBI. The secreted aspartic proteases (SAPs) from *C. albicans* showed inactivation of activity in presence of the inhibitor in vitro, indicating its probable mechanism of action. In addition to the antifungal activity, the efficacy of the inhibitor was also evaluated in an immunosuppressed mice model, where toxicity and lethal dose were determined. Significant reduction in the *C. albicans* cell count was observed per gram of kidney tissues; even though no reduction was observed in case of liver and spleen. These studies suggest the role of ATBI as a probable candidate for therapeutic use.

Cysteine protease inhibitor from endophytic fungus AAT-TS-4

The taxol producing fungus under different fermentation conditions produces protease inhibitors which lead to cancer cell apoptosis. Screening showed that these are cysteine protease inhibitors (CPI). CPI was stable in a broad range of temperature (37 to 100°C) and showed inhibitory activity against papain, clostripain, cathepsin L and cathepsin B. CPI is specific for cysteine proteases and failed to show inhibitory activity against other classes of enzymes. The purification was done on reverse phase column on HPLC. The purified CPI showed a molecular mass of 854 Da on analysis by mass spectroscopy (ESI-MS). Further characterization of CPI is in progress.

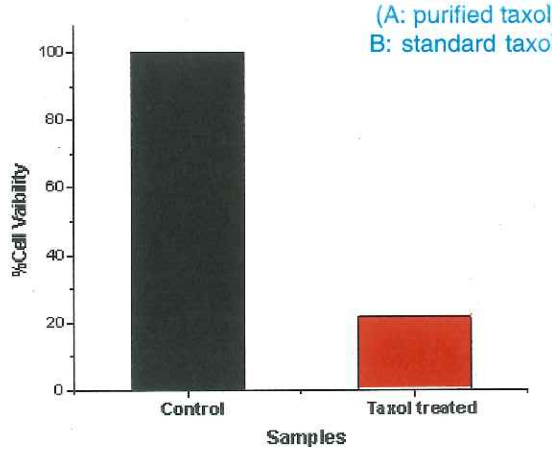
Taxol: isolation and purification

Taxol, a tubulin binding diterpenoid, originally isolated from the Pacific Yew (*Taxus brevifolia*) has been regarded as an important anticancer agent. Forty endophytic fungi were isolated from Indian Yew tree *Taxus baccata*, out of which one fungus AAT-TS-4 was found to produce Taxol. Fungal taxol was isolated and purified by thin layer chromatography and high performance liquid chromatography and characterized by ultra violet absorption, mass spectroscopy and by proton NMR spectroscopy. Taxol was quantified by competitive inhibition enzyme linked immunoassay. This strain yields 10.2 μg/L taxol. Cytotoxicity towards cancer cell line HL-60 (leukemia), A431 (epidermal carcinoma) and MCF-7 (breast cancer) was determined by MTT assay.



Endophytic fungus (AAT-TS-4) from *T. baccata*

TLC showing purified taxol alongwith standard taxol.
(A: purified taxol,
B: standard taxol)



Activity against epidermal carcinoma cell line A431

Biosynthesis of vinca alkaloids using an endophytic fungus of *C. roseus*

Vinblastine and vincristine, tubulin binding indole alkaloids, originally isolated from the *Catharanthus roseus* commonly known as sadabahar in India are regarded as important anticancer agents. Ten endophytic fungi were isolated from *C. roseus,* out of which one fungus AA-CRL-6 was found to produce vinblastine and vincristine. Fungal vinblastine was isolated and purified by thin layer chromatography and high performance liquid chromatography and characterized by ultra violet absorption and mass spectroscopy. Cytotoxicity towards cancer cell line HL-60 (leukemia), A431 (epidermal carcinoma) and MCF-7 (breast cancer) was determined by MTT assay. Further characterizations of vinblastine and vincristine are in progress.

Secondary metabolites from *Calophyllum and Garcinia*

Assessment of chemodiversity in plant species enables identification of new molecules and potential drugs of therapeutic value. Molecular characterization further assists in species identification and fixing of the superior plant species. Two members of the family Guttiferae *viz. Calophyllum* and *Garcinia* occurring along the Western Ghats of India were studied.

The genus *Calophyllum* is represented by four species *viz. C. inophyllum, C. polyanthum, C. apetalum* and *C. austroindicum*. About 200 accessions of this genus were collected and analyzed for inophyllums B and P which are anti HIV compounds. These terpinoids have been isolated, characterized and studied for the diversity assessment in *C.inophyllum*. Two elites were identified with high content of these bioactive compounds. *In vitro* protocol was developed for conservation of this species. *C. austroindicum* a rare and endangered species was also collected and screened for bioactive compounds. The most potent anti-HIV compounds calanoloids A and C (which are NNRT inhibitors) were isolated and their structures elucidated.

Garcinia is represented by thirteen species distributed along the Western Ghats. Nine species have been collected and authenticated. Total 185 accessions were collected for the species identified. A sound protocol for plant regeneration by *in vitro* somatic embryogenesis was developed for *Garcinia indica*. Regeneration using mature explants is also in progress for three species of *Garcinia*. Molecular characterization of the species is also underway. (-)-Hydroxy citric acid, an important anti lipidogenic constituent of *Garcinia,* was isolated from *Garcinia* species to study the chemodiversity.

1.2.5 Plant biotechnology

1.2.5.1 Bio-control and bio-pesticides

Aspartic protease inhibitor as biocontrol agent

We have demonstrated the antifungal activity of ATBI against phytopathogenic fungi in plate assays. In continuation of this work, experiments on infected plants with the inhibitor were performed. Pigeon pea wilt caused by *Fusarium udum* and powdery mildew of *mung* bean caused by *Erysiphe polygoni* were targeted. Biological control of phytopathogens is one of the key areas of research due to the increasing awareness of the hazards and drawbacks of chemical control agents. To effectively control the existing infection and to improve the yield of the standing crop safe antifungal agents from biological resources are receiving great attention. The ability of protease inhibitors to control physiologically important enzymes and their antinutritional interactions makes them suitable for biological control. The inhibitor was evaluated against wilt of pigeon pea caused due to *F.udum* and powdery mildew of mung bean caused by *E.polygoni* under field conditions. ATBI was found suitable in controlling 71% of Fusarium wilt of the highly susceptible pigeon pea variety ICP 2376 which was comparable to the chemical control agent carbendazim. Seed coating, drenching and seed coating and drenching were performed to analyse the method best suited for application of ATBI for pigeon pea. The results indicated that seed coating and drenching gave optimum results with 71% reduced the environmental hazards associated with the toxic effects of chemical fungicides. ATBI was analysed for its toxicity on non-target organisms like *Rhizobium*, *Trichoderma* and *Bacillus* species. No inhibition was found on the growth of these beneficial organisms confirming its suitability for application in the soil.

Microbial control of pests: Entomopathogenic fungi as mycoinsecticides

The technology transfer of a mycoinsecticide against *Helicoverpa armigera* in pulses, from the laboratory to the market based on *M. anisopliae*, has been supported under the Indo-Swiss collaboration in biotechnology (ISCB) project. The toxicity and non-target effect data was generated and the work on packaging and marketing is being carried out for the technology transfer. The identification of 3 back strains was done.

Scale-up, field demonstration and techno-economics of enzyme complex from *M.verrucaria* as a biocontrol agent

The plant-pathogenic fungi and insects share a common structural component, chitin, for their respective protective covers. Therefore, the fungal products such as mycolytic and cuticle degrading enzymes consisting mainly of chitinase as well the inhibitors that hamper the synthesis of chitin have proved their potential in controlling pathogenic pest. Similarly, the seed dressing with the microorganisms producing these enzymes extracellularly and/ or their soil application have also contributed significantly in controlling root infecting pathogens. Myrothecium verrucaria is one of the potential organisms that produces very high levels of mycolytic and cuticle degrading enzyme activities.

Under the CSIR rural development programme, fungi (*M. anisopliae*) and fungal products (cuticle degrading enzyme complex of *M. verrucaria*) were used to control woolly aphids in the sugarcane field. The successful demonstration trials were carried out Sugarcane Research Station, Padegaon as well as with a farmer at Pargaon in 2005.

1.2.5.2 Genetic markers

Molecular approaches to improve the bread making quality of wheat

After achieving considerable success in yield enhancement, the trend of wheat research in the country has been to improve the quality of wheat for the end use product. Taking into consideration the end products and end user of wheat, the important grain qualities which need to be improved are grain protein content (PC), grain size, grain hardness (GH) and bread making quality (BMQ). Of these, good BMQ is the major end use requirement for the baking industry. In order to decipher BMQ into its components and also to dissect the chromosomal regions associated with these components, a segregating mapping population was developed at Directorate of Wheat Research (DWR), Karnal. These were generated from a cross between HI 977 (a wheat cultivar with good BMQ) and HD 2329 (poor BMQ) consisting of 105 individuals. These populations were phenotyped at three different agroclimatic regions, for two consecutive years, for traits such as Loaf volume (Lv), Loaf score (Ls), sedimentation volume (SV), Thousand kernel weight (TKW), PC and GH as BMQ is influenced by all these traits. Linkage map for 19 chromosomes were constructed with 205 SSR markers and the composite interval mapping revealed presence of 21(Ls) and 30(Lv) QTL. The QTL for other traits like Sv, PC also collocated with Lv and Ls QTL. These QTL exhibited significant GxE interactions and shown that BMQ is a complex and composite trait, which is governed by many QTL. This will help breeders to construct beneficial allelic combinations and accelerate Indian breeding program for development of superior cultivars with good BMQ.

Development of disease-resistant wheat varieties using molecular marker technology

Wheat productivity is severely affected by two important diseases, leaf ruts and stripe rust especially in North-Western plains zone. Development of agronomically desirable lines with durable resistance to leaf and stripe rust using molecular marker technology is essential to ensure a rust-free crop. In order to achieve speedy and reliable incorporation of effective seedlings/ adult plant resistance genes, DNA marker(s) linked to such genes need to be employed along with breeding efforts. Based on the statistics of wheat production and productivity of individual states in the country and demand supply gap, it is necessary to increase production and productivity from central and peninsular zone of India. This region of country is predominantly marginal rain fed and semiarid. Genotype such as NI5439 recommended for this region adapted to rainfed and low irrigation conditions, high yielding with one or two irrigations, is completely susceptible against prevalent races in this region. In the present programme, it is therefore proposed to transfer two leaf rust resistance genes Lr 15 (seedling resistant) and *Lr* 34 (Adult Plant Resistant) in NI5439 background.

For identification of marker linked to *Lr* 15, mapping population consisting of 148 F_2 plants developed by crossing Tc x Tc *Lr* 15 at ARI was used by NCL. Twenty three polymorphic primers (ISSRs and SSRs from 2D) were attempted using only HR and HS lines. The phenotypic scores based on 162 A (Agharkar Research Institute, ARI, Pune and, Punjab Agricultural University, PAU, Ludhiana) were used for linkage analysis which revealed Xgwm102 to be linked with *Lr* 15 at LOD 6.0 in the preliminary screening. For mapping of *Lr* 34, 266 families (F_7/F_8) from a cross 90RN2491 x WL711 were developed and phenotyped for leaf rust resistance at adult plant stage during 2005 and observations on LTN were also recorded at PAU. SSRs from 7DS, 1BS and 2DS which are reported to be linked to *Lr* 34 are being attempted with these samples at NCL.

Stem rust caused by *Puccinia graminis* f. species *tritici* and leaf rust caused by *P.triticana* are major constraints to wheat production worldwide. In the present study F4 derived SSD population, developed from a cross between Australian cultivars 'Schomburgk' and 'Yaralinka' was used to identify molecular markers linked to various leaf and stem rust resistance genes using a total of 1,330 RAPD and 100 ISSR primers and 33 SSR primer pairs selected on the basis of chromosomal locations of these genes. The markers linked to these rust resistance genes will be exploited for marker assisted selection in wheat.

Improving the nutritional value of chickpea

Tagging of *Fusarium* wilt resistance genes, mapping of important agronomic traits and developing an intraspecific linkage map of chickpea using various DNA markers were studied. The F_9 RIL populations of three crosses (Vijay xJG62, JG61xICC 4958 and Vijay xICC 4958) were raised at MPKV, Rahuri and wilt data are collected from sick plants. Agronomic data and the leaf tissues for DNA analysis of RILs were collected from normal plants. An integrated intraspecific linkage map of chickpea based mainly on SSR as anchor markers was developed with JoinMap 3.0 using segregation data from two F_9 recombinant inbred populations (RIP 1 and RIP 2), with one common parent. Using 93 individuals from each population, 121 and 127 reproducible and segregating markers were obtained and used for linkage analysis, of which 91 and 83 markers were grouped into 12 and 15 linkage groups in RIP-1 and RIP-2, respectively. These two maps were combined using 26 common markers. At a LOD score of ≥ 3.0 and maximum recombination fraction of 0.4, 107 markers were mapped onto six linkage groups in the integrated map comprising 87 SSRs, 12 RAPDs, 5 ISSRs, 2 RGAs and 1 ASAP markers. The map had a total length of 384.2 cM with an average marker density of 3.59 cM. Comparative studies with previously reported inter and intra specific chickpea linkage maps confirmed the conservation of SSR markers across maps as well as the variation in terms of marker distance and order.

DNA based quality control of plants

The clonal fidelity and uniformity of the micropropagated plants are a major concern of tissue culture industry as well as of the farmers. The variation within the progeny results in serious losses to the end users, thus making quality control of Tc raised plants mandatory. In view of this, the research programme to ascertain clonal fidelity and to correlate progeny raised to the mother plant in case of the genotype is undertaken. This includes developing fingerprints for the mother plants and clones of the identified plant species using PCR based markers, thus testing quality of the TC raised plants. Apart from seven other plant species analyzed previously, molecular analysis of

Pongamia was completed using ISSR primers to select primers producing best profiles. A test protocol for this analysis standardized for *Pongamia* based on these specific profiles.

Improved profitability and sustainability of sheep production

A systemic effort has been made to enhance the prolificacy of Indian sheep breads. Towards this, DNA samples from four Indian sheep breeds, viz. Garole, Deccani, Bannur and Madras Red were screened by PCR–RFLP to determine the presence of *FecB* mutation in these breeds. The Garole was the only breed, which carried the *FecB* mutation. The *FecB* mutation was introgressed from Garole sheep into Deccani sheep and Bannur sheep, and the performance of the crossbred sheep is being monitored in subsequent generations. Approximately half of the first backcross ewes (progeny of *FecB* heterozygote F1 rams) was found to carry one copy of *FecB* mutation, as expected. The *FecB* PCR– RFLP test was found to be fast, accurate and useful as a tool for making breeding decisions.

Mitochondrial DNA sequence representing a partial sequence of control region and 12S RNA and complete tRNA-Phe (1060bp) of thre Indian sheep breeds viz Deccani represented by two subtypes (Lonand and Sangamneri), Bannur and Garole located in different geological and agro-climatic regions of India were analyzed for genetic variation and for intra specific phylogenetic relationship. These sequences were further compared with four reported European sheep, one Asian (Javanese thin tail) and one wild type (Mouflon) breed sequences. Comparison of all these sequences revealed 71 polymorphic sites with 75 total numbers of mutations and 73 haploytpes. Six haplotypes were shared among the breeds and majority of the other haplotypes were restricted to individual breeds. In case of Indian breeds, the nucleotide and haplotype diversity was the highest in Bannur (0.00355 and 0.981, respectively) and the lowest in Sangamneri (0.00167 and 0.882, respectively). The results of the sequence diversity calculated in terms of the average number of nucleotide differences (D) and average number of nucleotide substitutions per site (K) indicated a high sequence diversity between Asian and European breeds (D = 0.23165, K = 9.498), which was less than the diversity observed between the mtDNA lineage (D = 0.26812, K = 10.9930). The mismatch distribution among the haplotypes revealed two distinct peaks peculiar of the two mtDNA lineages A and B. All Indian sheep clustered together in clade 'A' while most of the European breeds and other Asian breed showed presence of both the haplotypes within the breeds. These results demonstrated that Indian breeds might be ancient compared to the European breeds and the founder population of the Indian breeds might be limited.

Improvement of sugarcane for high sugar yield

Sugarcane is a tropical plant with unusual photosynthetic efficiency and ability to store sucrose in stem cell vacuoles. In certain environments the plant can produce extremely high biomass, which can be used for production of sugar, ethanol for fuel and many other by-products. The ability to store high amount of sucrose, along with high biomass potential makes sugarcane one of the world's most productive agricultural crop. Against a backdrop of annual GDP growth exceeding 5% and a population growth rate around 2% it is essential to increase the sugar yield of sugarcane using modern tools of biotechnology to meet the needs of growing population. Soluble acid invertase (SAI), which catalyzes the hydrolysis of sucrose to glucose and fructose, has been suggested as the key regulator for accumulation of sucrose in sugarcane stem storage parenchyma. High levels of SAI activity in mature stem results in lowered levels of sucrose. The enhancement of sugar yield in sugarcane can be achieved by using SAI gene, in sense and anti-sense orientation to transform sugarcane with the aim at reducing or silencing SAI activity.

A genomic and a cDNA gene clone of the SAI were isolated from sugarcane. Sequence analysis showed >90% homology with other SAI genes at nucleotide level and ~98% homology at amino acid level. Genomic DNA and cDNA clones among themselves show ~98% homology, but there are distinct differences at nucleotide and amino acid levels to suggest that they are different genes. The cDNA gene clone of SAI was cloned in anti-sense and sense orientations in plant transformation vectors for transformation of sugarcane.

1.2.5.3 Host pathogen interactions

Transcript profiling during host-pathogen interactions in chickpea and *F.oxysporum*

Wilt caused by *Fusarium oxysporum* f.sp. *ciceri* (FOC) is an important disease of chickpea leading to heavy losses. Seven races of FOC are known world wide, of which race 1 and 2 are prevalent in central India. Although excellent resistant plant sources are available in chickpea germplasm, success in breeding for FOC-resistance is limited, mainly due to region specific races of FOC and gradual breakdown of resistance in chickpea cultivars. The molecular mechanisms involved are being explored in chickpea-FOC interactions by analyzing root cDNA libraries in established resistant and susceptible cultivars in response to FOC-race 1 (FOCR1).

Resistant and susceptible cultivars, Vijay and JG62, respectively, inoculated with FOC1 were analysed using cDNA-AFLP approach to identify differentially expressed TDFs. These TDFs were further characterized to get full-length clones and sequenced. Homology of these TDFs with the reported database revealed various classes of defense genes. One of these classes was the DNA transposon.

Among these, two transcripts CaFRi12 and CaFRi15 showed homology to non-LTR sequences and CaFRi20 was similar *Ty-copia* like element from *C. arietinum*, respectively. These transcripts were differentially regulated in roots of the resistant infected cultivar, Vijay, though the level of expression in its control was higher than the expression levels in the roots of uninfected and infected susceptible chickpea cultivar. The transcript level of CaFRi12 was high in resistant infected seedling even at 8 day after infection (DAI) as compared to the other two TDFs, CaFRi15 and CaFRi20 all representing the TE like sequences. Many transposons (Tnt1A, Tnt1B, Tnt1C, BARE-1 and Tto1) reported are induced during biotic and abiotic stress. Retroelements have known to be found in resistant gene clusters like the Fusarium wilt resistance locus in melon Fom-2 that contains two retroelement-like sequences and three sequences with similarity to other transposable elements, DNA transposons. Resistance gene clusters in plants conferring race-specific resistance are often large tandem repeats of highly polymorphic genes. Besides the unequal exchange between the different copies, it has been proposed that the high variability needed to evolve new resistance specificities is generated by the transposable element insertions.

Variation in the virulence within the isolates of a given forma specialis has led to the designation of seven pathogenic races of FOC. Management of this disease is done primarily using differential resistant chickpea cultivars. Thus, it is essential to know about the factors responsible for the virulence of FOC races towards chickpea, because the difference in virulence would help in identification of races, which in turn will facilitate the choice of corresponding chickpea cultivar. In the present work we analyzed FOC for the presence of virulence related genes. This involved the use of oligonuleotides designed from conserved regions of virulence genes or metabolically significant genes like *xylanase, Hop78, CLNR* and *Icl*, etc. of different phytopathogenic fungi. Presence of corresponding virulence genes in FOC was analyzed by polymerase chain reaction based approach, wherein the products were cloned, sequenced and characterized. Using these gene specific primers the presence of *Isocitrate lyase, Xylanase, Hop78, Mst12* and *CLNR* in FOC genome was identified.

Expression of such virulence related genes was determined during different stages of FOC-chickpea infection. At the same time expression of these genes was determined using Foc 1 and 2 cDNA when the pathogen was in culture growing on artificial media (in the absence of host plant). Two gene specific primers namely, Mst12 and CLNR showed amplification with 6 DAI samples and onward. The infection stage specific amplification product was cloned and sequenced.

1.2.5.4 Biocontrol / transgenic plants

Winged bean proteinase inhibitor for *H.armigera* resistance

In continuation of our work on wing bean proteinase inhibitors (WBPIs), PIs from a number of species have been screened and it was demonstrated that the pooled PIs from seeds of winged bean, which is a non-host plant of pod borer, inhibit the *Helicoverpa* gut proteinases and pod borer larval growth. Dry mature seeds of winged bean (*Psophocarpus tetragonolobus*) (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 WB. While *WCI2* has previously been identified, *PtCI5* represents a new member of the WCI family. *PtCI5* was exclusively expressed in winged bean seeds, whereas *WCI2* expression was the strongest in seeds but low levels of transcripts could also be detected in leaves, flowers and pod-walls. Predicted proteins of both the genes consisted of a polypeptide chain of 207 amino acids with 86% sequence similarity. The proteins contained four half-cysteine residues and a well-conserved Leu^{65}–Ser^{66} reactive site, typical for chymotrypsin inhibitors. *WCI2* and *PtCI5* were expressed in *Pichia pastoris* and the recombinant proteins were assayed against various proteinases. Both the inhibitors showed complete inhibition of commercially available bovine chymotrypsin. PtCI5 exhibited stronger inhibition of bovine trypsin as compared to WCI2. More importantly, gut proteinases of *H. armigera* larvae that damage many important crop plants were inhibited by WCI2 and PtCI5 to varying levels. Both the chymotrypsin inhibitors showed growth inhibition of *H. armigera* larvae feeding on inhibitor incorporated artificial diets. The results indicate candidature of *WCI2* and *PtCI5* as useful genes in developing transgenic plants to enhance plant defense against *H. armigera*.

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

Tomato (*Lycopersicon esculentum*, cultivar-Dhanashree) proteinase inhibitors (PIs) were tested for their trypsin inhibitory (TI) and *Helicoverpa armigera* gut proteinases inhibitory (HGPI) activity in different organs of the tomato plants. Analysis of TI and HGPI distribution in various parts of the plant showed that flowers accumulated 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. Field observation that *H. armigera* larvae infest leaves and fruits but not the flowers could be at least partially attributed to the protective role-played by the higher levels of PIs in the flower tissue. Tomato PIs inhibited about 50-80% HGP activity of *H. armigera* larvae feeding on various host plants including tomato, of larvae exposed to non-host plant PIs and of various larval instars. Tomato PIs were found to be highly stable to insect proteinases wherein incubation of inhibitor with HGP even for 3 hrs at optimum conditions did not affect inhibitory activity. Bioassay using *H. armigera* larvae fed on artificial diet containing tomato PIs revealed adverse effect on larval growth, pupae development, adult formation and fecundity.

Capsicum proteinase inhibitors and their interaction with insect gut proteinases

Two proteinase inhibitors (PIs), CapA1 and CapA2, were purified from *Capsicum annum* Linn. Var. Phule Jyoti leaves and assessed for their *in vitro* and *in vivo* activity against *Helicoverpa armigera* gut proteinases (HGPs). Both the inhibitors exhibited molecular weights of about 12 kDa with inhibitory activity against bovine trypsin and chymotrypsin indicating presence of probable two-inhibitor repeats of PIN II family. CapA1 and CapA2 inhibited 60–80% HGP (azocaseinolytic) activity of fourth instar larvae feeding on various host plants while 45– 65% inhibition of HGP activity of various instars (II to VI) larvae reared on artificial diet. The partial purification of HGP isoforms, their characterization with synthetic inhibitors and inhibition by *C. annum* PIs revealed that most of the trypsin-like activity (68–91%) of HGPs was sensitive to *C. annum* PIs while 39–85% chymotrypsin-like activity of HGPs was insensitive to these inhibitors. The feeding of *C. annum* leaf extracts and two purified PIs in various doses to *H. armigera* larvae for two successive generations through artificial diet demonstrated their potential in inhibiting larval growth and development, delay in pupation period and dramatic reduction in fecundity and fertility.

Chickpea proteinase inhibitors in defence against *H. armigera*

Chickpea (*Cicer arietinum* L.) seeds contain Bowman–Birk proteinase inhibitors, which are ineffective against the digestive proteinases of larvae of the insect pest *H. armigera*. We have identified and purified a low expressing proteinase inhibitor (PI), distinct from the Bowman–Birk Inhibitors and active against *H. armigera* gut proteinases (HGP), from chickpea seeds. N-terminal sequencing of this HGP inhibitor revealed a sequence homologous to legume Kunitz inhibitors. The identity was confirmed by matrix assisted laser desorption ionization – time of flight analysis of tryptic peptides and DNA sequence coding for the mature protein. Available sequence data showed that this protein forms a distinct phylogenetic cluster with Kunitz inhibitors from *Glycine max*, *Medicago truncatula*, *P. sativum* and *Canavalia lineata*. The isolated coding sequence was cloned into a yeast expression vector and produced as a recombinant protein in *Pichia pastoris*. The recombinant protein did not inhibit chymotrypsin or subtilisin activity but did exhibit stoichiometric inhibition of trypsin, comparable to soybean Kunitz trypsin inhibitor. The recombinant protein exhibited higher inhibition of total HGP activity as compared to soybean kunitz inhibitor, even though it preferentially inhibited HGP-trypsins. *H. armigera* larvae fed on inhibitor-incorporated artificial diet showed significant reduction in average larval weight after 18 days of feeding demonstrating potent antimetabolic activity. The over-expression of this gene in chickpea could act as an endogenous source of resistance to *H. armigera*.

Expression studies of *H. armigera* gut proteinases for the identification of proteinase inhibitor insensitive proteinases

Helicoverpa armigera is one of the severe polyphagous lepidopteran insects, which infest important crops like cotton, chickpea, pigeonpea, etc. Recently it has been reported that this pest has developed an ability to overcome the adverse effects of proteinase inhibitors (PIs), which is being used to produce insect tolerant transgenic crop plants. It has also been reported that this PI overcoming mechanism is mediated by larval gut proteinases.

We investigated the response of *H.armigera* larvae towards ingestion of *Cicer arietinum* Kunitz proteinase inhibitor (CaKPI), which caused antagonistic effects on developing *H. armigera* larvae. CaKPI-degrading proteinases were not detectable in either control or sensitized larvae. There were negligible increases in total proteinase activity, as well as in trypsin-like and chymotrypsin-like activities of *H. armigera* gut proteinases (HGPs). Decrease in sensitivity of HGPs to inhibition by CaKPI was not observed when the inhibitor was fed suggesting that the insect had not shown a specific adaptive response to dietary CaKPI. Semiquantitative reverse transcriptase polymerase chain reaction (Q RT-PCR) analysis showed a general up-regulation of proteases in larvae that ingested CaKPI and a specific regulation of individual transcripts was not observed. CaKPI had maximum inhibitory activity against HGP derived from fourth instar larvae. CaKPI was equally potent in inhibition of HGPs derived from larvae fed on different host plants, as well as various proteinase inhibitors (PIs) to which larval adaptation was previously reported. The lack of larval response to CaKPI was attributable to the atypical active site sequence and inhibitory activity of CaKPI and/or to the pre-adaptation of *H. armigera* larvae due to the constant exposure to basal levels of CaKPI in chickpea seeds or a chickpea seed-based diet. Two serine proteinases from the midgut of *H.armigera* were partially purified and characterized. One proteinase, HGP-1, was capable of hydrolyzing a synthetic substrate of elastase and was inhibited by elastatinal. The second proteinase, HGP-2, was inhibited by a trypsin inhibitor. Molecular weights of HGP-1 and HGP-2 were approximately 26.0 and 29.0 kDa, respectively. Both the proteinases exhibited alkaline pH optima in the range of 10–11. Furthermore, interaction of HGP-1 and HGP-2 with proteinase inhibitors (PIs) from host and non-host plants was studied. HGP-1 was not only insensitive to a PI from chickpea (host) but was also able to degrade it. The same PI from chickpea was able to inhibit over 50% activity of HGP-2. On the contrary, PIs from potato (non-host) showed strong inhibition of both, HGP-1 and HGP-2 and also demonstrated protection of chickpea seed proteins from digestion by both the HGPs. These results could provide important clues in designing strategies for sustainable use of plant PIs in developing insect-tolerant transgenic plants.

1.2.5.5 Secondary metabolites

Biomolecular prospecting of Gaultheria species

Inter simple sequence repeat (ISSR) markers were studied to analyse genetic diversity of an undershrub, *Gaultheria fragrantissima* Wall from two plant diversity hotspots in India, namely Western Ghats (WG) and North-Eastern Himalayas (NE). The plants from these two regions show no morphological differences but the total heterozygosity (H_T = 0.505) is high. Furthermore, the average heterozygosity of *G. fragrantissima* at WG (H_S = 0.433) is higher than that at NE region (Hs = 0.231). Within population variance is higher (15.56%) than among population variance (8.31%) as seen in outcrossing plant species. Mantel's test showed a strong positive correlation between the genetic and geographic distances. The plants within WG show high gene flow, which may be enough to prevent genetic drift, however, the gene flow in NE population is very low.

Essential oil (wintergreen oil) yield and methyl salicylate (MeSA) content of the oil of *G.fragrantissima* from the two biodiversity hotspots in India, NE and WG, sampled during different seasons were studied. A single population of *G. fragrantissima* representing sixteen samples was also studied for its essential oil yield, MeSA content as well as intergenic region of its chloroplast DNA was analysed using PCR-RFLP. The oil yield and content of *G. fragrantissima* was higher with leaf maceration and was similar to that with worldwide used oil of wintergreen from *G. procumbens*. Within India the oil yield and MeSA content was higher for NE plants as compared to WG plants. Significant positive correlation between oil yield and methyl salicylate was observed. Within NE population, no significant variation in oil yield and methyl salicylate content was observed indicating probable influence of macroenvironment of NE region on this trait. Three chlorotypes and four mitotypes were detected within NE population using PCR-RFLP markers. No correlation between oil yield, and methyl salicylate content and haplotypes represented by individual plant was observed.

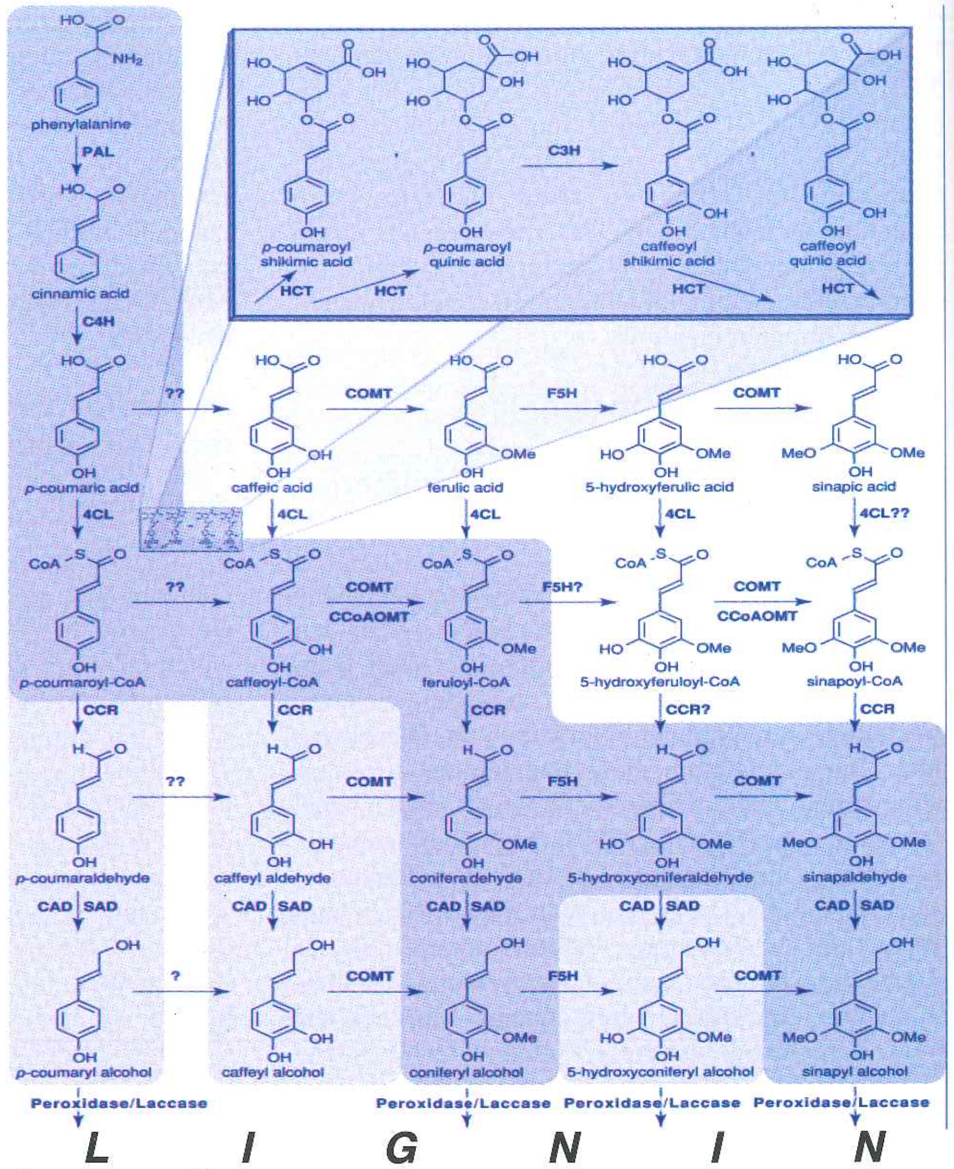
Molecular diversity in flax cultivars and their oil content

The genetic diversity using PCR based ISSR markers among 70 Indian flax (*Linum usitatissimum* L.) cultivars was studied. A total of 12 ISSR primers were used for the analysis yielding 136 loci, of which 87 were polymorphic. The average number of bands and the average number of polymorphic bands per primer were 11.3 and 7.25, respectively. The percent loci polymorphism ranged from 11.1 (UBC 809) to 81.8 (UBC 808) with an average of 63.97% across all the cultivars. The unweighted pair group method with arithmetic mean (UPGMA) was used to cluster the closely related cultivars based on the molecular data and a dendrogram was constructed using the software WINBOOT, based on the similarity matrix. The Jaccard similarity coefficient among the genotypes ranged from 0.20 to 0.97. The above data distinguished flax genotypes in five different groups in the dendrogram. The omega-3-ALA content of the individual cultivar when correlated with the groups formed in the dendrogram, the high ALA containing varieties formed two groups, III and V. This study further established relationship among the genotypes, which is the basis in defining strategies for the breeding programs.

Revealing secrets of mango flavour

Mango (*Mangifera indica* L) is the most popular and nutritionally enriched fruit. There is large diversity of mango varieties existing in India among which a few varieties are popular due to peculiar flavor, colour and pulp quality. Alphonso mango grown in costal belt of Maharashtra is considered as the king of mangoes. It is well known for its flavour and colour throughout the world.

However, the chemical constituents of the flavour as well as the molecular processes involved in the biogenesis of these compounds are poorly understood. We studied volatile composition of 23 different mango cultivars including Alphonso by head space gas chromatography mass spectroscopy. More then 200 different compounds belonging to alcohol, aldehyde, ester and ketone classes were detected. Eighteen cultivars were found to emit unique volatiles. Volatile profile of Alphonso was observed to vary with the process of ripening. In the GC chromatogram, progressive increase in the alcohol peak with progressive decrease in terpenoid peak was observed with the ripening process. In the RT-PCR based approach for targeting the genes involved in the terpenoid biosynthesis, a partial cDNA gene has been cloned, sequenced and annotated broadly as sesquiterpen synthase. A domain of 145 bases of this clone matched in parts with terpene synthase of plants of various genera like *Actinidia*, *Vitis*, *Citrus*, *Gossypium*, etc. Developing fruits of Alphonso mango were further collected from three locations, namely Dapoli, Deogad and Vengurle of the Konkan region along with non flavored variety Subja. Fidelity analysis of these specific plants was carried out using random nuclear markers such as ISSR. These are being used for differential expression of the sesquiterpene synthase gene.



1.2.5.6 Metabolic engineering

Metabolic engineering of the phenylpropanoid pathway in plants

Metabolic engineering the phenylpropanoid metabolic pathway of plants has the potential to order the content and the composition of the plant lignins. A change in the S/G ratio of the plant lignins, for example, would make lignin removal from lingo-cellulose materials easy and environmentally less hazardous. Regulated expression of the caffeoyl CoA-O-methyltransferase (CCoAOMT), caffeyl aldehyde dehydrogenase (CAD), caffeoyl CoA reductase (CCR), coumaryl CoA ligase (4-CL), coniferin β 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.

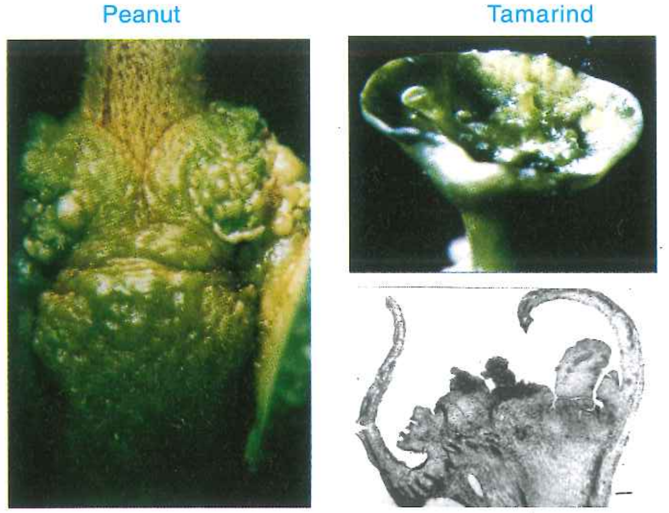
We isolated, sequenced and characterized all the above mentioned major genes of the lignin biosynthesis pathway. The cDNA gene clones have been cloned in antisense orientation in transformation vectors like pCAMBIA and pBINmgfp-5-ER. The vectors have been used to transform *L.leucocephala*. Putative transformants recovered by selection in presence of either hygromycin or kanamycin are being analysed for their lignin content and composition.

1.3 Plant tissue culture

1.3.1 Basic studies

Dual role of thidiazuron on in vitro morphogenesis

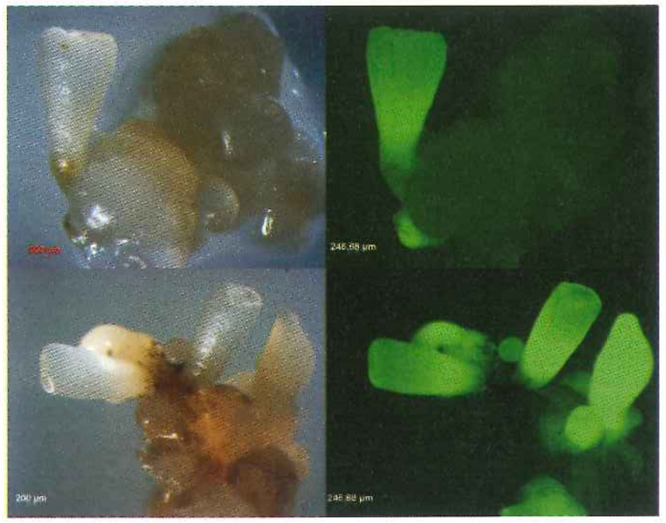
In vitro regeneration of plants using both herbaceous plants and tree species was studied. The effect of higher concentrations of Thidiazuron (TDZ) was demonstrated on the cells of meristems using peanut and tamarind as experimental systems. This has lead to the conclusion that TDZ targets the existing meristem to restrict differentiation and stimulate proliferation of caulogenic buds which differentiate on withdrawal of the inhibition exerted by the growth regulator. TDZ induced meristematic activity spread radially to the neighbouring non-meristematic cells without loosing continuity between the cells. This work revealed the differential roles of TDZ on induction and differentiation of caulogenic buds and provided a tool to study the mechanism of action of TDZ. Involvement of TDZ induced production and release of intermediate chemical transmitter(s) by the morphogenic cells to induce morphogenic activity in the neighbouring cells is now being explored.



Effect of TDZ on meristem cells of peanut (left) and tamarind (right). Proliferation of the cells in the meristems led to formation of caulogenic buds. Differentiation of the buds restricted

Repetitive embryogenesis in peanut system for genetic transformation

Plant transformation requires reliable regeneration protocols. *In vitro* regeneration of peanut from various explants via direct organogenesis and embryogenesis was studied and a lead in the area of peanut tissue culture has been established. The available protocols are extremely reliable and appropriate for both genetic transformation and for morphogenetic studies. These protocols were further refined and conditions for repetitive embryogenesis in Indian cultivars of peanut was achieved. These protocols will be used for developing transgenics.



Peanut embryo transformed with GFP, showing GFP expression in A) Visual light, B) in UV light; Multiple embryos C) in visual light, D) in UV light

1.3.2 Micropropagation for energy plantation

Tissue culture studies for micropropagation and genetic modification of Jatropha (*Jatropha curcas*), Karanj (*Pongamia pinnata*) and oriental cashew (*Semicarpus anacardium*) were carried out.

Keeping in view the contemporary issues on sustainable development of wasteland, production of bio-diesel and important biochemicals from plants the work on three potential plant species was initiated. Seeds of *P. pinnata* (oil 25-30%), and *J. curcas* (oil 31-37%) were identified for production of bio-diesel. *S. anacardium* also produces 25-30% oil. The potential of this plant as a candidate for sustainable development of wasteland is being explored in our laboratory.

All these plants produce oil which needs transesterification for more extensive use as biodiesel. Transesterification is commonly done by hazardous, cost intensive chemical methods. Possibility of producing improved quality oil in the seeds by developing transgenics or mutants needs to be explored. With this objective work is now being carried out in this laboratory to develop protocols for in vitro regeneration of these plants from various organs.


De novo organogenesis in Jatropha curcas


Micropropagation of Pongamia pinnata


Micropropagation of Semicarpus anacardium

In vitro raised plants of *P. pinnata* were supplied to a farmer for field testing. Testing of clonal fidelity among the *in vitro* raised *Pongamia* plants is in progress to confirm the reliability of the protocol for micropropagation.

1.3.3. Wasteland development

Identification of plants for phytoremediation of land degraded due toindustrialization

Under the program sponsored by CSIR for industrial waste minimization and clean-up, efforts are being made to identify the plants growing in the mining dumps and wastelands degraded due to mining activities. The survey showed that the coalmine dumps are often rich in carbon and are appropriate for growing energy plantations. The possibility of growing such plantations is now being explored. On surveying the manganese mine dumps of Gumgaon, near Nagpur it is apparent that some plants have potential to grow in metal contaminated soil without additional amendments. Identification and characterization of these plants are in progress to determine if the ability to withstand metal stress is the characteristic of the species found in the contaminated land or an acquired character or whether the particular plant is a mutant. Experiments are in progress to standardize protocols for clonal propagation of these plants for preservation of germplasm and for molecular characterization.

Mandaman coal mine dump, Dhanbad, Jharkhand (left). A single tree growing in a manganese mine dump, Gumgaon near Nagpur, Maharashtra (right)

Conditions of metal toxicity simulated *in vitro* and various economically important plants are being tested to determine their natural ability to withstand metal stress against chromium, cadmium and copper.

1.3.4 Saffron biotechnology

Saffron is the most exotic, versatile and costliest (Rs. 45,000-50,000 per kg in the domestic market and US $ 2000 per kg in the international market) spice. Saffron of commerce is the dried stigmas of *Crocus sativus* which contains, picrocrocin (a bitter principal), safranal (an odourous compound), and crocin (a colouring matter). Saffron has long been used as a food additive, flavouring agent, traditional medicine for a variety of afflictions, and as a dyestuff for silk and wool. In recent years there is much interest in the cancer chemo-preventive, tumericidal, and antidepressant properties of saffron and its bioactive compounds. The demand for saffron is witnessing a steady increase despite its high price. The high cost is because of: (i) specific agro-climatic requirement for cultivation, and (ii) low yield coupled with labour intensive, manual harvesting.

In the past 15 years, the world saffron production has increased five-fold from 50 to 250 tones. Earlier Spain was the largest saffron producer. Now it is Iran. Though Kashmiri saffron is considered as one of the best in the world, India's contribution has dwindled. Increasing saffron production has great economic potential, both for employment generation and export earnings. By traditional cultivation increasing saffron production is difficult. Biotechnological research in saffron are in three lines: (i) micropropagation and somatic embryogenesis, (ii) *in vitro* proliferation of stigmas, ovaries etc. to produce stigma like structures, and (iii) production of stigma-metabolites in cultured cells and tissues. Micropropagated plants need to be planted in the specific agro-climatic conditions to raise the crop. Stigma like structures (SLS) do not proliferate indefinitely, and their crocin and picrocrocin content is much lower than in natural stigmas.

At NCL, we are studying two approaches to increase saffron production: i) *In vitro* induction of flowering, to produce flowers in culture vessels (from these flowers stigmas can be harvested), and ii) high density greenhouse cultivation. *In vitro* culture can sometimes be a powerful mean for accelerating reproductive development, and maintenance of flowering state. If successful, *in vitro* induction of flowering can free saffron production from the narrow geographical belt, and requirement of specific agro-climatic conditions. Once the different parameters (planting medium, irrigation, fertigation, temperature, light, etc.) for high density greenhouse cultivation are standardized, saffron can be cultivated in places where traditionally saffron cannot be grown.

We have standardized protocol for callus induction and growth from corm explant, corm sprout and shoot regeneration, and micro-corm production in saffron. We could also grow saffron in a greenhouse and induce flowering (nearly coinciding with flowering in Kashmir).

1.4 Biochemical engineering Neera: A traditional palm beverage

Under this program, a new method for collection of *Neera* from palm trees was developed whereby the microbial count present in *Neera* was considerably reduced. Further pilot plants are being planned at two locations, one in 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*

Optimization of growth parameters of useful lactobacilli was studied. Different strains of lactobacilli were investigated for their nutritional requirements and environmental conditions. A variety of commercial nutrients were investigated for their effect on the growth and viability of the cells. The experiments were performed in shake flasks and in laboratory fermentor. Suitable techniques for cell separation were used followed by desiccation to obtain excellent survival of the biomass. The standard operating procedure (SOP) was developed and transferred to the company.

Gibberellic acid fermentation

The work on strain improvement and fermentation optimization of *G.fujikuroi* for production of gibberellic acid was continued under the DBT funded project. Several hundred mutants were selected and screened or GA3 production in shake flasks. Laboratory scale 10 L fermentor with sophisticated control of pH, temperature, dissolved oxygen and feed profile was used in the work to understand the exact role of individual factors on gibberellic acid biosynthesis. Batch, fed-batch, repeated fed-batch and extractive fermentation were performed to maximize the product concentration in the fermented broth using the best mutant obtained through a mutagenesis program. The process of extraction of gibberellic acid patented earlier by NCL was used in the work with further modifications. The recovered gibberellic acid was analyzed by HPLC, NMR, IR techniques for purity and chemical identification and confirms to all the necessary parameters. The process will require further strain improvement to become competitive in the open economy.

Cloning, expression and production of haeme-proteins by yeast

Iron deficiency in the Indian population, especially in the rural community is very high. Anaemia is one of the most common nutritional disorders worldwide because of iron deficiency.

NCL has initiated a multi-institutional project for cloning of the human hemoglobin in *Saccharomyces* (NCCS, Pune) and lactoferrin (NDRI, Karnal) gene in an effective generally regarded as safe (GRAS) yeast expression system that gives high yield of intracellular hemoglobin/ lactoferrin.

NCL plans to optimize the growth and intracellular accumulation of hemoglobin protein in shake flask and 10 L fermentor. This will be followed by purification and recovery of the hemoglobin protein using techniques such as cell disruption, membrane separation, chromatographic separations, etc., for obtaining a food grade dietary supplement with high iron bioavailability.

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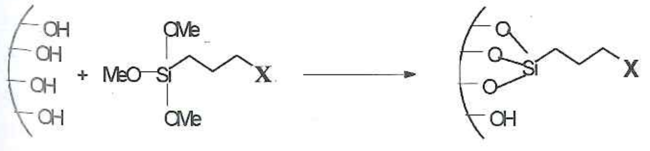
2 CATALYSIS

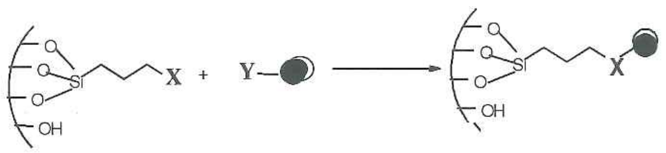
2.1 Novel catalysts

2.1.1 Mesoporous metallosilicates and organic-inorganic hybrid materials

The demand for environmental friendly and efficient technologies has enhanced considerable interest in the use and development of porous solids as catalysts. Among the various methods opted for creating pores, the templating fabrication method created a variety of porous networks with a wide range of pore sizes, well defined morphologies on controllable length scales and various chemical functionalities to match the needs for different applications. Siliceous mesoporous MCM-41, MCM-48, HMS and SBA-15, synthesized by the supramolecular templating approach using alkyl trimethyl ammonium halide (e.g., CTMABr), alkyl amines and block co-polymers (e.g., P123/P103) as the structure directors in basic and acidic conditions, respectively, relies as a novel support surface for the introduction of active metal/ organometallic species (V-MCM-41 (48), Ti-MCM-41, Cr-MCM-41 (48), Co-HMS, V/ SBA-15, etc) because of its variable internal pore diameter, large surface area and abundant silanol sites. Subsequently, the unique features of these mesoporous materials can be well utilized for the synthesis of novel organic-inorganic hybrid mesoporous materials using various organo silanes having active donor sites (-NH_2, -Cl, -SH, -$(PPh_3)_3$, -OH), by *in situ* method or by post synthesis grafting methods, for the heterogenization of various active metal complexes/ chiral metal complexes. Thus the heterogenization of useful homogeneous catalysts over hybrid mesoporous materials having active donor sites finds improved catalytic properties than the conventional amorphous silica supported metal catalysts, due to the periodicity in the pore walls which inturn will inhibit the mass transfer related problems and hence are less prone to deactivation resulting in a higher level of productivity.



X= -Cl, -NH_2, -SH, etc. & Y is a chiral moiety

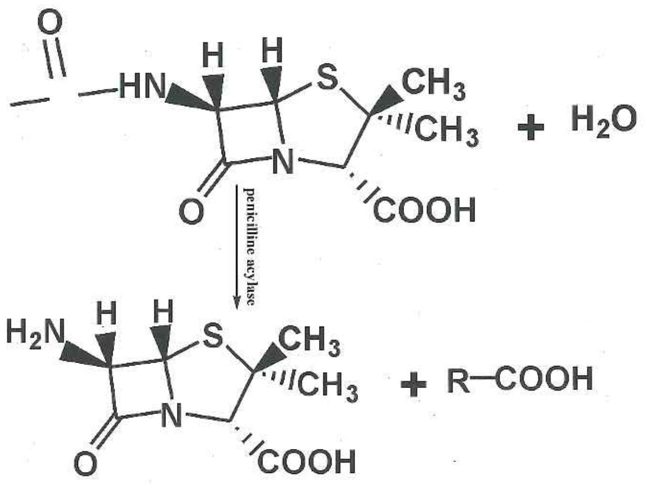


The combination of organic and inorganic fragments inside the structure of porous materials that are self-assembled into architectures with dimensions spanning multiple length scales can give rise to new materials preserving the unique characteristic of both organic and inorganic materials. Periodic mesoporous organosilicas (PMO) having various designed organic groups in the frame wall positions can be synthesized from silsesquioxane precursors having the general formula $(R'O)_3SiRSi(OR')_3$, where R = -$(CH_2)_x$-, -C_6H_5-, -CH=CH-, etc. Various metal containing PMOs (Ti-PMO, V-PMO, Cr-PMO, etc.) were synthesized as efficient heterogeneous catalysts for oxidation and epoxidation reactions. These materials have improved hydrophobicity and their frameworks contain completely uniform distribution of organic groups integrated within the inorganic framework at the molecular level. The materials used in their synthesis are: silica source - bridged silsesquioxanes, $(R'O)_3SiRSi(OR')_3$, where R = -(CH_2)x-, -C_6H_5-, -CH=CH-, and surfactants - cationic or polymeric surfactants.

In a novel approach, mesoporous silica supported molybdenum oxide nanoparticles have been synthesized without using any additional template. These solid materials have shown very high catalytic activity in various acid-catalyzed reactions such as nitration, acylation, and transesterification. Catalyst synthesis was scaled up to one kg batch level.

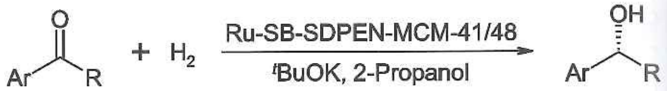
In the course of developing stable mesoporous acid catalysts, Si^{4+} incorporated SBA-15 materials have been synthesized. Tetraethylorthosilicate (TEOS) and $SnCl_4$ (Si/ Sn = 114 – 15) were used as silica and tin precursors. Sn^{4+} was incorporated by the *in situ* synthesis technique using carrinon-ionic surfactants under a slightly higher pH conditions. Location and speciation of Sn^{4+} ions in the silica materials were investigated by XRD and ^{29}Si MAS NMR, Sn-Mössbauer and UV-spectroscopic techniques. Part of the Sn^{4+} ions has tetrahedral coordination while the rest possess octahedral coordination.

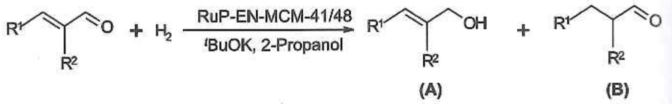
Ordered mesoporous silicas, SBA-15, have been extensively used as a potential support material for enzyme immobilization because of their controllable pore dimensions (20–500 A°), large specific surface area (1000 m^2/g), and highly ordered pore structures. For the first time, penicillin acylase (PA) has been immobilized on APTES functionalized SBA-15 and its catalytic activity was investigated. PAs are important in pharmaceutical industry in the commercial production of semi-synthetic β–lactam antibiotics *via* key intermediates, 6-aminopenicillanic acid (6-APA) and 7-amino-3-deacetoxycephalosporanic acid (7-ADCA). Immobilization enhanced the temperature stability of the enzyme.



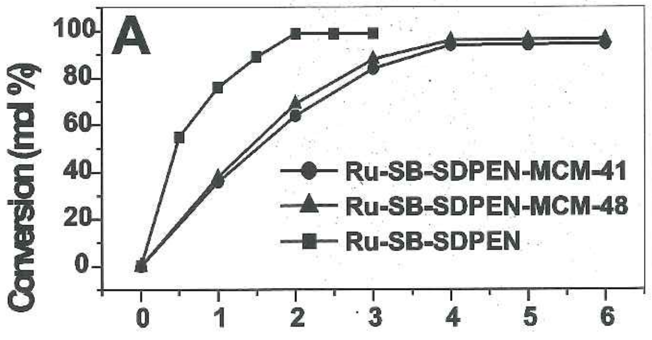
2.1.2 Solid enantio- and chemoselective catalysts

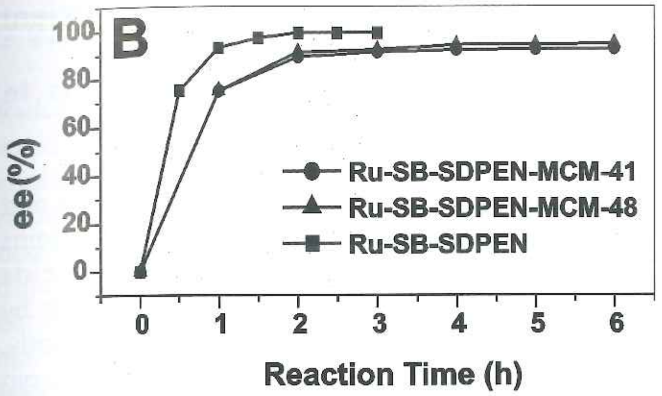
Asymmetric catalysis is the most attractive method for the production of optically pure compounds from the atom economic point of view. Asymmetric heterogeneous catalysis is a vivid branch of catalysis due to its reusability, stability and constraint effects and site isolation in higher selectivity. Mesoporous silica supported binol and salen derived complexes have been designed for the heterogeneous asymmetric organic transformations. An efficient heterogeneous catalyst system for enantio- and chemoselective hydrogenation of α,β unsaturated aldehydes was synthesized, involving anchoring of Ru^{II}-complexes on the inner surfaces of organo-functionalized (propylamine and propylethylenediamine) mesoporous MCM-41, MCM-48 and SBA-15 materials. Powder XRD, SEM and TEM experiments revealed highly ordered hexagonal and cubic patterns of the organically modified MCM-41 and MCM-48 materials, respectively, even after incorporation of Ru-complexes, as supported from FTIR, ^{31}P CP MAS NMR and XPS analyses. This heterogeneous catalyst showed promising activity and enantioselectivity (ee = 95-99%) and chemoselectivity towards hydrogenation of carbonyl groups in prochiral ketones and a,b-unsaturated aldehydes, respectively.



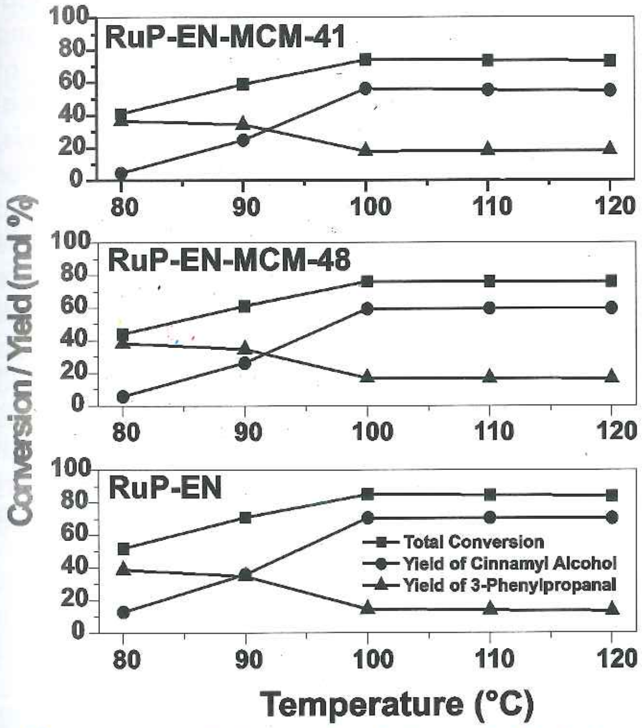


The effects of reaction temperature, reaction time and hydrogen pressure on the activity and selectivity were studied in detail. The anchored solid catalysts could be recycled effectively and reused several times without any loss in activity and selectivity. Although, the initial activity of the same Ru-complex when grafted onto the organically modified surfaces of fumed silica is comparable to corresponding MCM-41/ MCM-48 catalysts, the activity and enantioselectivity and chemoselectivity significantly decreased during recycle of the catalyst due to leaching. However, the Ru-complex-SBA-15 system allowed the preferential hydrogenation of C=O over coexisting conjugated C=C linkages in unsaturated carbonyl compound to give ca. 76%ee.





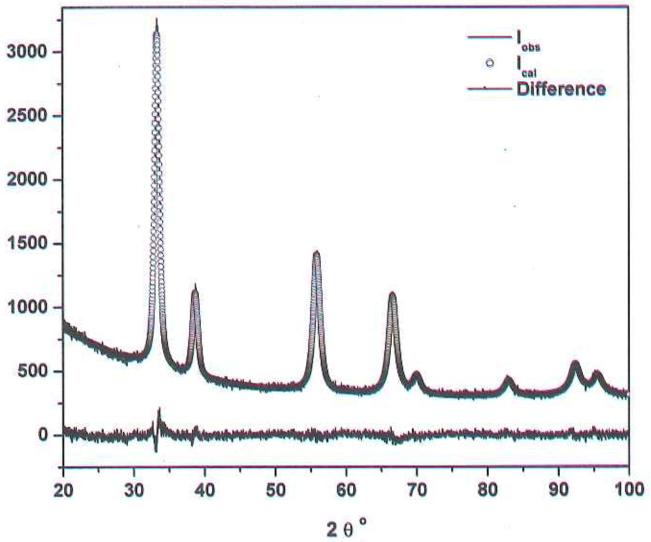
Enatioselective hydrogenation of acetophenone by the Ru-SB-SDPEN-MCM-41, Ru-SB-SDPEN-MCM-48, and homogeneous Ru-SB-SDPEN catalysts. Influence of reaction time over (A) conversion and (B) enantioselectivity.



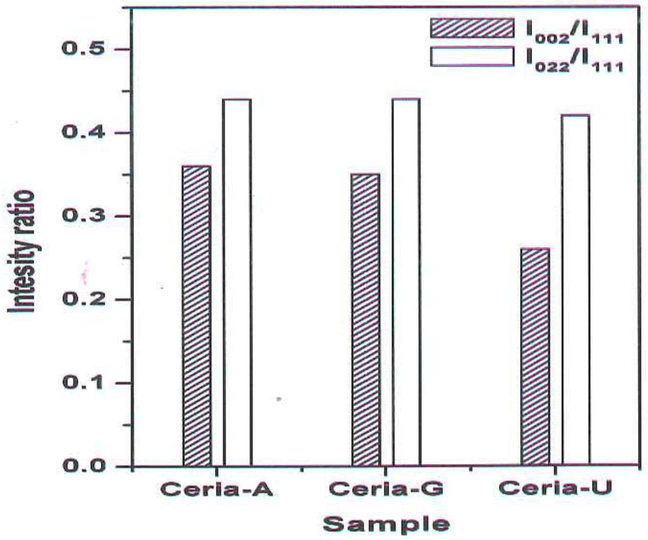
Chemoselective hydrogenation of cinnamal dehyde by RuP-EN-MCM-41, RuP-EN-MCM-48, and homogeneous RuCl2(PPh3)3-ethylenediamine catalysts. Incluencfe of reaction time over conversion and chemoselectivity.

2.1.3 Novel fluorite structures – cerium oxide-based catalysts

The effect of fuel on the nature of manganese species in $Ce_{1-x}Mn_xO_{2-\delta}$ solid solutions synthesized by solution combustion method has been investigated. The results revealed a strong influence of the nature of the fuel and its concentration on the physical and chemical characteristics of Mn/ CeO_2 samples. Nanocrystalline ceria catalysts were prepared by three different methods, viz. alcoholysis route and solution combustion method using glycine and urea as fuels. The method of preparation influenced the size, defect Ce^{3+} ions concentration and hence the catalytic activity for oxidative dehydrogenation of ethylbenzene. Among the three ceria catalysts, the one prepared by alcoholysis method exhibited superior properties than the other two samples.



Rietveld refinement of XRD profile of ceria sample prepared by alcoholysis method



Intensity ratio of (002)/ (111) & (022)/ (111) planes for ceria samples prepared by different methods

Structure-activity correlations indicated that the enhanced activity of ceria sample prepared by alcoholysis method is not only due to its high surface area but an enriched concentration of Ce^{3+} defect sites and preferred exposure of the crystalline planes (022) containing these active defect cerium sites. The on-set temperature for the dehydrogenation of ethylbenzene was found to be as low as 598 K over such a ceria catalyst prepared by the alcoholysis route.

An efficient ceria/ã-alumina nanocomposite prepared by gel-combustion method was found to be highly active at temperatures much lower than reported so far in the ODH of ethylbenzene with a high selectivity towards styrene. The catalyst showed stable activity without deactivation. The overall reaction occurs via Mars-van Krevelen mechanism. The surface Ce^{3+}-O-Ce^{4+} acid-base pair induces the polarization of the hydrogen atoms of ethyl group and the lattice oxide ion is utilized in the dehydogenation of ethylbenzene. The lattice vacancy is subsequently replenished by the effective decomposition of N_2O by this composite catalyst.

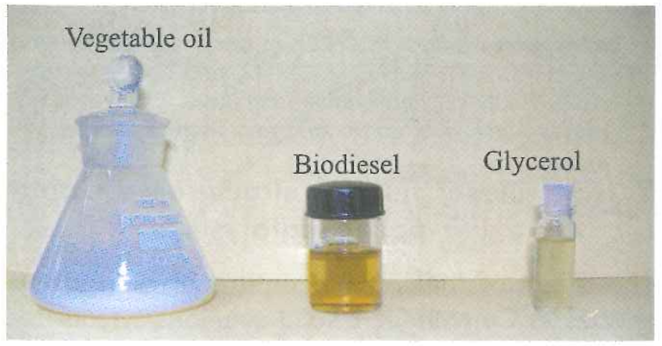
2.1.4 Iron Pillared Clays (Fe-PILC)

Fe-PILC with uniform interlayer basal spacings (1.62–1.76 nm) were successfully prepared with reduced preparation time (20 minutes) by ultrasonication for both Na- and Ca-montmorillonite using the trinuclear Fe (III) acetato complex. The weight loss of the Fe acetato complex takes place in two steps whereas for the pillared clay it takes three steps. Successful pillaring of iron in the pillared clay samples was confirmed by the increase of interlayer distance, higher surface area, the strong FTIR bands of the complex and Fe_2O_3 content determined by XRF. The average pore diameters were in the range of 1.9 to 2.45 nm agreeing fairly well with basal spacings. The proportion of the delaminated structure is found to be smaller in the Fe-PILC sample prepared by ultrasonication compared to the stirring method. The surface acidity in Fe-PILCs is predominantly of Lewis type introduced by iron oxide pillars. The Brÿnsted acid sites were found to be absent. The catalytic activity of these samples is being tested.

2.2 Catalysis – green and efficient catalytic processes

2.2.1 Conversion of vegetable oils to biodiesel and biolubricants

Biodiesel is a biodegradable, cleaner burning and renewable alternative to petrodiesel and contains mono alkyl esters of long chain fatty acids produced from vegetable oils or animal fats by transesterification with lower alcohols. Similarly, biolubricants can be produced when longer chain alcohols (like octanol) are used. Use of non-edible oils containing large excess of free fatty acids (FFAs) as raw material oils leads the biodiesel and biolubricants production cost effective and economical. Additionally, a catalytic process that operates at moderate reaction temperatures and employs efficient solid catalysts instead of conventional homogeneous alkali and mineral acid catalysts are highly desirable. In view of this, novel solid catalysts were prepared. These heterogeneous catalysts are hydrophobic and acidic and transesterify both edible and non-edible vegetable oils with a range of alcohols to produce biodiesel and biolubricants. These solid catalysts are active even in the presence of a large excess of free fatty acids (40 wt% of oil) and water (30 wt% of oil). Another major advantage of this heterogeneous catalytic process is the very high quality of glycerol co-produced (~98%) as compared to the quality of glycerol co-produced in conventional homogeneous route.



2.2.2 DeNOx

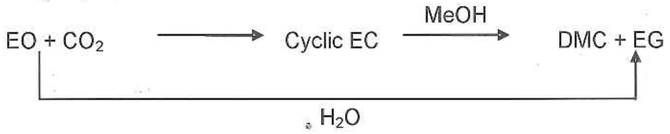
Reduction of NOx from automobile diesel engine exhaust operating under lean conditions is a challenging task for catalysis community. Non-noble metal based catalyst has been synthesized and found to be active for removal of NOx from automobile engine exhaust under lean burn conditions. The catalyst composition is being optimized. After screening of various catalysts for selective catalytic reduction of NOx, Ag/ Al_2O_3 has been proved to be very efficient catalyst for SCR using hydrocarbon. More than 90% NO conversion was obtained at relatively low temperature (340°C). Efforts are in progress to wash-coating coat the catalyst on monolith, to test its catalytic activity and compare the activity with that of the powder catalyst.

2.2.3 Silicon tetrachloride process

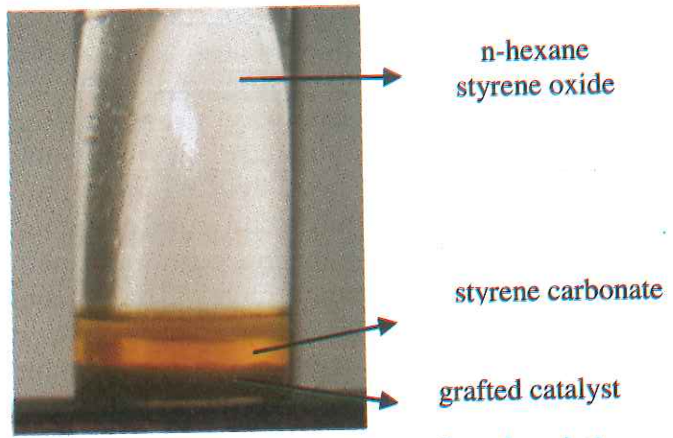
Silicon tetrachloride ($SiCl_4$) is an important compound widely used in semiconductors and optical fiber manufacture. It is also used as a basic raw material in many specialty polymers and paints. A multinational company (MNC) entrusted NCL to suggest and demonstrate a process for the production of high purity silicon tetrachloride at lower cost ($ 0.49/lb) for its use in special paint manufacture. A process for low cost production of silicon tetrachloride was suggested to MNC, which was accepted for further development. A pilot plant of 1 kg per hour of silicon tetrachloride was designed, fabricated, installed and operated successfully. The process demonstrated to MNC met the cost as well as the purity targets. The MNC is planning to set up a commercial plant for the production of silicon tetrachloride and NCL is involved in the design of the commercial plant.

2.2.4 Synthesis of cyclic carbonates and dimethyl carbonate utilizing CO_2

Production of cyclic carbonate precursors of polycarbonates from CO_2 and epoxides is an efficient approach for CO_2 utilization. This approach has already been put to practice and cyclic carbonates are being manufactured in large quantities. The synthesis of dimethyl carbonates (DMC) from methanol and CO_2 (instead of the conventional carbonylation route) is challenging. Towards this goal, several solid catalysts have been designed and catalyst evaluation is in progress. Transesterification of cyclic carbonates with methanol yields DMC. Glycol is co-generated along with DMC in this process. Two types of solid catalysts – (a) double metal cyanides and (b) simple oxide-based catalysts have been developed for this transformation. These catalysts were highly efficient. DMC yields of more than 85 mol% were obtained over the oxide-based catalyst in the transesterificaiton of ethylene carbonate with methanol at ambient temperatures. The process has been scaled up to 50 g catalyst loading. In a fixed-bed reaction, the catalyst was found stable up to 60 h with no loss in activity. Solid double metal cyanide catalysts were efficient even to transesterify propylene carbonate with a variety of alcohols producing different dialkyl carbonates in high yields.



Carboxylation of styrene oxide (SO) to styrene carbonate was investigated. 1-(tri-ethoxy-silyl-propyl)-3-methyl imidazolium chloride, an immobilized ionic liquid on SiO_2, was used as a catalyst. Effects of various reaction parameters like solvent, temperature, and catalyst loading effects etc. on the yield and selectivity of styrene carbonate were investigated. The activities of immobilized ionic liquids are compared with that of unsupported ionic liquids as well as classical ionic liquids. It has been shown that immobilized ionic liquids performed equally well to that of classical ionic liquids like butyl methyl imidazolium chloride and octyl imidazolium chloride. The activities of immobilized ionic liquids were also compared to that of ionic liquid on silica prepared by incipient wetness method and with pure silica gel, which was used as support. Leaching of the catalyst occurred in the case of ionic liquid on silica prepared by incipient wetness whereas pure silica gel did not give any activity. With n-hexane as a solvent, reaction mixture was triphasic in nature, upper n-hexane layer, middle viscous product layer and bottom solid catalyst layer. With this catalyst, styrene carbonate was produced with 99.5% selectivity and 99% yield in 4hr under mild reaction conditions. Above all, n-hexane system has its own advantage of easy product separation and solvent recovery. Catalyst could be easily recovered by filtration and reused by single washing with acetonitrile without any major loss of activity.



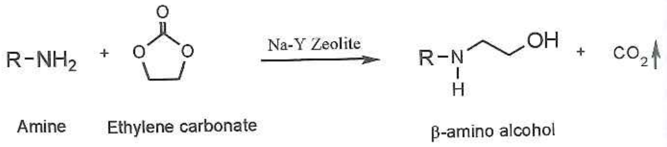
Reaction mixture showing separation of product, reactant and catalyst

2.2.5 Utilization of organic carbonates as reagents in chemicals synthesis

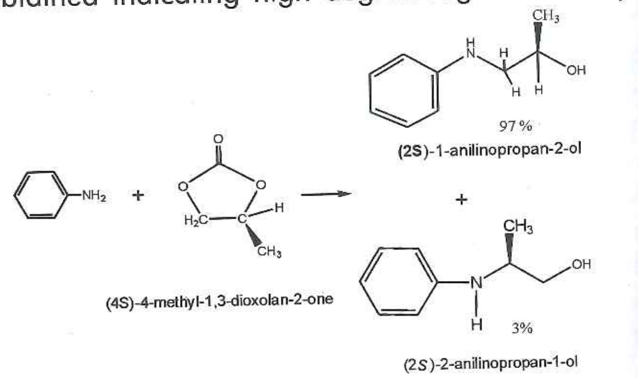
Dimethyl carbonate (DMC) enjoys the status of being a clean reagent for making industrially useful compounds. As an example, carbamates, N-alkylated amines and β-amino alcohols can be synthesized by eco-friendly methods using DMC. NCL has developed solid base catalysts for the synthesis of these chemicals by reacting substituted ureas with carbonates.

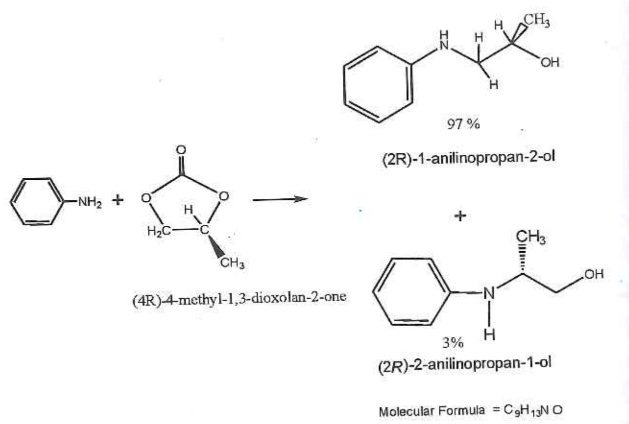
2.2.5.1 Synthesis of β-amino alcohols from alkylene carbonates

β-Amino alcohols find applications in medicinal chemistry in the preparation of biologically active natural and synthetic products, artificial amino acids and chiral auxiliaries for asymmetric synthesis. They are also useful as intermediates in the synthesis of perfumes, dyes, photo developers, and oxazolidones useful in biological field. The synthesis of β-amino alcohols from alkylene carbonates and anilines is attractive due to non-hazardous nature of alkylene carbonates over alkylene oxides used as starting material in conventional production. The drawback of the conventional methodology is that it involves handling of potentially hazardous alkylene oxides and often the catalysts used are corrosive and expensive. Alkylation employing an alkylene carbonate does not require the high-pressure equipment often necessary when working with the highly volatile oxiranes. A simple, efficient and environmentally benign methodology for the synthesis of β-amino alcohols (100 % yield) from aromatic amines and alkylene carbonates in the presence of highly active solid base catalysts like Na-Y and Na-X zeolites has been completed.



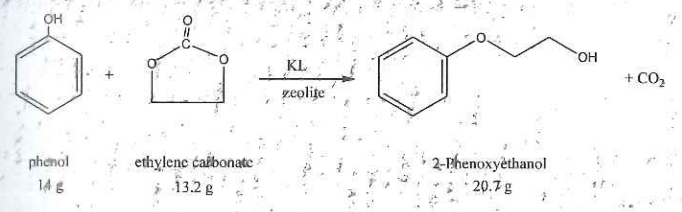
The effect of process parameter on the synthesis of N-phenyl ethanolamine (NPEA) from aniline and ethylene carbonate has been investigated. The reactivity study of various cyclic carbonates towards β-amino alcohol formation has been explored. The catalyst Na-Y has been found to be the most suitable catalyst for this reaction based on its reusability (up to five recycles without any loss in catalytic activity). Experiments were carried out using chiral propylene carbonates (pure S and R) to synthesize chiral amino alcohols. It was observed that under experimental conditions the chirality is preserved and 97% of 2S-1-anilinopropan-2-ol or 2R-1-anilinopropan-2-ol is obtained indicating high degree regio-selectivity.





2.2.5.2 Synthesis of ethylene glycol mono phenyl ethers from ethylene carbonate

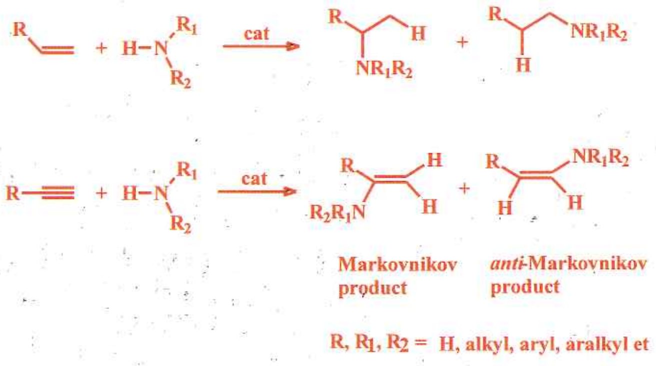
Aryl alkyl ethers, especially aryl methyl ethers are valuable intermediates for the preparation of dyes, agrochemicals, fragrances and pesticides. They are conventionally synthesized by O-methylation of the corresponding phenols with dimethyl sulfate or methyl halides. However, these methods require not only corrosive and toxic reagents but also require stoichiometric amount of strong base to neutralize acidic by-products, which results in large quantities of inorganic salts that require disposal. This philosophy has been extended for synthesis of ethylene glycol mono phenyl ethers from cyclic carbonates such as ethylene carbonate and phenols. The methodology allows one to retain alcohol functionality in the product during O-alkylation reaction.



Glycol ethers are conventionally manufactured by reaction of phenols with ethylene oxide. This route is hazardous and dangerous since ethylene oxide is highly carcinogenic and needs to be handled under pressure. Their wide range of hydrophilic and hydrophobic nature put them in the category of important fine chemicals and specialty solvents. o-Methylation of phenols with methanol in the presence of a strong acid catalyst or a heterogeneous catalyst in vapor-phase at high temperature has been extensively studied. In most of these reactions, the conversions of phenols are not satisfactory and the selectivity to aryl methyl ethers is complicated by C-methylation. The route developed in this study utilizes highly active, selective and recyclable zeolite catalyst. In a typical reaction between phenol and ethylene carbonate, ethylene glycol mono phenyl ether is produced in quantitative yields. Several substituted phenols including bisphenol-A (2,2-bis-(4-hydroxyphenyl) propane) were screened and the yields obtained were nearly quantitative.

2.2.6 Hydroamination reactions

The direct addition of amines to carbon-carbon double and triple bonds known as hydroamination offers the most attractive route to prepare numerous classes of organo-nitrogen molecules such as alkylated amines, enamines and imines. Eco-friendly and cost effective heterogeneous catalysts, which include transition metal ions exchanged on solid supports like clay and mesoporous materials, were designed for intra and intermolecular hydroamination of activated and inactivated alkenes and alkynes.

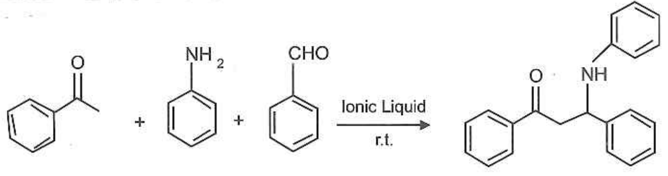


2.2.7 Alkylation reactions

Heteropoly acids (HPAs) of Keggin structures are anionic metal cluster compounds having the molecular formula $XM_{12}O_{40}$, where, X is a central tetrahedrally coordinated metal atom connecting to 12 peripherial octahedrally coordinated "M" metal atoms. Keggin structure of HPAs demonstrates activity as both acid and redox catalysts. A detailed investigations on the thermal and hydrothermal stability of HPAs like phosphotungstic acid (PTA), molybdophosphoric acid (MPA) and silicotungstic acid (STA) using zirconia and titania supports as well as mixed oxides with mesoporous silica (MCM-41, MCM-48 and SBA-15) have been carried out. HPAs were found to be highly dispersed in nano sizes over oxide supports and provided excellent acidic properties and improved activities and product selectivities in an industrially important alkylation, acylation and esterification reactions, e.g., esterification isoamyl alcohol by acetic acid to isoamyl acetate under milder conditions.

2.2.8 Mannich reaction in Brönsted acidicionic liquid: A facile synthesis of β-amino carbonyl compounds

Brönsted acidic ionic liquid containing nucleophile 1-methylimidazole and triphenylphosphine with 1,4-butane sultone and inorganic anions *p*-toluenesulfonic acid (PTSA) and trifluoroacetic acid (TFA) catalyzed Mannich reaction smoothly to afford β-amino carbonyl compounds in excellent yield and less time. Effect of addition of water on the product yield and effect of anions and cations of the ionic liquid on the reaction rate have been investigated. The ionic liquid was easily separated from the reaction mixture by water extraction and was recycled four times without any loss in activity. An efficient process for a simple and fast reaction of different aldehydes, ketones and amines (Mannich reaction) to afford corresponding β-amino carbonyl compounds is demonstrated. The reaction proceeded very fast with high yield. of the desired Mannich base using catalytic amount of ionic liquid.

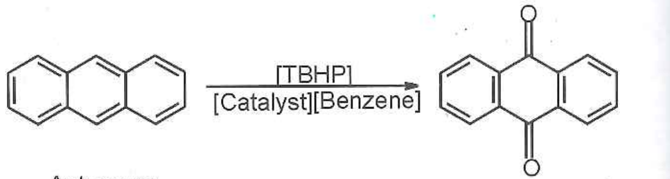


2.2.9 Chemoselective aerial oxidation of terpenic compounds

Terpenes and their oxyfunctionalized products are important perfumery chemicals and fine-chemical intermediates. Selective oxidation of terpenic compounds mainly to a particular desired compound has been a challenging task. The conventional methods of preparation give lower selectivity and generate chemical waste. Oxidation by molecular oxygen instead of peroxides, PhIO, $KHSO_5$, etc is an important step in developing eco-friendly, cleaner catalytic processes. Towards this goal, organo-functionalized mesoporous SBA-15 materials and immobilized Mn complexes have been designed. By Mukaiyama-type oxidation reaction using molecular oxygen these catalysts are found to be efficient in chemo-, regio- and stereo-selective oxidation of terpene compounds.

2.2.10 Selective oxidation of aromatic hydrocarbons

Polyoxometalates are unique class of materials, which posses both acidic and tunable redox properties. In recent years, there has been a great interest in heterogenizing these materials using mesoporous silica supports by surface modification for improving their catalytic performances in oxidation of aromatic substrates such as limonene and anthracene. Keeping in mind the above hypothesis, we are trying to develop inorganic – organic hybrid materials based on polyoxometalates, which could be used as catalysts under milder conditions and easily recyclable like heterogeneous catalysts. Another field of interest is coordination polymers, which we are working on the development of new coordination polymers using metals like tungsten, molybdenum and vanadium which could be efficient catalyst systems for oxidation reactions.



Antracene

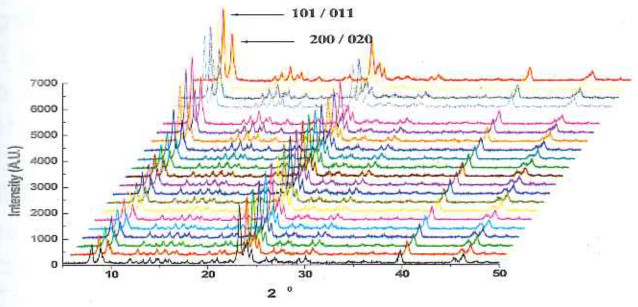
9,10 - Anthraquinone

2.3 Mechanistic investigations – in situ characterization

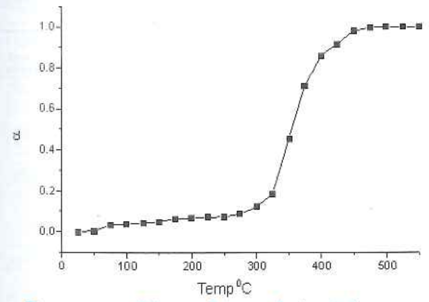
2.3.1 High temperature X-ray diffraction

2.3.1.1 Studies on template decomposition in microporous molecular sieves

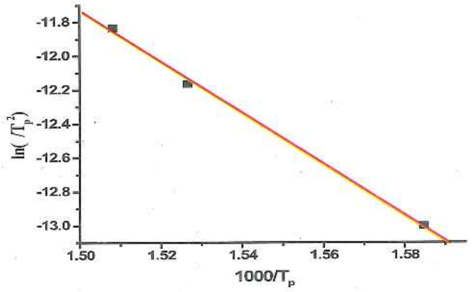
Molecular sieves are used in the preparation of the membranes due to their ability to separate various gases from the mixtures where other separation methods fail. For making the defect (crack)-free membranes of the molecular sieves one should know the mechanism of template decomposition. In situ High Temperature X-ray Diffraction (HTXRD) technique was used to study template decomposition in silicalite-1, FeS-1, TS-1 having MFI structure. Different heating rates have been employed to investigate the non-isothermal reaction kinetics for template decomposition and apparent activation energy. Non-isothermal calcinations of the molecular sieves have been carried out to know the order of reaction, activation energy for the process of template decomposition and changes in the lattice after calcination at different heating rates. The changes in the intensities of the 101/ 011 and the 200/ 020 reflections during in situ calcinations have been followed to study the kinetics of the reaction. Determination of activation energy of template decomposition using Kissinger method and Flynn-Wall-Ozawa method yielded values agreeing with literature. Template decomposition was found to be a bi-dimensional diffusion reaction, which may be due to the interaction of zeolites framework with the template molecules or may be due to the crystallographic orientation of two types of TPA molecules in the channel system of the MFI structure.



HTXRD patterns ofTPA-Silicalite-1 scanned at a heating rate of 1ÚC/min



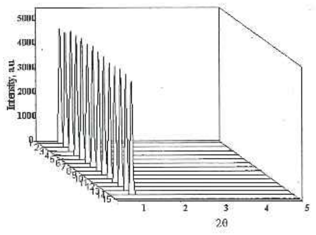
Decomposition of template (α) as a function of temperature



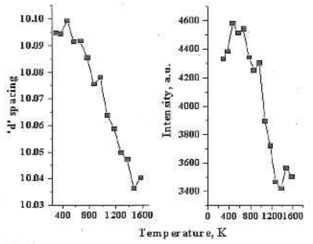
Plot of ln (β/T_p^2) versus $1/T_p$ according to Kissinger method

2.3.1.2 Thermal stability of mesoporous metallo silicate molecular sieves

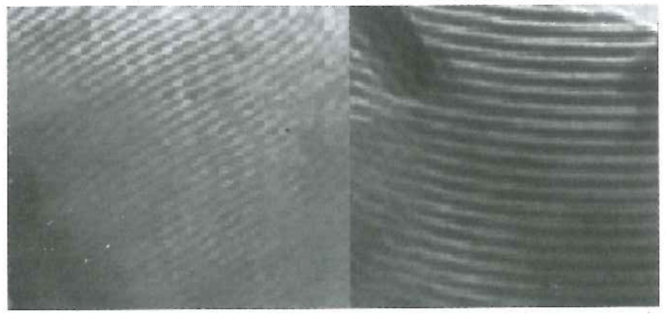
The thermal stability of mesoporous SBA-15 and SnSBA-15 material and the effect of isomorphous substitution of Sn on the thermal expansion behavior were investigated by HTXRD analysis for the first time in literature. The high angle region of the XRD profile of SBA-15 sample indicates the appearance of α-Cristobalite phase at 1473 K and increases further with increase in temperature but at the same time the 100 reflection at low angle was intact. Significant lattice shrinkage is observed with a marked decrease in *d* spacing upon gradual increase in temperature. The decomposition behavior of template ions located within the pores is strongly influenced by the presence of Sn in the framework and a 'soft' interaction probably exists between the template ions and the Sn sites. α-Cristobalite phase does not form even at 1473 K in Sn-SBA samples. TEM of the Sn-SBA after HTXRD scans shows the existence of hexagonal array in the material, which is supported from the presence of 100 reflection even at 1473K.



HTXRD patterns of SBA-15 sample in the range 298-1623 K



Change in interplanar distance d and intensity as a function of temperature of SBA-15



TEM of SnSBA samples after HTXRD scan

2.3.2 Powder XRD

2.3.2.1 Phase composition studies in highly disorder materials using DIFFaX routine

The phase composition of the different polymorphs of zeolite beta was determined by Rietveld refinement studies. Broadening in the reflections of the observed patterns is due to the heavy faulting /disorder in the material. The structural parameters were not refined, due to the disorder inherent to the beta samples and hence simulation of the powder patterns was carried out using the DIFFAX routine. Phase composition is derived using the simulated patterns for the random intergrowths of polymorph A and B by DIFFaX routine. Integrating the diffraction intensities layer-by-layer resulted in the simulation of the XRD pattern. By changing the layer composition or the stacking sequence, it was possible to build in different types of disorder into the lattice and compute the changes in the pattern. During the simulation of powder pattern using DIFFaX, only the stacking probabilities of the different layers were changed while using the standard stacking vectors. The stacking direction c' is perpendicular to the a' b' plane of the layer. The compositional data on the different polymorphs A, B and C obtained by both Rietveld refinement and DIFFAX were slightly different.

2.3.2.2. Structure-Activity correlations in moVAlOx catalysts

To understand the structure-activity correlations using powder XRD in MoVAlOx type catalysts used for selective oxidation of ethane to produce ethylene and acetic acid selectively, detailed XRD analysis of the samples prepared at different pH was carried out. Catalysts of general formula MoVAlOx prepared at different pH conditions showed pH dependant elemental compositions. From powder XRD and other spectroscopic studies, the high activity at PH = 2 was attributed to the presence of MoV_2O_8 and other reduced species like Mo_4O_{11} phases supported on MoO_3. Although presence of any amorphous phase is not clear at present, presence of V and Mo ions in partially reduced form, as confirmed by other techniques, plays a crucial role in the selective oxidation of ethane.

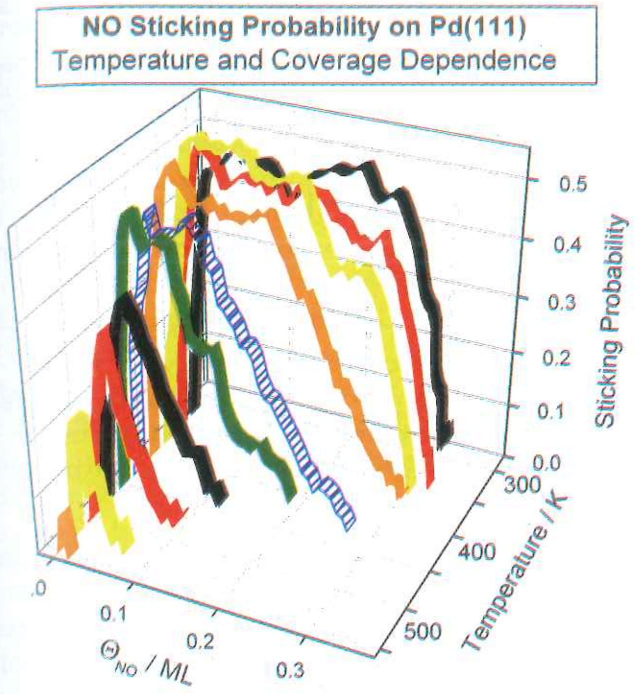
2.3.3 In situ spectroscopic characterization

In situ spectroscopic characterization techniques help to understand the interaction of adsorbed surface species on catalysts and highlight the chemical and orientation changes of the adsorbate, short-lived intermediates and surface complexes that are formed during the reaction.

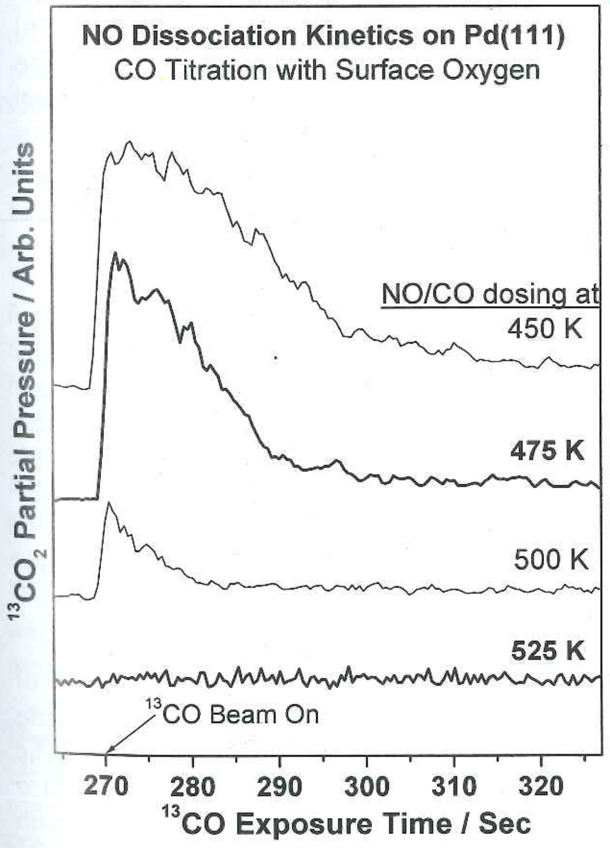
2.3.3.1 Adsorption studies using molecular beam instrument

A molecular beam instrument (MBI) developed at NCL is a unique tool to study the fundamental phenomenon such as adsorption, competitive adsorption etc. and transient and steady-state reaction kinetics of catalytic reactions in an ultra-high vacuum environment. MBI was employed to study the kinetics and mechanistic aspects of reactions occurring in automotive catalytic converters (fitted in all automobile units), especially on nitric oxide (NO) reduction under technically relevant conditions on palladium (Pd) surfaces. Sticking probability of NO on Pd surface determined as a function of temperature and NO-coverage is shown in figure. It is also interesting to note that oxygen, a product of NO dissociation disappears from the surface but diffuses/ moves into the bulk of Pd above 475 K due to high oxygen solubility in Pd. A systematic research might enable to take advantage of this fact to use Pd-based catalyst under technically relevant oxygen-rich conditions to convert NO into innocuous nitrogen.

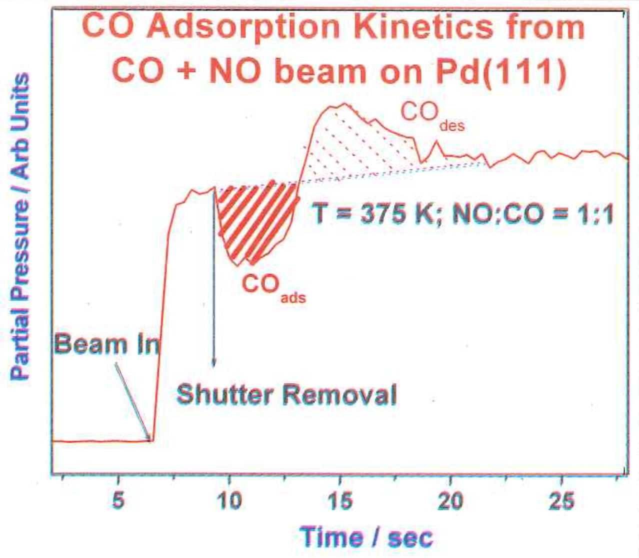
A competitive NO adsorption from NO+CO beams and hence a displacement of adsorbed carbon monoxide (CO) by incoming NO could be observed and it highlights the importance of the MBI method for catalysis research. Details given in figure are the amount of CO adsorbed initially, CO desorbed subsequently, difference between both of them and the amount of NO adsorbed. The major interest in this work is the actual composition of surface coverage of adsorbed components is entirely different from the composition of NO + CO mixture. The actual surface coverage decides the course of the reaction and the specific information on surface coverage of different species could be determined from the above method.

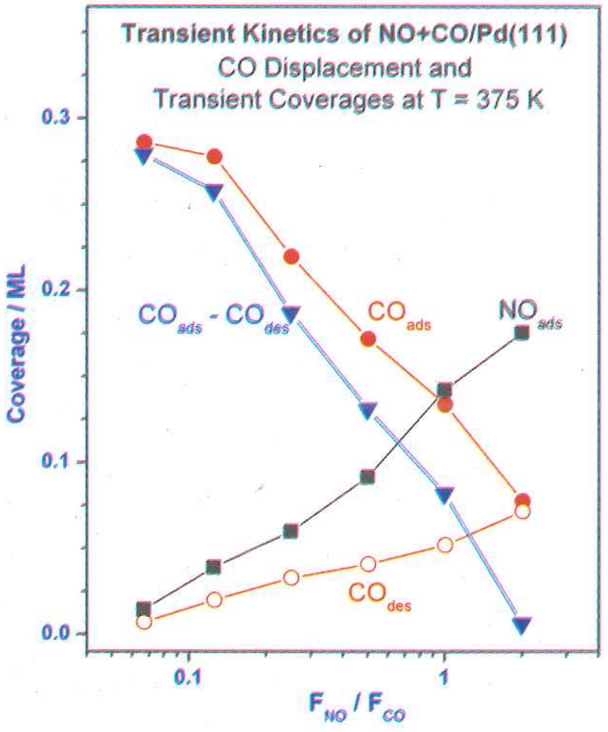


Temperature dependence of coverage (Θ_{NO}) and sticking probability calculated from the nitric oxide uptake data



Surface oxygen due to NO dissociation on Pd(111) was measured by oxidizing ^{13}CO beam to $^{13}CO_2$ at the same NO adsorption temperatures





The coverage of NO and CO in the transient state on NO+CO /Pd(111) system at 375 K. NO_{ads}, CO_{ads} and CO_{des} corresponds to the coverage of NO, CO immediately after shutter removal and coverage of desorbed CO, respectively

2.4 Engineering studies in hydrogenation reactions

2.4.1 Hydrogenation of butynediol

Hydrogenation of 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 (olefinic diol) and butane-1,4-diol (saturated diol). Therefore, a catalyst and a continuous process in a fixed bed reactor was developed for the hydrogenation of B_3D to give 2-butene-1,4-diol (B_2D) and butane-1,4-diol (B_1D) without formation of any other side products. 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. Further, a mathematical model for reactor performance was also developed based on the kinetic data obtained previously in a batch slurry reactor. The predicted values of conversion, selectivity and rate of hydrogenation were found to agree with the experimental data over a wide range of conditions.

2.4.2 Hydrogenation of meta-dinitrobenzene

Another important hydrogenation reaction investigated was the hydrogenation of m-dinitro benzene (DNB) to m-phenylene diamine (MPD), which proceeds via formation of m-nitro aniline. MPD is an important raw material for the synthesis of aramid fibers, which find applications in interiors of aircrafts where high temperature resistance and high tensile strength is needed. In this process, the hydrogenation of the intermediate nitroaniline to MPD is difficult due to the presence of nitro group in meta position which deactivates the benzene ring. NCL has developed a novel bimetallic Ni-Pt catalyst supported on carbon which gave very high turn-over frequency numbers and almost complete selectivity to m-phenylene diamine in m-dinitrobenzene hydrogenation as compared to the monometallic nickel catalysts. The XRD and XPS characterization revealed that most of the nickel remains as Ni^{+2} in a monometallic catalyst while, the addition of platinum leads to the stabilization of Ni^0 state, in case of bimetallic catalysts.

2.4.3 Organo-catalysis

The work in the area of organocatalysis was started recently in which diastereoselective synthesis of 2-amino-1,3,5-hexane triols was achieved with *de* > 95% using L-proline catalyzed Aldol reaction. The de was established by high resolution proton and ^{13}C NMR.

In case of catalysis in supercritical carbon dioxide medium, it was found that enhanced hydrogen solubility and a dramatic change of adsorption characteristics of the catalysts in supercritical carbon dioxide influence the activity and selectivity pattern of hydrogenation of various functional groups. The most important among these was selective hydrogenation of naphthalene to *cis*-decalin which is being considered as an ideal organic hydride for hydrogen storage for the application of fuel cell. This work was carried out jointly with National Institute of Advanced Industrial Science and Technology, Japan.

Pilot Plant for *p*-aminophenol

A know-how for p-aminophenol (PAP, a starting material for paracetamol) has been successfully transferred to an industry. Based on NCL process, a pilot plant erection will be completed at the client's site. A commercial process of 10,000 TPA for PAP will be operational within 2 years period.

Vinyl esters by transvinylation of vinyl acetate and carboxylic acids

The project was undertaken with an objective of development of a catalytic process for vinyl laurate for M/s Transmetal Ltd, Vadodara. The catalytic process was standardized and demonstrated at a 60g vinyl laurate scale, in a 300 ml reactor, with catalyst recycle. Scale up of the process to a two liter rector (~ 400g vinyl laurate) is in progress.

2.4.4 Hydroformylation

The program has been initiated to investigate the reaction kinetics of hydroformylation of olefins in a biphasic non-aqueous ionic liquid -organic medium. Synthesis of numerous ionic liquids (IL) and correlation of their structure with the activity etc in hydroformylation will also be investigated. A new method for the synthesis of halide free water soluble ILs has been developed and ILs like $BMIMBF_4$ and $BuPyBF_4$ have been synthesized. The applicability of these ILs as reaction media in rhodium complex catalyzed hydroformylation of olefins has been demonstrated. Hydroformylation of octene and decene in the water immiscible ILs- $BMIMPF_6$ and $BuPyPF_6$ has also been standardized using Rh complex catalysts.

Heterogenization of the water soluble Rh-TPPTS hydroformylation catalyst has been achieved by ossification and demonstrated for the hydroformylation of higher olefins in high selectivity. A new method for heterogenization of metal complex catalysts by precipitation of its water-soluble analogue as a Group 2 metals (Ca, Sr or Ba) salt on porous supports has been proposed. This technique yields a highly dispersed catalyst having a significantly higher activity (TOF) for hydroformylation of olefins compared to other known heterogenized catalysts. The catalyst can be recycled with ease.

The role of Lewis acids in enhancing the activity of Pd catalysts in Heck reactions has been investigated. Significant enhancement in the rate of Heck reactions has been achieved when catalytic amount of Lewis acid (like $FeCl_3$) promoters in the presence of trace amounts of water (>2000 ppm) are used along with Pd complex catalysts. Experiments with different aryl halides, bases as well as olefins have been carried out to demonstrate the role of Lewis acid promoters. The increase in the reaction rates is due to the weakening of Ar-X bond by the Lewis acid in the manner similar to Friedel- Crafts reaction.

The kinetics of vinylation of 4′ -bromo acetophenone (4′ -BAP) with n-butyl acrylate (n-BA) has been studied using palladacycle catalyst, in the presence of sodium acetate (NaOAc) as a base and tetrabutylammonium bromide (TBAB) as a promoter in N-methyl 2-pyrrolidinone (NMP) solvent. The rate was found to be first order with respect to 4′ -BAP, fractional order with the catalyst, and first order tending to zero order with NaOAc concentration. The rates passed through maxima with variation of TBAB and n-butyl acrylate concentrations. The rate data have been analyzed to propose an empirical model which is in good agreement with the mechanism already established for Heck reactions using Palladacycle catalyst.

Development of catalysts for the chemo selective hydrogenation of benzoic acid selectively to cyclohexane carboxylic acid or cyclohexyl methanol or benzyl alcohol has been achieved with more than 95% selectivity to the desired products.

2.4.5 Heck reactions in bi-phasic conditions

Biphasic - glycol-organic system has been developed for the Heck reaction of olefins with a $PdCl_2$(bipy) catalyst. This catalyst is soluble in glycol media and has been demonstrated for the Heck coupling of numerous substrates in the presence of organic and inorganic bases. The catalysts has also been recycled a number of times with no drop in the activity. The major advantage of this system is that it utilizes a conventional organic phase soluble ligand to achieve biphasic catalysis unlike typical biphasic systems which rely on ligands with hydrophilic moieties like sulfonates, phosphates etc. to ensure solubility in the aqueous phase.

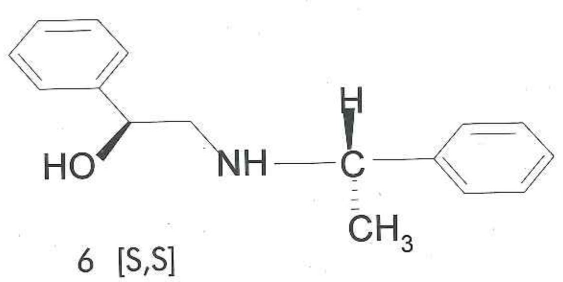
Kinetics of the Heck coupling of styrene with iodobenzene using the $PdCl_2$-bipyridine complex was studied over a temp range of 393-413 K in a biphasic (organic-glycol) medium. An empirical rate model has been proposed to fit the observed data. This is the first time that kinetic modeling has been attempted for the Heck reaction in a biphasic medium.

Water-soluble catalysts have been developed for the Heck coupling of olefins with aryl halides in aqueous media. In general it has been observed that biphasic Heck reactions are conducted in aqueous glycol or similar systems, wherein the objective is to use water present in the catalyst phase. In this work the catalyst phase is totally aqueous and hence a proper biphasic aqueous – organic system has been demonstrated. The catalysts are stable and can be recycled number of times without any deactivation or precipitation.

2.4.6 Chiral auxilliaries and asymmetric synthesis

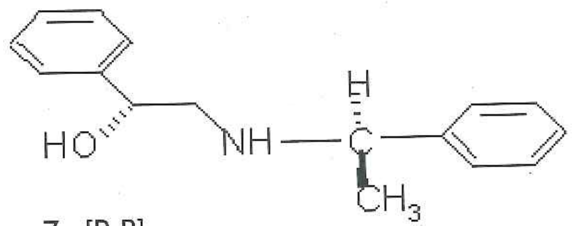
Two new ligands were prepared by condensation of S-mandelic acid and phenethyl amine derivatives. Structures and single crystal X-ray structures of the ligands are as follows:

Transfer hydrogenation of acetophenone has been carried out using these ligands and $[Ru(Benzene)Cl_2]_2$, $[Ru(p\text{-}Cy)Cl_2]_2$, $[Ir(Cp^*)Cl_2]_2$, $[Rh(Cp^*)Cl_2]_2$ as catalyst precursors. The results obtained are presented in the table:

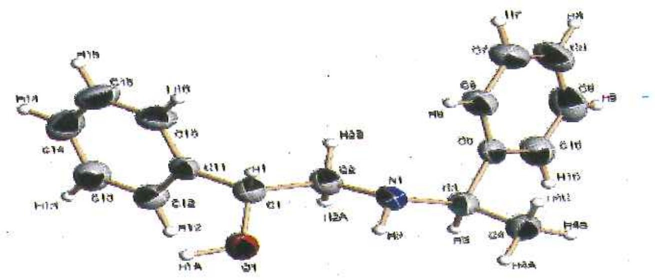


6 [S,S]

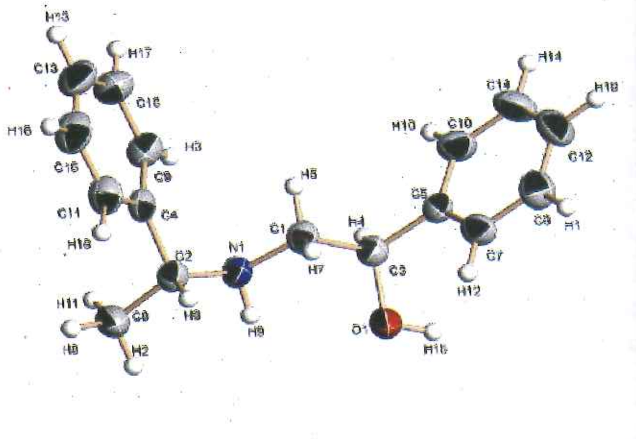
Transfer hydrogenation of various ketones such as 4-isobutyl acetophenone, 6-methoxy-2-acetyl naphthalene, substituted acetophenone derivatives have been carried out and good conversion and ee in a range of 50 to 75% have been obtained. Thus the ligands prepared are good for asymmetric transfer hydrogenation of various ketone derivatives. Further work on asymmetric transfer hydrogenation is in progress.



7 [R,R]



(S,S) α-[(1-phenylethyl)amino]methyl]-benzenemethanol



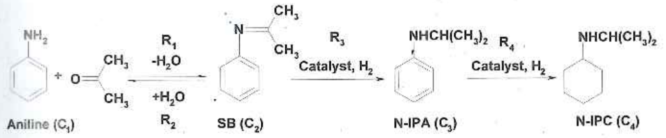
(R,R) α-[(1-phenylethyl)amino]methyl] benzenemethanol

Sr. No.	Catalyst used	(S,S) α-[(1-phenylethyl)amino]methyl]-benzenemethanol		(R,R) α-[(1-phenylethyl)amino]methyl]-benzenemethanol	
		Conversion (%)	ee (%)	Conversion (%)	ee (%)
1	$[Ru(benz)Cl_2]_2$	92	50 (S)	93	50 (R)
2	$[Ru(p\text{-}cymene)Cl_2$	91	76 (S)	91	76 (R)
3	$[Ir(Cp^*)a]_2$	56	60 (S)	55	63 (R)
4	$[Rh(Cp^*)Cl_2]_2$	95	79 (S)	95	79 (R)

2.5 Reaction engineering of multiphase reactions

2.5.1 Reductive alkylation of aniline with acetone using Pd/Al_2O_3 catalyst: kinetic modeling and trickle bed reactor studies

N-alkyl anilines are important products for the dyes, fuels and rubber industries and are synthesized by the reductive alkylation of aromatic amines and carbonyl compounds in the presence of supported transition metal catalysts. The first step in the synthesis is a non-catalytic homogeneous reaction, followed by hydrogenation in the second step to the desired N-alkylated product. But, after formation of N-alkyl aniline (N-IPA), hydrogenation of the aromatic ring can occur to give N-alkyl cyclohexylamine (N-IPC), which is of lesser importance than the former. The reaction scheme for reductive alkylation of aniline with acetone is shown below:



Experiments were carried out to understand the reaction engineering issues like the role of mass transfer parameters and reaction kinetics, which is important to select suitable reaction conditions to obtain improved selectivity of the intermediate product, N-IPA.

The experiments were carried out in a stirred slurry reactor under isothermal conditions in a temperature range of 378 to 408 K. Experimental data on concentration-time as well as hydrogen consumption-time profiles were obtained to study the effect of concentration of aniline, catalyst loading and partial pressure of hydrogen. Separate controlled experiments were performed to understand the nature of the condensation reaction between aniline and acetone, which forms the Schiff's base (SB) intermediate. It was observed that the Schiff's base formation was neither influenced by the presence of hydrogen nor the catalyst used.

From the concentration-time profiles and the effect of reaction conditions, it was found that the non-catalytic equilibrium formation of the Schiff's base intermediate was the slowest step in the multistep reaction sequence. Several rate equations were considered to fit the batch slurry reactor data and a rate models (Eq. 1 and 2 below) based on competitive dissociative adsorption of hydrogen followed by reaction with the liquid phase substrates as rate limiting catalytic steps was found to represent the experimental data satisfactorily. The kinetic parameters were evaluated by fitting the integral batch reactor data at different temperatures.

$$R_1 = k_1C_1 - k_2C_2(C_0 - C_1) \quad \text{for equilibrium reaction} \quad (1)$$

$$R_i = \frac{k_i w C_i (A^*)^{1/2}}{(1 + K_H (A^*)^{1/2} + \sum_{i=2,3} K_i C_i)} \quad \text{for catalytic steps} \quad (2)$$

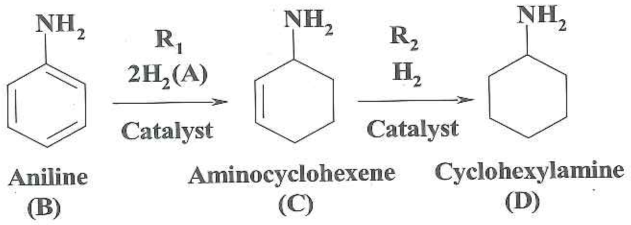
where, R_1 and R_i were the rate of equilibrium and i-th catalytic steps respectively, kmol/m^3/s . C_0 was the initial concentration of aniline, kmol/m^3. C_i represented the concentration of i-th species, kmol/m^3.

Further, reductive alkylation of aniline with acetone was also investigated in a trickle bed reactor. Based on the intrinsic kinetics, a theoretical model for trickle bed reactor was derived. A model considering partial wetting and stagnant liquid holdup, as was used to develop the trickle bed reactor model, which also incorporated the effect of external and internal mass transfer. Experimental data were collected in a 0.3 m length and 1.5×10^{-3} m inner diameter trickle bed reactor with a concurrent down flow of gas and liquid at different inlet concentrations of aniline (0.55-2.2 kmol/m^3), inlet temperatures (37-408K) and liquid flow rates (0.8×10^{-4}-7×10^{-4} m/s). The results on conversion of aniline, selectivity of all the products, global rate of hydrogenation and temperature change in the inlet, middle and exit of the reactor were observed. The experimental results were compared with predictions by the theoretical model, which showed a very good agreement. This study revealed that partial wetting of catalyst particles (under lower liquid velocity) and intra particle diffusion effects were significant under trickle bed conditions.

2.5.2 Analysis of a gas-liquid-liquid-solid catalytic reaction: Kinetics and modeling of a semi batch slurry reactor

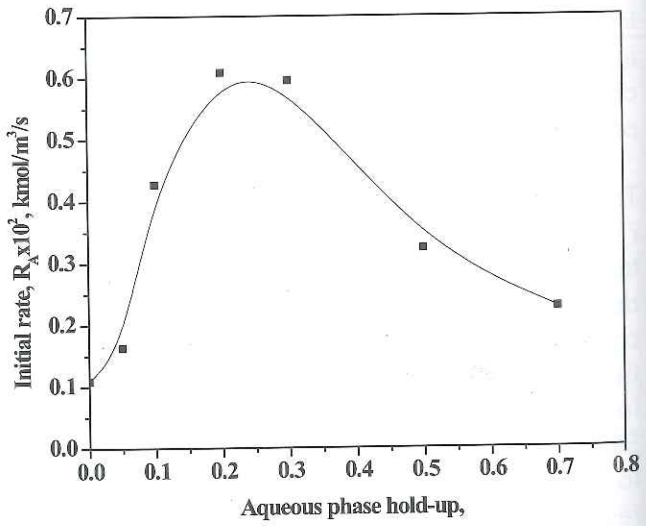
Four phase reactions (gas-liquid-liquid-solid) are advantageous in many cases with respect to the corresponding three phase catalytic reactions. But the issues like phase behavior, mass transfer of the reactant and product molecules, swelling or shrinking of a particular phase during the course of a reaction and their effects on overall reactor performance and phase behavior are not well studied. Therefore, a detailed kinetic model and importance of mass transfer parameters for hydrogenation of aniline in presence of Ru/Al_2O_3 catalyst in a gas-liquid-liquid-solid four-phase system was studied.

The Ru/Al_2O_3 catalyst was synthesized by a precipitation technique and characterized by XRD, TEM and ICP-OES. XRD results showed that the ruthenium metal exists in hexagonal close pack (hcp) crystal structure. The hcp structure is believed to make ruthenium a suitable catalyst for aromatic ring hydrogenation where as other common transition metals (such as Pd, Pt, Ni, Rh, Co, Ni) exist in the face centered cubic (fcc) structure and hence are not suitable for this reaction. Therefore, Ru/Al_2O_3 catalyst was used for ring hydrogenation of several aromatic substrates in three phase (gas-liquid-solid) and four phase (gas-liquid-liquid-solid) systems. It was observed that the four phase system showed better activity, selectivity and stability for all the studied substrates with respect to the corresponding three phase system. Due to the hydrophilic nature of alumina (Al_2O_3), the Ru/Al_2O_3 catalyst remained in the aqueous phase and hence the four phase system also provided an easy separation of the catalyst from the product. Among the studied reactions, hydrogenation of aniline to cyclohexylamine was chosen as the model reaction system for a detail study. The reaction scheme is shown below:



The intrinsic kinetics of aniline to cyclohexylamine in a gas-liquid-liquid-solid system was studied in a 3×10^{-4} m^3 slurry reactor in a temperature range of 378-418 K. Aniline in cyclohexane and water constituted two immiscible liquid phases in the four phase reactions. All the reactions were carried out keeping aqueous phase and total volume of liquid as constant. Experimental data on concentration-time as well as hydrogen consumption-time profiles were obtained to study the effect of concentration of aniline, catalyst loading and partial pressure of hydrogen. A detailed analysis of gas-liquid, liquid-liquid, liquid-solid and intraparticle mass transfer was carried out using initial rate data to ensure the kinetic regime. Based on these data, several rate equations were evaluated. A rate model considering adsorption of hydrogen on the catalyst surface followed by reaction with the liquid phase components as the rate-limiting step was found to give the best fitting of the experimental concentration-time as well as the hydrogen consumption-time data.

When the aqueous phase hold-up was changed keeping the total liquid volume constant, it was observed that the initial rate of hydrogenation passes through a maxima.



Effect of aqueous phase hold-up on initial rate of hydrogenation for hydrogenation of aniline in a four phase system using 2% Ru/Al_2O_3

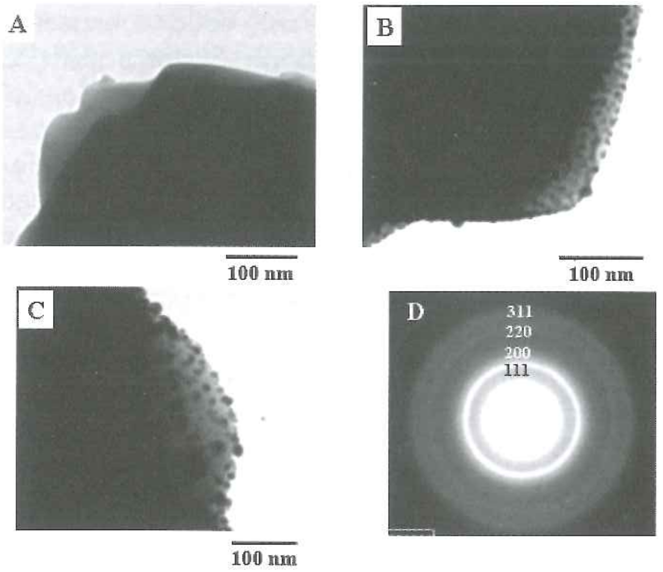
Reaction conditions: aniline, 0.1 kmol; catalyst (2% Ru/Al_2O_3), 0.6×10^{-3} kg; $P_{H2,}$ 4.8 MPa; temperature, 398K; total liquid volume, 100×10^{-6} m^3.

As the aqueous hold up increased, interfacial area of water and organic phase changed and hence contribution of mass transfer steps changed. Also, the organic phase holdup decreases passing through a phase inversion. Therefore, two independent models, considering aqueous and organic phases as the continuous phases, were developed to explain the holdup effect.

2.5.3 Pt and Pd nanoparticles immobilized on amine-functionalized zeolite: catalytic applications for hydrogenation and Heck reactions

Among the various new concepts, catalysis by metal nanoparticles received immense interest to the researchers because of its potential in achieving higher catalytic activity. At the same time, agglomeration at higher reaction temperature, separation and reuse of metal nanoparticles from the reaction systems are considered as the major challenges for their practical applications.

Amine groups bind very strongly to platinum and palladium nanoparticles. Therefore, an attempt was made to entrap aqueous platinum and palladium nanoparticles on the surface of micron-sized zeolite particles functionalized with amine groups. Platinum and palladium nanoparticles bound at high surface coverage on 3-aminopropyltrimethoxysilane (APTS)-functionalized Na-Y zeolites were found to be the excellent heterogeneous catalysts ([Pt]-APTS-Y and [Pd]-APTS-Y) for hydrogenation and Heck reactions. A detailed characterization by UV-VIS., FTIR, TGA, XRD, XPS and TEM has been done to understand the exact nature of the nanocomposites. It was observed from FTIR and TGA that the platinum and palladium metal nano particles were immobilized due to the amine functionality of the zeolite surface modifier. XRD results ensured that zeolite structure was not affected during the synthesis steps. [Pt]-APTS-Y and [Pd]-APTS-Y showed very good catalytic activity for hydrogenation (both Pt and Pd) and Heck coupling (Pd) reactions. XPS was used as an important tool to confirm the active species for these two important classes of reactions. TEM images of the fresh and used catalysts indeed showed that the platinum and palladium nanoparticles supported on amine-functionalized zeolite remain unchanged at the end of the reactions.



Representative TEM images (A-C) of amine-functionalized zeolite, [Pt]-APTS-Y before reaction and [Pt]-APTS-Y after reaction respectively on a carbon-coated TEM grid. Selected area diffraction (SAED) pattern (D) recorded from the platinum nanoparticles shown in B. The diffraction rings have been indexed.

The rates of hydrogenation and Heck reactions over these catalysts were found to be much higher than those obtained using conventionally prepared catalysts. Thus, a simple protocol for synthesis of heterogenized Pt and Pd nanoparticles as truly heterogeneous catalysts for hydrogenation and Heck reaction has been established.

2.5.4 Catalytic carbonylation reaction of various substituted olefins and alcohol derivatives

Catalytic carbonylation reaction of various substituted olefins and alcohol derivatives leads to commercially important non-steroidal anti-inflammatory agents. While Suzuki coupling reactions lead to the synthesis of fine chemical and pharmaceutical intermediates. Synthesis of various catalytically active organometallic complexes for these reactions was undertaken, with special emphasis to palladium complexes. Detailed catalytic studies with respect to activity and selectivity issues were pursued. Catalyst-product separation and effective catalyst reuse are being studied whereby numerous immobilization techniques have been practiced and expertise attained, with novel findings. Systems such as aqueous biphasic catalysis, supported metal complex catalysis, supported liquid phase catalysis, anchored and encapsulated complex catalysis on various porous matrices have been studied. Characterization of these immobilized catalysts have been perfected with the use of analytical tools as solid state CP-MAS NMR, XPS, powder XRD, AAS, TG-DTA, SEM, TEM, FT-IR etc. to prove the integrity of the catalysts beyond ambiguity. Catalysis kinetics studies involving previously mentioned catalyst systems are also subjects of investigation. Very recently, a novel and facile methodology have been developed for immobilization of the complex catalysts by transformation of the soluble complex to its inherently insoluble counterpart. A new terminology 'Ossification' has been coined for the method. Palladium complexes thus immobilized were shown to have excellent performance for both the reactions.

2.5.5 Esterification of acetic acid with methanol

A detailed study on the ion exchange resin (Dowex 50W) catalyzed esterification of acetic acid with methanol and butanol in a batch slurry reactor was carried out. Since esterification can also occur in the liquid phase, the kinetics of homogeneous non-catalytic esterification was investigated separately to assess its contribution. Experimental study on homogeneous reaction was carried out over a temperature range of 308-328 K. For the heterogeneous catalytic esterification reaction, the effect of various reaction parameters such as temperature, catalyst loading, and catalyst particle size and reactant concentration on the initial rate of reaction was also studied in a temperature range of 308-328 K. These data were used to develop intrinsic kinetics of homogeneous and heterogeneous reactions. A rate model has been developed incorporating the effect of intraparticle diffusion for [1,1] order reversible reaction. The initial rate data were used to determine the significance of liquid-solid and intraparticle mass transfer resistances. For interpretation of the kinetics, the observed concentration-time data were used to estimate the kinetic parameters using a batch reactor model. The model predictions for different operating conditions are compared with experimental data.

2.5.6 Esterification of maleic acid with methanol

The esterification of maleic acid with methanol, a multi-step reaction was investigated in a batch slurry reactor. The kinetics of homogeneous esterification was investigated separately to assess its contribution. For the heterogeneous catalytic reaction, the ion exchange resin with a smaller particle size (0.46 µm) was used where the intraparticle diffusion resistances were negligible. The effects of temperature, methanol concentration, catalyst loading, and particle size were investigated to evaluate the intraparticle diffusion resistance. For interpretation of the kinetics, the observed concentration-time data were used and the rate parameters were evaluated at each temperature using a batch reactor model.

The esterification of maleic acid with methanol was also carried out in trickle bed reactor using ion exchange resin as catalyst. A simple homogeneous model has been developed to predict the performance of the reactor. Experimental data were obtained over a wide range of operating conditions and compared with model predictions. The agreement between the model predictions and experimental data was very good.

2.6 Desulfurization of diesel

High content of sulfur in diesel fuel is one of the main causes of automobile pollution. E.U. countries have mandated sulfur reduction to 30 - 50 ppm from the year 2005. It is likely that diesel containing 50ppm sulfur will have to be produced in India in the near future. Typically, sulfur-removal from diesel fraction is carried out by

hydrodesulfurization (HDS) over Co-Mo-(Ni-Mo-)-sulfidealumina catalysts at high pressures (> 30 bars) and temperatures (>30°C). Last few hundred ppm of sulfur compounds in diesel are dialkyl dibenzothiophene compounds and are difficult to desulfurize. Moreover, the desulfurization of diesel by catalytic HDS is expensive due to severe conditions of operations to destroy the dibenzothiophenes that constitute the major sulfur-compounds of diesel at this sulfur-level.

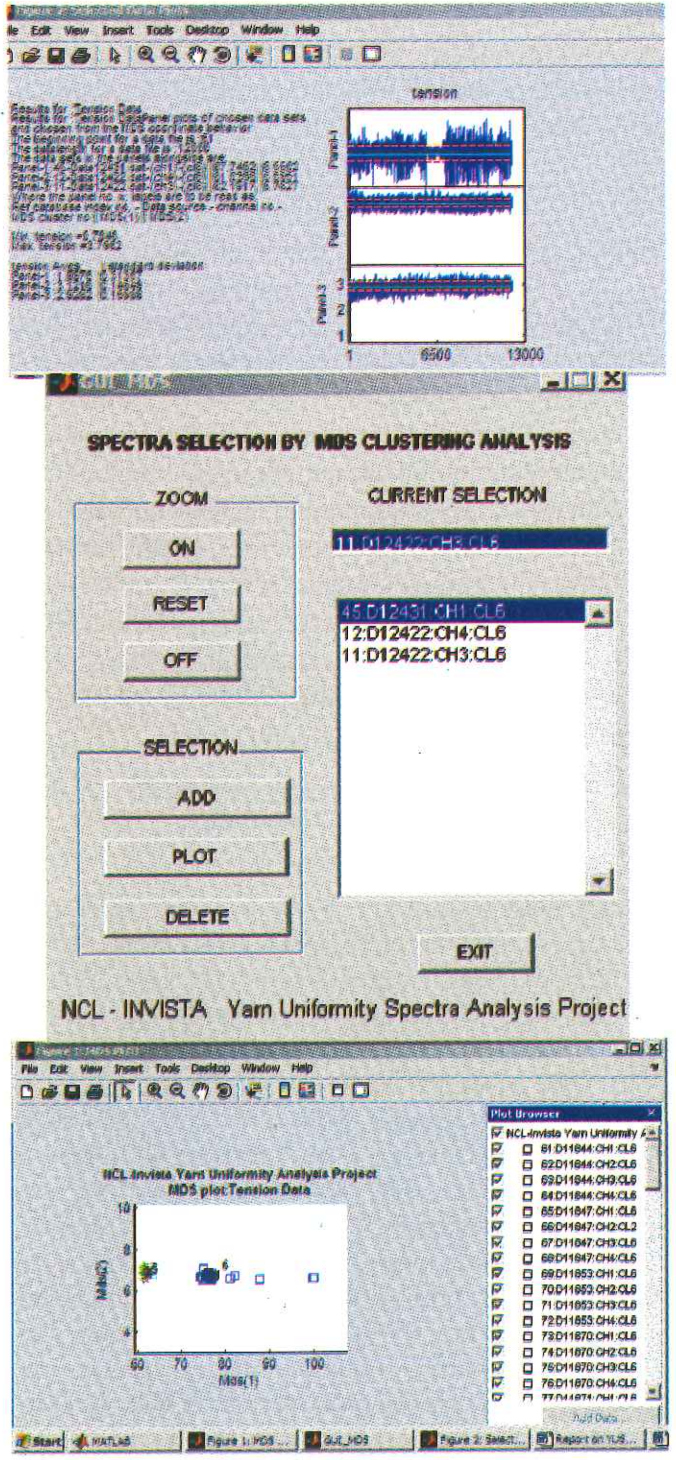
The alternate approach is the oxidation of sulfur-compounds and adsorptive removal of the oxidized products. The advantage of this approach stems from the slightly greater electron density of the 5- atom in alkyl-substituted dibenzothiophenes making them more prone to oxidation. Thus, the *reactivity* under oxidation conditions of the above mentioned typical sulfur-compounds is expected to be: 4,6-dimethyl dibenzothiophene > 4-methyl dibenzothiophene > dibenzothiophene. Thus, selective catalytic oxidation (oxidative desulfurization, ODS) of sulfur-compounds offers an economically attractive alternate process for the desulfurization of diesel to less than 10 ppm sulfur. The economic attractiveness arises mainly from the very mild process conditions (30 - 80°C; atmospheric pressure) used in ODS compared to catalytic hydrodesulfurization (300 - 340°C; 20 - 50 atmospheric pressure).

Novel solid oxidation catalysts based on mesoporous oxides were prepared and evaluated in the oxidation of three model sulfur-compounds that are typically present in diesel fractions. Two catalysts based on V and Ti showed promising results in that the difference in the rate of oxidation of the three compounds is not as large as observed over hydrodesulfurization catalysts. Another exceptionally good catalyst is a HPA based catalyst. This catalyst possesses an activity order for the three model sulfur-compounds (DBT, 4-MDBT and 4,6-DMDBT) that is reverse of that observed over HDS catalysts. Moreover, the catalyst is also more active than the other catalysts. Similarly, the homogeneous catalysts based on polyoxometallate complexes are also substantially efficient when decalin is used as the solvent. As diesel is a mixture of aromatic, aliphatic and naphthenic compounds and is more polar than cetane, it is likely that these complexes will also perform well in desulfurizing diesel fractions. The studies point out significant possibilities in ODS of diesel fractions to very low sulfur-levels.

3. CHEMICAL ENGINEERING SCIENCE

3.1 Modeling and simulation studies with applications

3.1.1 Yarn uniformity spectra analyzer (YUSA)



Snapshot of the Yarn Uniformity Analyzer (YUSA)

A project was sponsored by Invista Inc. (USA) for analysis of historical data collected from its yarn spinning plants. The company wished to analyze the data obtained over batches because an understanding of the variability in the data could lead to improved quality control and fault detection.

Gigabytes of data were transferred to NCL and the project entailed creating new algorithms that could search and recognize patterns in the dynamically monitored plant performance data over batches and within batches. The aim was to link up disparate batches, taken even widely apart in dates and months, so that similar faults occurring in different batches can be automatically recognized. The algorithms developed at NCL using multidimensional scaling, wavelet transforms and clustering analyses were found to be extremely successful in pattern recognition and fault detection from data. In fact, software modules along with a graphical user interface (GUI) were used to develop a user friendly package that could be installed online in the production process. The package built completely at NCL has been tested on-site in the yarn production plants of Invista, Waynesboro, USA. The results obtained have now made it easier for plant data analyzers and operators to take suitable corrective actions for increased productivity by the accurate diagnosis of the operating behavior of their yarn producing plants.

3.1.2 Knowledge incorporated SVM formalisms for process fault detection

Invariant support vector machines (SVM) are used in the present work by incorporating the knowledge of invariance in process engineering datasets to improve the classification performance. Tennessee Eastman Process, a benchmark chemical engineering problem, was studied for this purpose from the fault detection perspective. This knowledge of invariance is particularly useful for process engineering applications wherein one finds that the class membership has wide ranges in terms of their attribute values and one can safely assume that it will not change after small local transformations. The results obtained on binary as well as multiple fault detection have shown substantial improvements in terms of correctly classifying the faults. In case of multiple faults detection, simply by incorporating the local transformations, we were able to reduce the error by 20.84% as compared to simple SVM and 8.34% as compared to FDA. Selection of appropriate SVM parameters further improved the results. Our results corroborate the fact that the application of prior knowledge, i.e., valuable information about the learning task, makes it possible to build a classifier with less structural complexity. Such a classifier solves the over fitting problem thereby facilitating better generalization from training examples to unseen test examples. Thus, knowledge about the invariance can be exploited to improve online fault detection accuracy.

3.1.2.1 Symbolization assisted simultaneous denoising-cum-feature selection for SVM classification

This work describes an efficient and robust scheme that discards the noisy, irrelevant and redundant information present in data, while still retaining the discriminating power of the data. A combination of filter and wrapper approaches is suggested to get improved accuracy, efficiency and better generalization. Here filter provides an intelligent starting feature subset for a wrapper—a process that is likely to result in a shorter, and hence faster search for the wrapper. The proposed scheme applies the method of data symbolization for solving the dual problem of filtering and noise reduction. Data symbolization involves discretization of the raw data features into a stream of limited set of values called symbols, which retain dominant deterministic features while suppressing measurement noise. Further the conditional entropy of class label with respect to the feature attribute (converted into symbolic form) is computed to determine whether the feature is decidedly correlated to the class or not. Here lower the conditional entropy, higher is the coupling. Similarly we can find the degree of coupling of a feature to other features. Quantities such as the correlation coefficient or the correlation function often do not provide unequivocal indication of the coupling feature variables and class information (since these can be sparse and noisy). Symbolization scheme, on the other hand, works even in presence of external noise. The data symbolization method can be applied to deterministic or stochastic, linear or non-linear systems, without any a-priori assumptions about the nature of the underlying dynamical process and has a practical advantage of simplifying and speeding up subsequent computations as data space is changed from continuum to discrete form.

3.1.2.2 Hybrid wavelet assisted SVM classification of process, biological and biomedical signals

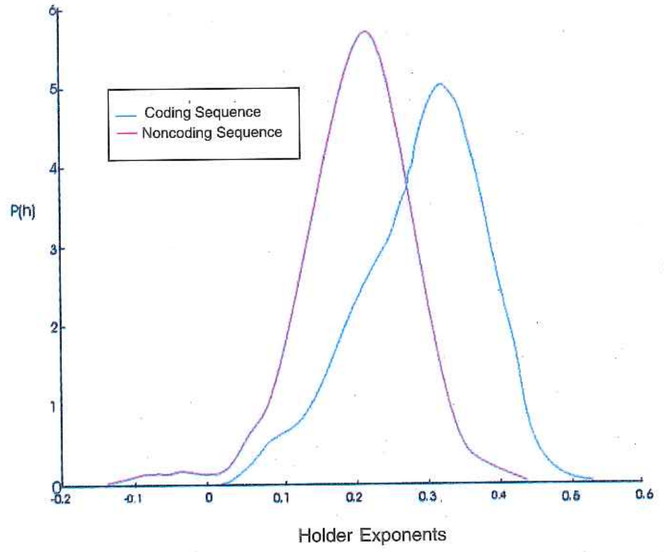
Hybrid strategies involving synergistic combination of wavelet transformation, nonlinear dynamics theory (mean local Hölder exponent formalism) and support vector machines (SVM) were employed for characterization of process, biological and biomedical signals. The basic idea is that the distinct behavior of dynamical systems can be rigorously characterized by singularity analysis. The distribution of local singularities of a time series can serve as its unique signature. Hence, the features of the singularity distribution of different time series can be employed for identifying the class and function of process/ biological/ biomedical signals of a time series. Wavelets were used as a mathematical microscope to enable identification and computation of and local Hölder exponents (singularity spectrum) profiles. The ability of wavelet transform to reveal the hierarchy of singular features was found to be particularly advantageous to tackle the problems at hand. Further, these singularity profiles were employed as the most informative input features to SVM. Further, SVM as the state-of-the-art classifier was used to:

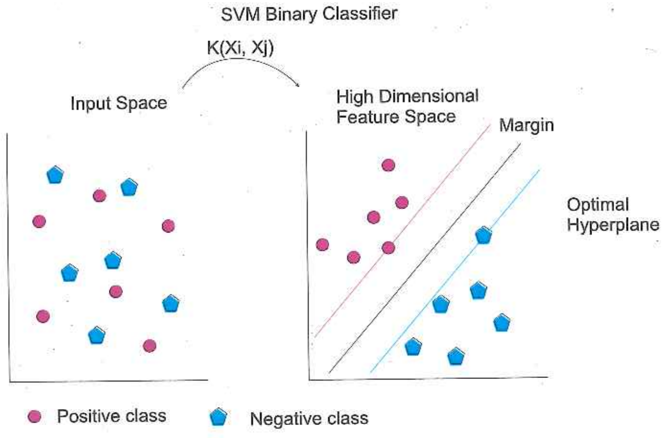
Identify regimes of operation in multiphase reactors

The case example of flow regime identification in gas–liquid stirred tank equipped with Rushton turbine was studied. Pressure fluctuations time series data obtained at different operating conditions were first analyzed to obtain the distribution of local Hölder exponents' estimates. The relevant features from this distribution were then used as input data to the SVM classifier. Employing this method, flow regimes with 98% accuracy could be classified. The results highlight the fact that the local scaling behavior of a given regime follows a distinct pattern. Further, the singularity features can be employed by intelligent machine learning based algorithms like SVM for successful online regime identification. The method can be readily applied to the other multiphase systems like bubble column, fluidized bed, etc.

Classifying arrhythmia signals

The hybrid system performance was evaluated using the benchmark MIT-BIH Arrhythmia database. The implemented model classifies 160 of normal sinus rhythm, 25 of ventricular bigeminy, 155 of Atrial fibrillation and 146 of nodal (A-V junctional) rhythm with 96.94 % accuracy. The distinct scaling properties of different types of heart rhythms may be of clinical importance.





Identification of genes

Accurate prediction of genes in genomes has always been a challenging task for bioinformaticians and computational biologists. The discovery of existence of distinct scaling relations in coding and non-coding sequences has led to new perspectives in the understanding of the DNA sequences. This has motivated us to exploit the differences in the local singularity distributions for characterization and classification of coding and non-coding sequences. The local singularity density distribution in the coding and non-coding sequences of four genomes was first estimated using the wavelet transform modulus maxima methodology. SVM classifier was then trained with the extracted features. The trained classifier was able to provide an average test accuracy of 97.7%. The local singularity features in a DNA sequence can therefore be exploited for successful identification of coding and non-coding sequences.

3.1.2.3 Soft-sensor development for fed-batch bio-reactors using SVR

In this study, a state-of-the-art machine learning based nonlinear modeling formalism known as support vector regression (SVR), has been introduced for the soft-sensor applications in the fed-batch processes. The SVR method possesses a number of attractive properties such as a strong statistical basis, convergence to the unique global minimum and an improved generalization performance by the approximated function. Also, the structure and parameters of an SVR model can be interpreted in terms of the training data. The efficacy of the SVR formalism for the soft-sensor development task has been demonstrated by considering two simulated bio-processes namely, invertase and streptokinase. Additionally, the performance of the SVR based soft-sensors is rigorously compared with those developed using the multilayer perceptron and radial basis function neural networks. The results indicated that the SVR is an attractive alternative to ANN for the development of soft-sensors in bio-processes.

3.1.2.4 SVM-based method for predicting the propensity of proteins to be soluble or to form inclusion bodies

Inclusion body formation has been a major deterrent for overexpression studies since a large number of proteins form insoluble inclusion bodies when overexpressed in Escherichia coli. The formation of inclusion bodies is known to be an outcome of improper protein folding; thus the composition and arrangement of amino acids in the proteins would be a major influencing factor in deciding its aggregation propensity. There is a significant need for a prediction algorithm that would enable the rational identification of both mutants and also the ideal protein candidates for mutations that would confer higher solubility-on-overexpression instead of the presently used trial-and-error procedures.

Six physicochemical properties together with residue and dipeptide-compositions have been used to develop a SVM-based classifier to predict the overexpression status in E.coli. The prediction accuracy is high, suggesting that it performs well in predicting the propensity of a protein to be soluble or to form inclusion bodies. The algorithm could also correctly predict the change in solubility for most point mutations. This algorithm can be a useful tool in screening protein libraries to identify soluble variants of proteins.

3.2. Kinetics and reaction engineering of complex process system

3.2.1 Performance enhancement of steam methane reforming in tubular packed-bed microreactors

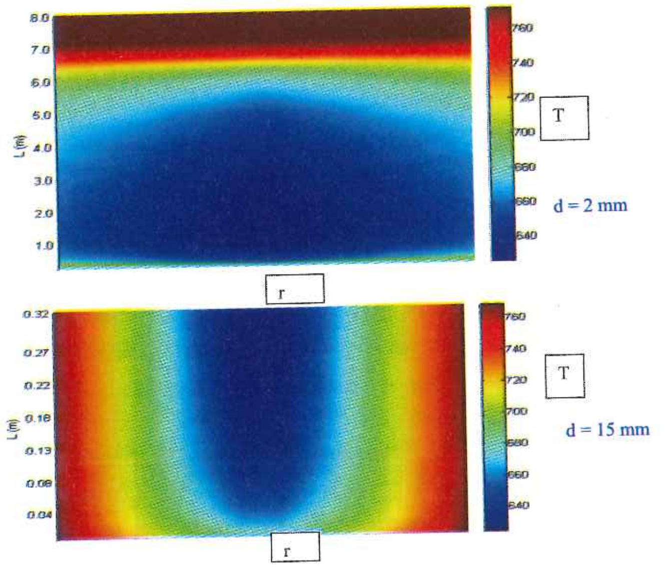
The key issue regarding the widespread commercialization of fuel cells is the ability to reduce cost and reactor dimensions to acceptable levels in both stationary and transport applications. The fuel processor which produces hydrogen rich stream from hydrocarbon based feedstock has a major impact on overall system cost. The processes are traditionally carried out in fixed bed reactors packed with catalysts. The reactions taking place are highly exothermic or endothermic in nature and controlling the reactor temperature is very crucial for optimum reactor performance.

The heat transfer rates in the packed-bed reactor depend strongly on interparticle temperature gradients and controlling interparticle heat transfer in packed-bed reactor by decreasing the reactor diameter may prove to be advantageous. Tubular packed-bed reactors (TPBMs) with small diameter have the advantage of providing higher surface to volume ratios. This results in decreasing mass transport and heat transport resistances and makes them attractive for achieving efficient thermal and mass transfer rates.

Natural gas, available in good supply, is a promising fuel for on-board and on-site production of hydrogen for fuel cells, provided pure hydrogen can be obtained and separated from it. Steam methane reforming (SMR) is a well established technology for the production of hydrogen and proper design and optimization is required for reducing cost and improving overall efficiency of operation. Work done at NCL showed that catalyst dilution by solids in the packed-bed reactor could improve the isothermicity while simultaneously suppressing other effects that adversely affect performance e.g., nature of axial dispersion, channeling loss. The use of TPBMs, therefore, enhances the performance of SMR by controlling the temperature gradient in the bed and improves the hydrogen productivity for this mode of operation. Studies for the SMR process performance in TPBMs was carried using a dynamic 2-D pseudo-homogeneous model. The model incorporates component and overall mass balance principles, pressure distribution in the packed bed, energy balance and is coupled with the general SMR reaction kinetic model.

Simulation studies were carried out first to assess the heat transfer limitation on SMR behavior and the results indicated significant temperature gradient even for 6 mm diameter and this becomes even more dominant at higher feed temperatures(T_f). We therefore studied the effects of decreasing reactor diameter on performance and the results showed that for acceptable catalyst loadings, the methane conversion increases from 20% to 100%, on reducing diameter from 25 to 2.8 mm. A reactor with diameter 2.8 mm and corresponding length can therefore be designed for full methane conversion. Process miniaturization by appropriate design and integration is indeed feasible.

The dynamics of SMR process in time as a function of reactor length was also studied. It was observed that the transient period is longer as the reactor diameter is reduced from 25 mm to 4 mm. For a 2 mm diameter reactor 100% conversion at the reactor outlet is seen throughout the operation of the process. This suggests that for a TPBM with lower diameter a smaller catalyst loading (W_c) would suffice for achieving complete conversion. The calculation showed that for 2 mm diameter reactor and length corresponding to a W_c of 5.5 gm yields 100% conversion.



Advantageous radial temperature profiles in reactors of lower diameter for the steam methane reforming reaction with catalyst dilution by adsorbent

3.2.2 A general kinetic model framework for the interpretation of adiabatic calorimeter rate data

Notwithstanding the variety and complexity of the reactions studied by adiabatic calorimeters like (AC), the data interpretation techniques are not general enough. Traditional thermokinetic analysis primarily lumps a complex multi-step reaction into a single overall reaction and ignores possible thermal effects in some of the possible side reactions. With detailed chromatographic/ mass spectrometric analysis of the headspace gases and the condensed phase residues, the pressure profile becomes an additional source of identification of the mechanism and the kinetics of the overall reaction. Finally, in the context of new multiphase catalytic processes of greater efficiency and environment friendliness and with reference to the storage of potentially incompatible fluid mixtures in metallic containers, AC studies of heterogeneous reaction systems are becoming part of the mandatory safety evaluations. With a few additional measurements, a proper kinetic interpretation of the AC data on such systems seems possible. A general model has been developed that was shown to be easily adaptable to a number of published reactions of various complexities referred to above. Standard thermal hazard characteristics like the onset temperature, adiabatic temperature rise, self-heat rate, time-to-maximum rate, pressure–temperature profile, etc. could be accurately calculated by the model and these compared closely with the experimental data. It is hoped that the model would be useful as a general-purpose tool for the interpretation of adiabatic calorimetric data for the purpose of process hazard assessment.

3.2.3 Modeling a continuous multistage liquid phase cyclohexane oxidation reactor network

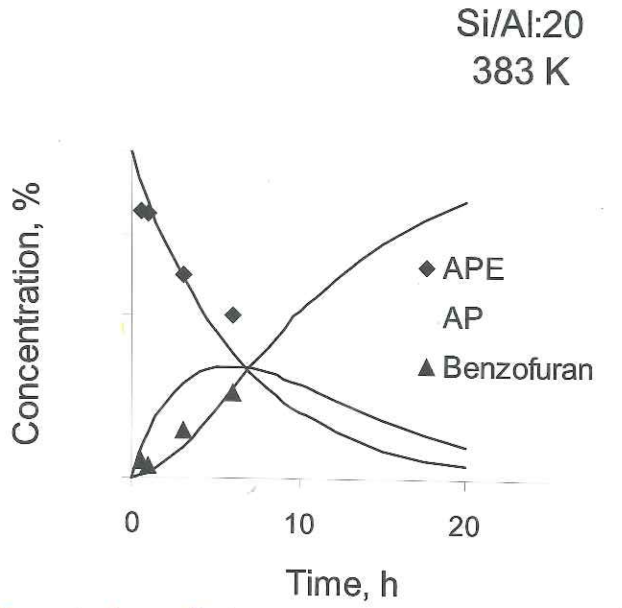
A model has been developed for a continuous multistage liquid phase cyclohexane oxidation reactors-in-series network, which uses a closed form rate model that (unlike previous efforts) is derived on the basis of the well-known free-radical kinetic mechanism of the oxidation reaction leading to a more generalized representation of the oxygen dependence of the rate. The model calculates the required transport and hydrodynamic parameters by an efficient set of correlations that has been successfully used in cyclohexane oxidation. Process sensitivities with regard to variables such as air rate, residence time, head pressure, inlet air composition and sparger configuration have been predicted. Some of these trends compared very well with the limited published experimental data in a three (35 L) agitated and sparged tank-in-series reactor system. The model has highlighted a fairly generalized way of correlating performance data from a given reactor, namely, in terms of yield–conversion characteristics, which can change depending on the mass transfer efficiency and the effective kinetics. Hence, it can aid in plant monitoring and optimization. It has also been shown how to use the same as an aid in preliminary scale-up studies based on laboratory or pilot plant reactor performance data.

3.2.4 Kinetics and optimization of reaction intermediates

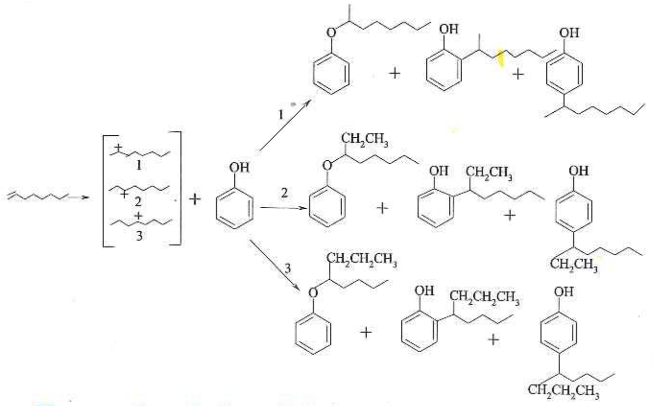
We have been studying the kinetics of important organic reactions and using this as a tool for understanding the reaction behavior and its relation to the catalyst characteristics. The development of the kinetic equation helps in generating the concentration profiles for the complete reaction based on limited experimental data. For example, in series reactions, it is possible to predict the reaction time for the maximum concentration of the intermediate. A typical example of a system studied is the methylation of catechol. The study of the sensitivity of the reaction rate constants of individual steps in series reactions helps in obtaining the desired product profile for altered reaction temperature. Again the study of the variation of rate constants with the number of carbon atoms in a homologous series helps in predicting the values of the rate constants when reaction is carried out with a new compound belonging to the same series. A study of the change in the rate constant with change in catalyst material characteristics (surface area, acidity, etc.) further helps in understanding and identifying the critical properties that contribute to the catalyst performance. For these aims we have been analyzing several series/ series-parallel organic reactions which fall under the common category, alkylation, acylation and Claisen rearrangement.

Alkylation/ acylation of aromatics is an important step in the preparation of various chemicals used in pharmaceuticals, fine chemicals, agrochemicals, etc. For example, octyl, nonyl and decyl phenols are important intermediates in the production of fine chemicals, and are widely used as surfactants in detergent formulations. 2,6-Naphthalenedicarboxylic acid (NDCA) is a valuable monomer used in the synthesis of novel polyester resins. NDCA is made by the oxidation of 2,6- dimethylnaphthalene, which is prepared by dialkylation of naphthalene with methanol. Silmilarly o-methylated dihydroxybenzenes (catechol, resorcinol and hydroquinone) are important synthetic intermediates in the production of fine chemicals and pharmaceuticals.

In the alkylation of phenol with octene, the complete spectrum of possible products was considered for the analysis. The product distribution obtained from the experimental data was used to select the steps relevant to the reaction on zeolite catalyst. The rate constants obtained from the resultant series-parallel reaction model was able to describe well the observed experimental results. The Claisen rearrangement of allyl phenyl ether produces allyl phenol and benzofuran, which is a series reaction. A kinetic analysis based on the experimental data could generate the complete concentration profile of the reaction and the time at which the formation of the intermediate product, allyl phenol is maximum. Other reactions studied include tertiary butylation and isopropylation of naphthalene, methylation of dihydroxybenzenes (catechol, resorcinol and hydroquinone), etc.



Concentration profile for the catalyst Claisen reaction of allyl phenyl ether



The reactions in the alkylation of phenol with 1-octene forming phenyl octyl ethers and octyl phenols

3.2.5 Downstream separation for improved productivity

Downstream separations are critical in deciding the success of any process industry as they contribute to as much as 30 to 70% of the manufacturing cost of products. NCL has skill base covering different aspects of downstream processing such as synthesis and characterization of new advanced materials, the process development and engineering, understanding of the dynamics, control and optimization etc. which can be pulled together to generate innovative separation strategies of practical relevance. In view of the requirement for flexible separation process systems, efforts have been directed towards development of hybrid systems and development of new materials for effective separations. The strategy is to incorporate development of new materials with increased selectivity/separation factors, collection of data for new systems, studies for improving separation involving dilute solutions for "real world" applications, process integration studies including reactive separations and development of computer models for predicting performance.

3.2.5.1 Zeolite-based adsorbents

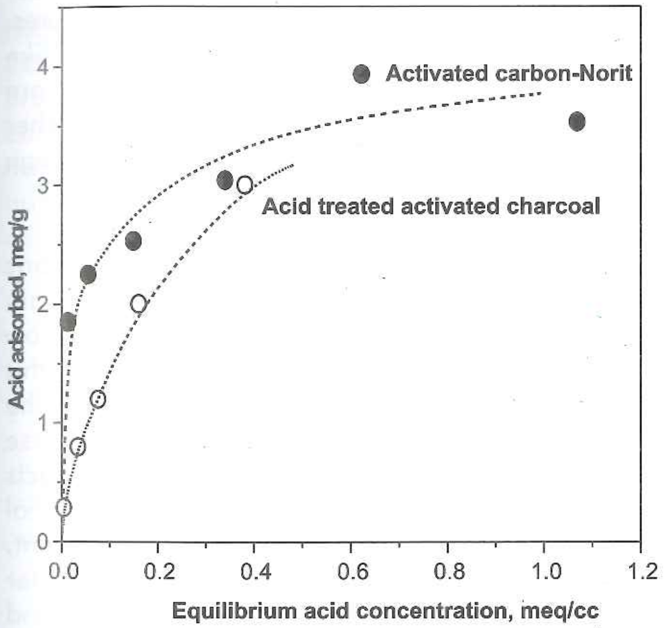
Aromatic isomers of cresols, cymenes, naphthols etc. are compounds of wide industrial importance and are used in a variety of applications, e.g., pharmaceuticals, cosmetics, surfactants, antioxidants, phenolic resins, plasticizers, inhibitors, agricultural chemicals, ore floatation chemicals, germicides, antiseptics, disinfectants etc. In many of these applications the purity of the isomer is of paramount importance. These compounds form azeotropes and the separation/purification of these compounds by normal distillation route is possible only up to the azeotropic composition. The final purification is carried out commercially by adsoption using zeolite-based adsorbents. We work on the development of novel adsorbents for these types of separations. We have developed some clay-based adsorbents that show good adsorption characteristics (comparative to that of commercial zeolite adsorbents) for these compounds. These adsorbents also have good adsorption characteristics for the sorption of fluoride and heavy metals from effluent/ground water. These programs are supported by CSIR / NCL (in-house) and the Department of Science and Technology (DST), New Delhi.

3.2.5.2 Fuel desulphurization

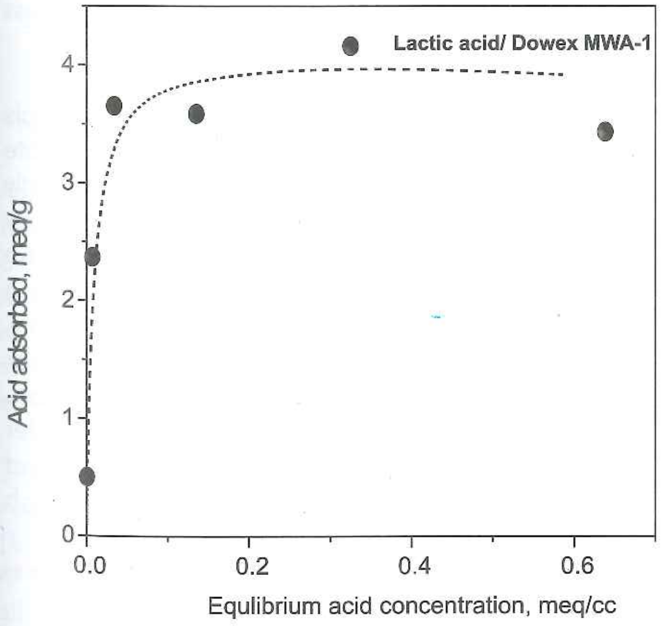
In recent years, the problem of removal of sulfur from the transportation fuels has gained wide attention and importance since governments worldwide now mandate significant reduction in the sulfur levels of transportation fuels— a maximum of 15 ppmw in diesel from the existing levels as high as 10 times of this value. Sulfur in the transportation fuels has been a major concern not just from environment point of view, but also from the viewpoint of application in Fuel Cells. These aspects make desulfurization a crucial research subject for the mankind and attach a high priority to it! The conventional process of hydrodesulfurization has limitations and involves a very high operating cost with severe process conditions. A sorption process is believed to offer an economically viable option to the existing processes. Hence research on sorption and sorbents is the key to new technology development. We have identified some ion-exchanged zeolites and modified activated carbons which have good desulfurization capacity and potential for technology development.

3.2.5.3 Enhanced recovery of lactic acid

In recent years, there has been increased concern on depleting petroleum reserves and this has prompted increased focus on biorefinery—bioprocesses for the production of variety of chemicals via fermentation using biomass. Manufacture of organic acids such as acetic acid, lactic acid, citric acid etc. can be most promising in this regard and is particularly important since its functionality enables further downstream production of many different compounds. Although fermentation processes are known for over 100 years, even today, they have many limitations due to rates of conversion and in efficiently separating desired products. Thus, although a wide range of acids can be made using fermentation using known microorganisms, the processes have great difficulty in real world due to technical problems associated with the recovery from dilute solutions and abnormally high cost of separation. We have studied adsorption of lactic acid on various adsorbents from the class of activated carbon, polymeric adsorbents and ion exchange resins. Both conventional as well as modified adsorbents were studied. It was found that the capacity of adsorption is better with adsorbents having surface modification through specific treatment. A good capacity of adsorption of about 350 mg/g of adsorbent was obtained with carbon-based adsorbents as compared to polymeric adsorbents.



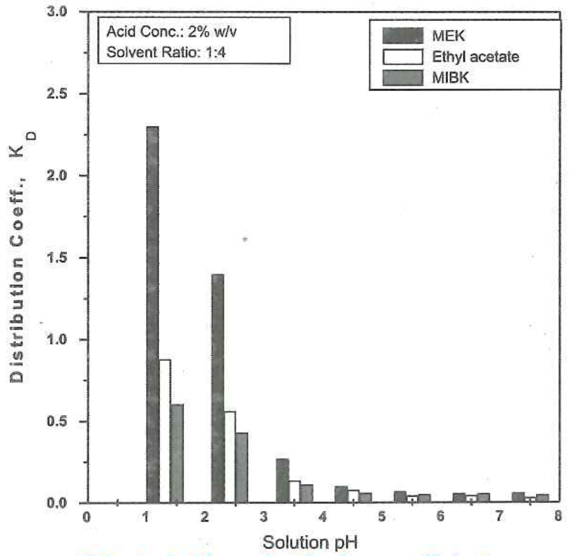
Lactic acid sorption isotherm on carbon based adsorbents



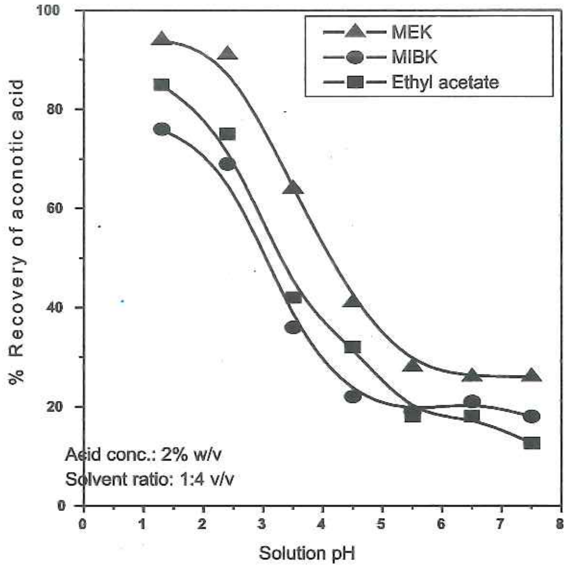
Adsorption of lactic acid on weak base resin

3.2.5.4 Separation of aconitic acid from sugar molasses

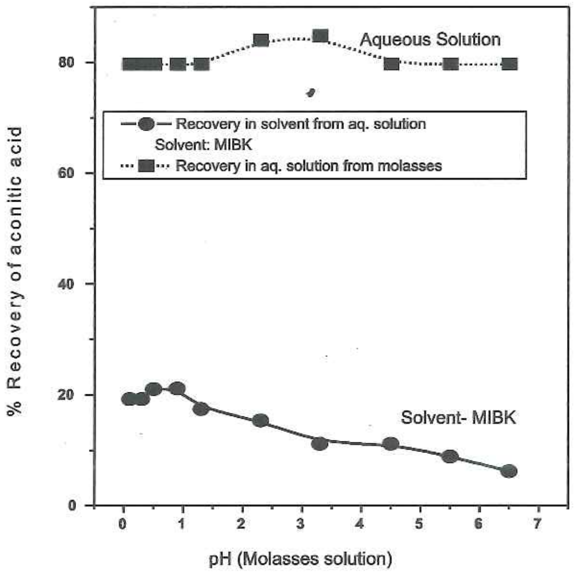
Separation of aconitic acid is an important problem in the sugar industry due to its potential as a value added chemical from the sugar manufacturing process, its impact on the sugar recovery, environmental pollution and its nuisance value in scale formation in juice heaters and evaporators. Solvent extraction of aconitic acid from aqueous solutions was studied. Experimental studies were carried out using both synthetic solution of aconitic acid of known concentration as well as on extraction of aconitic acid from molasses. A number of solvents were studied and effects of various parameters such as pH, temperature, solvent ratio etc. were evaluated to maximize the recovery of the acid. It was found that methyl ethyl ketone and ethyl acetate as solvent showed promising results on recovery of aconitic acid. Lower pH was found to enhance the separation and an acidic pH of about 1.3 was found to be most suitable for extraction. Up to 94% of aconitic acid recovery was achieved from synthetic solution using MEK as solvent while that with ethyl acetate and MIBK was about 82% and 72% respectively. Experimental studies on actual molasses showed up to 35% recovery of aconitic acid, which is quite high as compared to that obtained using the conventional precipitation method. The reason for lower values of recovery with molasses solution as compared to synthetic solution can be attributed to the presence of other organic acids in the molasses. The encouraging results of the present work clearly point towards useful application of solvent extraction as an alternative to the existing precipitation method.



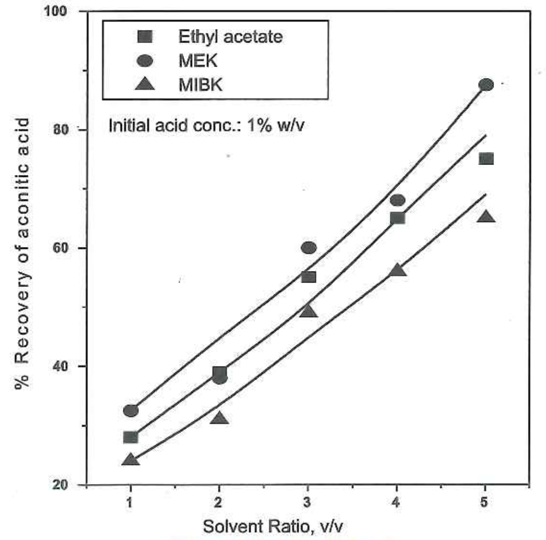
Effect of pH on distribution coefficient



Solvent Extraction- Effect of pH



Effect of pH on extraction of acid from molasses



Effect of solvent ratio

3.3 Studies in carbon sequestration

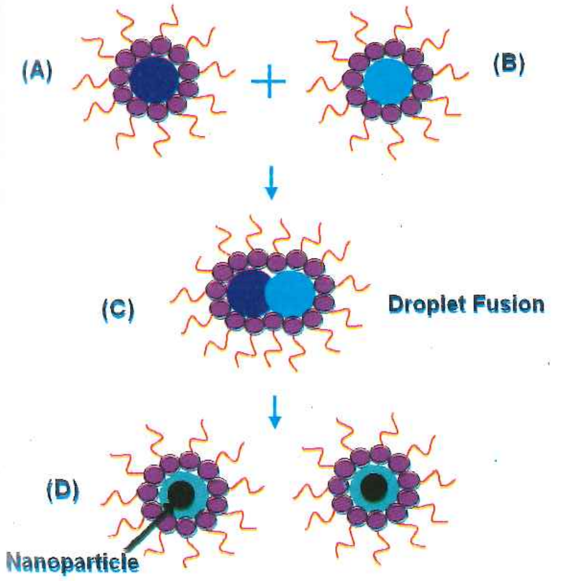
Flue gases from the coal-burners, chimneys and power plants come out hot with temperatures varying from a few hundreds to about a thousand degrees Celsius. It is highly desirable to separate carbon dioxide from these gases at high temperature. The need to capture carbon dioxide from these processes is important because of global warming considerations. Considerable efforts are being made to find ingenious ways of sequestering carbon dioxide at high temperatures. Also, the existing separation technologies like absorption and low-temperature distillation are not able to separate carbon dioxide over other small gases such as nitrogen or hydrogen at high temperatures.

Synthesis of nanoparticles in microemulsions media has been an useful method to obtain nanoparticles with controllable size and narrow particle size distribution. The main idea behind this technique is that by appropriate control of the synthesis parameters one can use these nanoreactors to produce tailor-made products down to a nanoscale level with new and special properties. A microemulsion is a transparent, isotropic liquid medium with nanosized water droplets dispersed in a continuous oil phase and stabilized by surfactant molecules at the water/oil interface. These surfactant-covered water pools offer a confined microenviornment for the formation of nanoparticles and inhibit their excess growth and agglomeration.

The synthesis of nanocrystalline ceramic materials imposes a challenge on the traditional solid-state synthesis methods which fail to offer a sufficiently narrow size distribution and desired homogeneity at the nanometer level. However, the solution methods using alkoxide precursors show promising potential for control over particle size, high purity, good chemical homogeneity at the nanometer level and therefore good carbon dioxide sorption. The lithium metasilicate is used as a strong breeder material due to its good tritium solubility and chemical and mechanical stability at high temperatures.

3.3.1 Synthesis and characterization of lithium silicate nanoparticles using reverse microemulsion

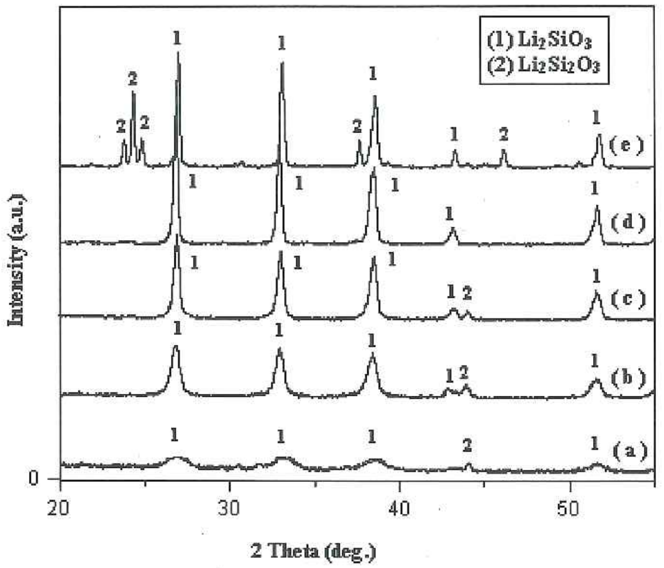
We have studied the synthesis of lithium silicate nanoparticles by using the inherent characteristics of microemulsions of Triton X-100/cyclohexane-n-hexanol/water and advantages of the sol–gel process and study the influence of conditions such as calcination temperature, starting material compositions, etc. on the characteristics of nanoparticles. The advantage of this technique is that the particle size as well as stoichiometry of the product can be controlled. The method also allows controlled hydrolysis of alkoxide and forms nanoparticles at low temperatures. The nanoparticle formation mechanism in reverse microemulsion is shown in figure.



The formation mechanism of lithium silicate nanoparticles in reverse microemulsion

Parts A and B in the scheme show the reverse micelles containing TEOS + lithium nitrate and ammonium hydroxide respectively. Part C shows the mixing of the two types of micelles and fusion of droplet upon collision. Part D in the scheme shows the formation of the nuclei, immediately after the hydrolysis of the precursors.

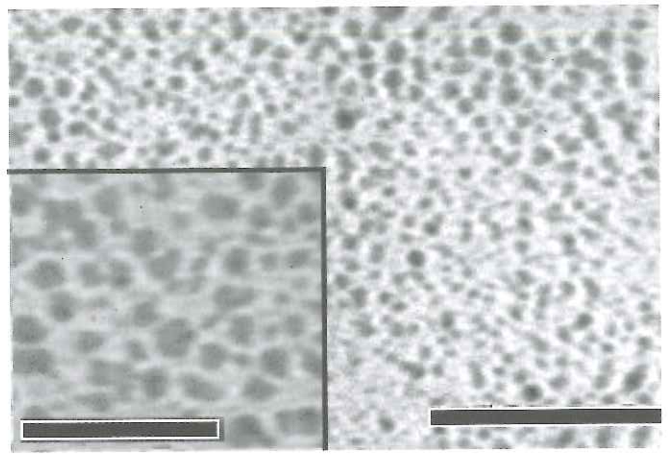
The powder X-ray diffraction patterns were recorded using Ni-filtered Cu-K ∝ radiation (λ=1.5418 Å) at 30KW and 20mA and a scan rate of 5°min^{-1} 2 θ. The XRD of the as-synthesized lithium silicate (Li:Si=2:1) sample after ageing for 12 hours shows small diffraction peaks indicating the formation of some crystal phase while the XRD of calcined samples show the highly crystalline lithium silicate compound present in the powder obtained by the microemulsion method sol-gel method.



XRD of the synthesized lithium silicate nanopowder and phase development after heat treatment at different temperatures for 4 hr, (Li:Si=2),(a) synthesized after ageing at 110°C for 12 hours,(b) 600°C,(c) 700°C, (d) 800°C (e) 1000°C.

X-ray diffraction of the powder calcined at 800°C for 4 hr shows the characteristic XRD peaks of single phase lithium meta silicate (Li_2SiO_3) while the other sample show formation of Li_2SiO_3 as well as $Li_2Si_2O_5$ in different proportions. Effect of varying the Li to Si ratio on the final product was also studied by XRD. For Li:Si ratio of 1, $Li_2Si_2O_5$ and Li_2SiO_3 was obtained. As the Li:Si ratio increased to 2, only pure Li_2SiO_3 was formed. For Li:Si ratio of 3&4, both $Li_2Si_2O_5$ and Li_2SiO_3 were obtained.

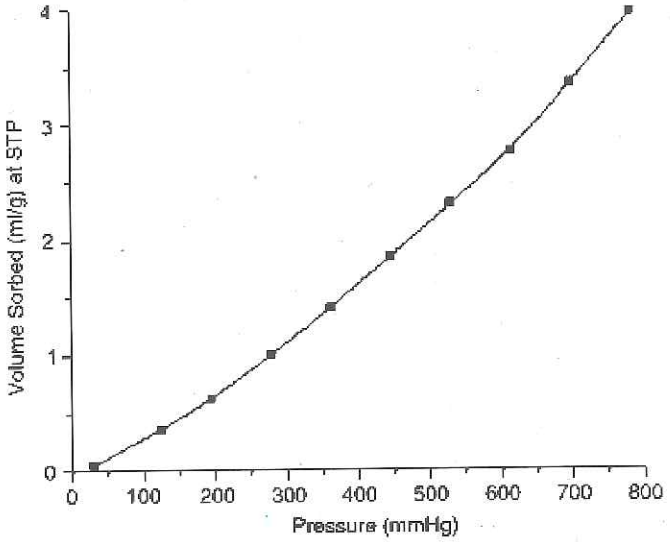
The size and morphology of the powder calcined 800°C for 4 hours observed by TEM is shown in figure below. It can be seen that lithium silicate powder prepared by microemulsion mediated sol-gel method is very fine, uniform without any agglomeration. The particle size ranges over 4-12 nm with an average particle size of 7 nm.



TEM of lithium silicate powder synthesized in microemulsion (Li:Si=2). The bar displays 200nm (Inset TEM. The bar displays 50nm.)

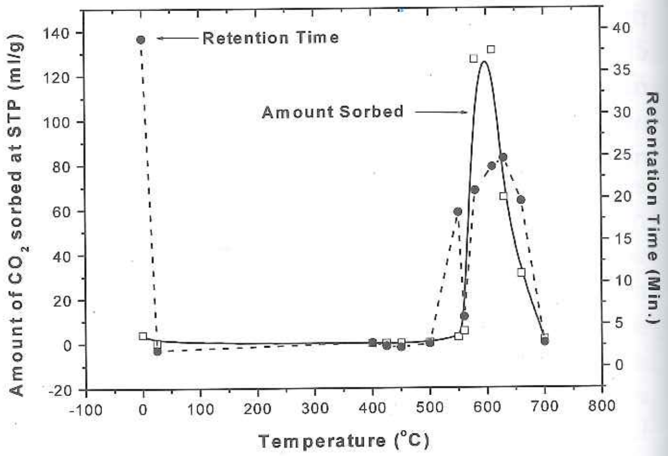
3.3.2. Carbon dioxide adsorption studies

The high-temperature sorption measurements for CO_2 were carried out using a volumetric technique by pulse chemisorption method after activation of sample in helium up to 800 °C. The volume adsorption of CO_2 increases with higher pressure leading to greater storage, but due to experimental limitations we have measured adsorption at 30–782 mm Hg pressure at 273 K. CO_2 adsorption using volumetric apparatus seems to be an accurate method as compared to change in weight method. In view of this, high-temperature sorption measurements for CO_2 were carried out using a volumetric technique by pulse chemisorption method after activation of sample in helium up to 800 °C.



Effect of pressure on sorption of carbon dioxide

The effect of temperature on CO_2 sorption capacity and retention time, i.e., time required for saturation at 1.5kg/cm² pressure shown in figure below, clearly indicates that sorption value slowly decreases from 0 to 450 °C and then slowly increases up to 580 °C (127.05 ml/g at STP). Beyond this temperature and up to 610 °C (131.04 ml/g at STP) the increase is very sharp. It has further been observed that sorption starts decreasing beyond 630 °C (65.35 ml/g at STP) to small volumes near to 700 °C (1.62 ml/g at STP). The time required for saturation is at least an order of magnitude faster than reported so far.



Effect of temperature on sorption of carbon dioxide

3.4. R&D applications employing CFD formalism

3.4.1 Gas-liquid flow/ solid-liquid flow in stirred reactors

Comprehensive mathematical models were developed to simulate gas-liquid and solid-liquid flows in stirred reactors. A new sub-model to estimate effective drag coefficient acting on gas bubbles or suspended solid particles in stirred reactors was developed. The model was applied to simulate gas-liquid and solid-liquid flow generated by different impellers. Model predictions were validated with the help of available experimental data. Wall pressure fluctuations and torque fluctuations in stirred vessels were carried out for several impellers over a wide range of operating conditions. The results were analyzed to develop robust criterion and methodology to identify different operating regimes in multiphase stirred reactors. The methods can be applied to industrial reactors.

3.4.2 Dynamics of air-lift loop reactors

A new program on understanding gas-liquid flows in air-lift loop reactors was initiated. A laboratory loop reactor was set-up. Extensive experimental data was collected to understand influence of sparger and superficial gas velocity and gas-liquid flow in air-lift loop reactors. Wall pressure fluctuations were measured to characterize the dynamics. Gas hold-up profiles were measured using conductivity probes. The probes, signal-conditioning units, and data processing software were developed in-house. The new type of conductivity probes, dual-tip probes are being developed to measure chord length distribution and bubble velocities. The experimental techniques are also being extended for studying dynamics of slurry bubble column reactors. Detailed computational fluid dynamics (CFD) - based models were developed to simulate dynamics of gas-liquid and gas-liquid-solid flows. Both, Eulerian-Eulerian and Eulerian-Lagrangian approaches were used to simulate these gas-liquid flows. These models were shown to capture key features adequately.

3.4.3 Modelling of hydrodynamics of trickle bed reactors

A CFD based model was developed to simulate gas-liquid flow through packed beds. The CFD model was used to investigate periodic operation of trickle bed reactors. The computational model was extended to simulate hydro-processing trickle bed reactors. Influence of mal-distribution and scale-up was studied using the computational model. The model predictions were verified by comparing simulated results with available experimental data. The model and the results would be useful to extend application of CFD models for simulating TBRs.

3.4.4 Fluidized bed reactors

The fluidization of glass and polypropylene (PP) particles was studied experimentally to understand differences and similarities between glass and PP fluidization. Long term bubbling characteristics of these fluidized beds were studied. A comprehensive CFD model was developed to capture long term bubbling characteristics of glass and PP fluidized beds. CFD model was able to capture key trends of these fluidized beds.

Fluid catalytic cracking (FCC) riser reactor has also been modeled. These FCC riser reactors exhibit dynamic formation of clusters of solid particles. It is essential to understand the implications of formation of such clusters on effective drag between gas and solid phases. Currently, CFD models rely on empirical drag coefficient correlations which do not account for such clusters. The state-of-the-art CFD models therefore are still not able to simulate high solid flux risers adequately. The multi-scale approach, which accounts for different scales occurring in high solid flux risers, appears to be promising for enhancing the ability to predict high solid flux risers. The energy minimization multi scale (EMMS) model was investigated for estimating drag between gas and solid phases flowing in risers. Though, the overall picture postulated in EMMS looks promising, the critical examination of EMMS for simulating gas solid risers reveals significant limitations of EMMS model. Characteristics of EMMS were computationally investigated to bring out key limitations with an intention of providing a basis for improvement.

3.4.5 Polymerization reactor simulator: PoRE

A comprehensive framework to simulate chain growth polymerization for different reactor configurations and different mode of operations (batch/ continuous) is developed. Wherever required, a population balance based model to simulate particle size distribution was integrated with this framework to account for the effect of average polymer particle size. The model is developed in a way to make it capable of predicting the effects of operating conditions such as monomer flow rates, temperature, pressure and catalyst feed rate and catalyst properties on polymer properties and PSD of product stream. The model can also be effectively used to understand the dependency of macroscopic variables such as temperature, monomer conversion, polymer grade transitions and PSD on the catalyst properties. The model can be used as a tool to generate sets of operating conditions and reaction kinetics schemes to design the process conditions and catalysts to evolve a specific set of output polymer characteristics. Apart from developing mathematical models for simulating polymerization reactors, a user-friendly software product called PoRE is being developed. The software is intended to provide a powerful platform to practicing engineers and researchers working on chain growth polymerization reactors. It will provide unique facilities to understand and to optimize polymerization reactors behavior to researchers as well as practicing engineers running large polymerization plants.

3.4.6 Coal fired boiler

Pulverized coal fired boiler is one of the key equipments governing the overall energy efficiency of coal fired power stations. A comprehensive three year project was therefore initiated at NCL. Appropriate multi-stage methodology was developed to implement the project. As a first stage, the CFD models were developed to simulate cold air velocity tests (CAVT) carried out at 210 MW coal fired boiler at Dadri plant of NTPC. Internal tube bundles e.g., platen, super heaters, economizers, were modelled using a porous media approach. The resistances offered by these various internal tube bundles were studied by employing a 'unit cell' approach. Appropriate resistance coefficients obtained via this were implemented in user defined functions and were then incorporated in FLUENT. Simulation studies for CAVT were then carried out. CFD models along with the user defined functions developed in this work were able to simulate CAVT tests adequately well. The models developed in this work will be useful for extending the application of CFD for the simulation of coal fired boilers.

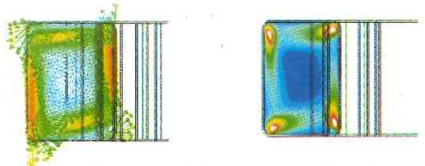
3.4.7 Vortex diode

Vortex diodes are used as replacements for leaky non-return valves in applications and where it is desirable to avoid moving parts. Despite their use in practice for several decades, no clear guidelines for design and optimization of vortex diodes are available. Detailed experimental study on flow and pressure drop characteristics of vortex diodes was therefore carried out to evolve such guidelines. The study covered a wide range of vortex diodes. The variation of diodicity (ratio of pressure drop for reverse and forward flow for the same flow rate) with respect to diode geometry, diode size, aspect ratio, nozzle configuration and Reynolds number was studied. The experimental results were critically analyzed to develop suitable design guidelines. Detailed CFD models were developed for simulating flow within diodes. CFD models were able to predict to diodicity of a wide range of vortex diodes. The methodology, CFD models and results obtained in this work will be useful for enhancing performance of vortex diodes.

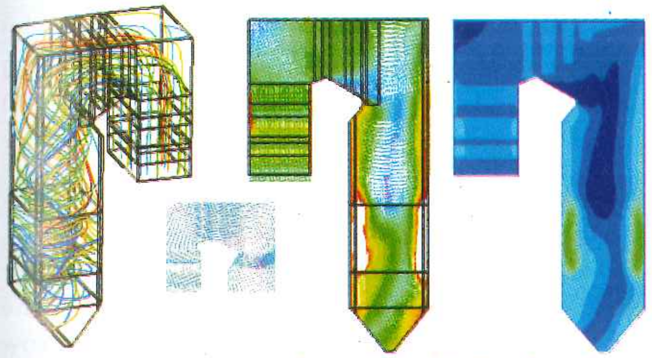
3.4.8 Ballast water treatment

A variety of physical and chemical techniques have been proposed for ballast water treatment. However, chemical disinfection techniques suffer from disadvantages like formation of possible carcinogenic byproducts, thereby posing health / environmental hazards. Therefore there is a need for developing novel and efficient disinfection technology, which could eliminate or reduce the use of these disinfecting chemicals. In this work, a proof of concept technology to achieve ballast water disinfection without generating any toxic byproducts was developed. This is based on the concept of hydrodynamic cavitation. Detailed CFD models were developed and used to evolve new types of cavitation chambers. The ideas, models and the results generated in this work will have significant implications in the development of large scale dis-infection system for ballast water. This work was carried out in collaboration with ICT, Mumbai and NIO, Goa.

Other industrial projects (Fleetguard Filters Pvt. Ltd., Invista Inc., USA) were also carried out during the last year. These projects were related to multiphase flows, CFD modeling and reactor engineering. Work was also done on CFD simulations of short stopping of runaway reactors. A case of bulk polymerisation was considered. Potential pitfalls in using conventional completely mixed assumption for arresting runaway situations were highlighted using this case

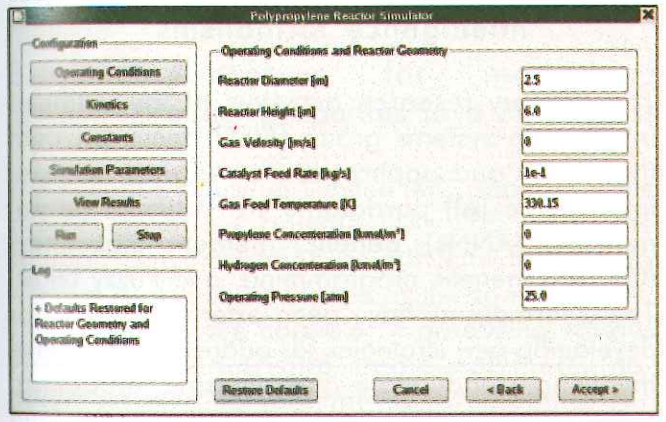


New insights about the 'fire ball' in boilers



Phenomenological model for coal fired boilers based on insights gained by CFD model

PoRE SOFTWARE



Operating Conditions and Reactor Geometry

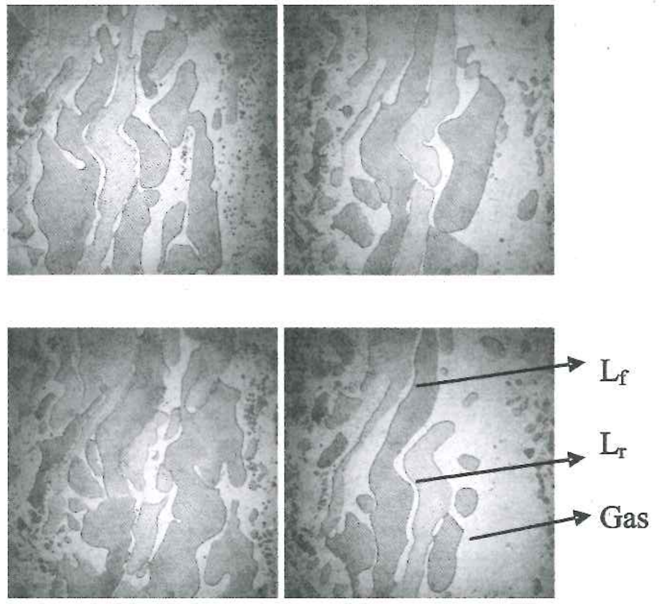
Reactor Diameter [m] 2.5
Reactor Height [m] 6.0
Gas Velocity [m/s] 0
Catalyst Feed Rate [kg/s] 1e-1
Gas Feed Temperature [K] 330.15
Propylene Concentration [kmol/m³] 0
Hydrogen Concenteration [kmol/m³] 0
Operating Pressure [atm] 25.0

+ Defaults Restored for Reactor Geometry and Operating Conditions

Easy to use, GUI based tool for reactor optimization (control on product quality, grade changes)

3.4.9 Microreaction technology

Recently, microreaction technology has gained importance in synthesis chemistry, process intensification and process engineering. Although a lot of thrust has been given at looking into its feasibility for synthesis, very little attention has been given on the engineering aspects of the design of microreactors. In view of this, a new laboratory entirely devoted to the studies of microreaction technology for process development purpose and fluid dynamics in microsystems is being established. The laboratory would have the facilities to carry out multiphase reactions using the in-house designed and fabricated microreactors as well as those that are commercially available. New micro-devices, viz., mesh microreactor for gas-liquid-solid catalytic reactions, micro fixed-bed reactor and micro heat exchanger have been designed and fabricated in-house. Hydrodynamic studies (hold-up, RTD, mass transfer coefficient, etc.) for certain processes are presently under investigation. The gas-liquid flow in small capillaries ~1 mm has been investigated using a high speed camera to capture the slug flow. CFD simulations of the same for understanding the intrinsic transport phenomena are also in progress.

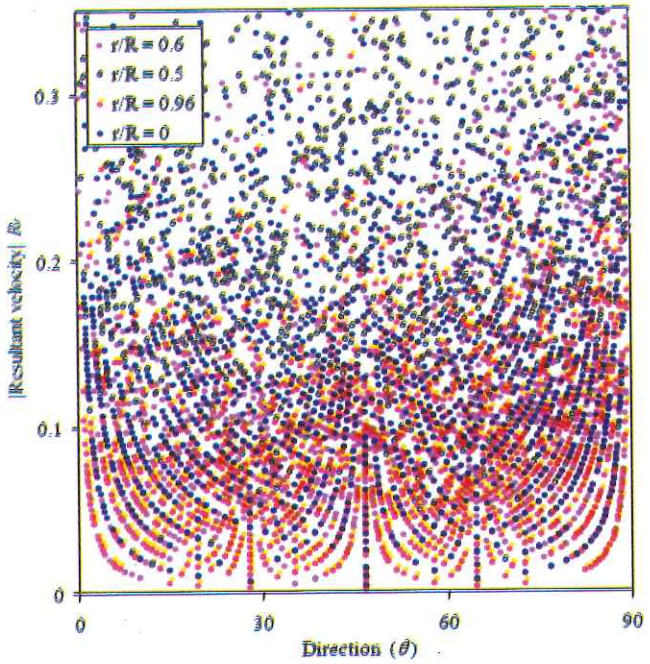


Two phase flow inside the mesh microreactor for different gas-liquid flow rates. Liquid film: (between mesh and front plate → L_f, between mesh and rear plate → L_r

3.4.10 Analysis of nonlinear and non-stationary data in bubble column reactors

A novel methodology is developed for the characterization of the sparger type on the flow patterns in a bubble column reactor. The methodology uses the simultaneously measured instantaneous velocity-time data (two orthogonal velocity components). The data sets are transformed into their equivalent description in terms of polar co-ordinates, viz., resultant velocity vector and angle and subsequently represented in terms of symbolic data in a binary number format. The covariance matrices obtained from the binary data are analyzed for their eigenvalues and the spectra are used for the identification of the dominant, energy containing modes in the data.

The plots in polar co-ordinates showed systematic patterns for the data from single point sparger and the covariance plots as well as the eigenvalue spectra showed existence of dominant features. These features were markedly different for a multipoint sparger and thus helped in the sparger characterization. The spectra indicated the higher level of complexities due to hydrodynamics for the multipoint sparger.



Patterns in the complex nonlinear and non-stationary velocity data on transformation in polar co-ordinates for a bubble column with a single point sparger

In a different analysis, the velocity-time data from many locations in a bubble column was analyzed to understand the local distribution of spectral energy and the possible constancy in the local value of energy dissipation rate. At each location, the data was obtained at every ten degrees, which corresponds to different directions from radial to axial component The spectral analysis could bring out the above features in a systematic manner, while the analysis based on number density plots showed some trends in the number density variation for data obtained from near wall regions. Further studies from this work will focus on intrinsic features of turbulence in two phase flows and are under progress.

A study was also done to bring out some interesting observations about the contribution of bubble size distribution to the mass transfer in a bubble column reactor. The true mass transfer coefficient measured in a bubble column reactor using chemical method was compared with those estimated using the physical data in terms of bubble size and rise velocity distribution. The information was used for verification of the regime of mass transfer with chemical reaction. The analysis showed that the regimes of mass transfer with reaction are a strong function of bubble size and hence depending upon the bubble size distribution, i.e., the true regime is a result of the statistical mean of the regimes due to individual bubble classes. Importantly, a significant number of bubbles can always lie in undesirable regimes. To achieve a better performance of the bubble column or any multiphase reactor, operating within a narrow bubble size distribution is therefore recommended.

3.5 R&D applications in artificial intelligence formalisms

The primary research activities of the artificial intelligence systems group (AISG) focus on both the theory and applications of various artificial intelligence (AI) paradigms viz. artificial neural networks (ANNs), genetic/ memetic algorithms (GA/MA), genetic programming, and Fuzzy Logic. These formalisms have been extensively used for developing new strategies for addressing problems involving steady-state and dynamic modeling, optimization, nonlinear control, fault detection and diagnosis, dimensionality reduction, classification, and selection of significant model inputs, encountered in chemical, biochemical, chemical engineering/ technology systems. Highlights of the work carried out using AI formalisms are brought out below.

3.5.1 Optimization of fermentation media for exopolysaccharide production from *L. plantarum*

A *Lactobacillus* strain was isolated from the fermented *Eleusine coracana*. This strain characterized as *Lactobacillus plantarum* was found to produce an exopolysaccharide (EPS) in quantitative amount. The objective of the study was to determine an optimum media composition and inoculum volume for the stated fermentative production of the PS. Towards this objective, a hybrid methodology comprising the Plackett–Burman (PB) design method, ANN and GA was designed and implemented. Specifically, the PB, ANN and GA formalisms were used for identifying the influential media components, modeling of the non-linear fermentation process and optimizing the process, respectively. Among the five media components only three were found influential namely, lactose, casein hydrolysate and triammonium citrate. Further, an ANN-based process model was developed for approximating the non-linear relationship between the fermentation operating variables and the EPS yield. The input variables of this ANN model were subsequently optimized using the GA formalism with a view to obtain the maximum EPS yield in the batch fermentation. The optimized media composition so obtained when verified experimentally resulted in a substantially improved product yield of 7.14 g/l.

3.5.2 Soft-sensors for monitoring product properties in a PE process

The Reliance Industries Limited (RIL), sponsor of the project produces polyethylene (PE) using the solution polymerization of ethylene technology wherein α-olefins are utilized as the co-monomers. The RIL plants are capable of producing various PE grades comprising homo-polymers, co-polymers and ter-polymers, for meeting the requirements of a wide spectrum of consumer applications. The quality of the final polyethylene is measured in terms of three quality control (QC) variables, namely, stress exponent, density and melt flow index (MFI). The RIL assigned the task of developing software-based sensors (Soft-sensors) for the three QC variables to NCL. Soft-sensors are software based sophisticated monitoring systems, which 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 values of less accessible and difficult-to-measure process variables. The soft-sensors can also reduce the extent of off-spec product and aid in better and faster process related decision-making. Accordingly, a number of AI based accurate soft-sensor models were developed for the prediction of three QC variables of the PE process. An AI strategy, which helps in the development of ANN models possessing excellent prediction accuracy and generalization ability in the presence of data comprising instrumental noise and measurement errors, was specially developed for building the soft-sensor models. These soft-sensors were installed on the distributed control systems (DCS) of the PE plants and have helped in improving the performance of the PE plants while cutting down the need for frequent laboratory analyses of the PE product.

3.5.3 Optimization of the ammonia injection based flue gas conditioning system

Restricting the amount of suspended particulate matter (SPM) in the exit flue gas of a coal-fired boiler (CFB) is critical from the viewpoint of controlling environmental pollution. The state regulating authorities such as the Pollution Control Board specify the tolerance limit for the SPM and the limits are very stringent. The commonly employed equipment for bringing down the SPM levels within the permissible limit is the electrostatic precipitator (ESP). The Heavy Water Board (HWB) has studied the ESP-augmented CFB system extensively and it has been observed that although the ESP is designed for 99.9% efficiency, in actual practice its efficiency is close to 95%. For improving the efficiency of the ESP, the Heavy Water Board has developed a patented ammonia injection technology. The said ammonia injection (dosing) technology has been implemented in various thermal power plants in India.

The extent of ammonia dosing required reducing the SPM value to the desired level depends on several factors, such as flue gas flow rate, coal and ash characteristics, flue gas temperature, inlet dust burden and outlet dust burden. Since the ESP-augmented CFB is a complex nonlinear process, its modeling via the phenomenological approach and the subsequent optimization of the model—for obtaining the optimal magnitudes of the ammonia dosing—is a difficult, tedious and time-consuming task. The augmented system however can be efficiently modeled and optimized using novel AI formalisms such as ANN and GA. The AI-based modeling formalisms are exclusively process data based and since a large number of historical process data were available with the HWB, these were gainfully leveraged to model and optimize the ESP-augmented CFB process. The specific task given NCL was to develop a CFB process-specific optimal ANN model and optimize the most important process operating variable, i.e., ammonia dosing rate, in a manner such that the process efficiency improves significantly and thereby the SPM amount exhibits substantial reduction.

An accurate ANN based model for the ESP-augmented CFB process has been developed. The inputs to the model are operating conditions of the ESP-augmented CFB process, physical and chemical properties of the coal used in boiler operation as also the ammonia injection rate. The model predicts as its output the magnitude of SPM. The ANN based model was optimized with a view to obtain the optimal values of ammonia dosing rates that would reduce the magnitudes of SPM to the desired levels. User-friendly software comprising the ANN model and GA-based process optimization was developed and given to HWB. The project was sponsored by Heavy Water Board, Mumbai.

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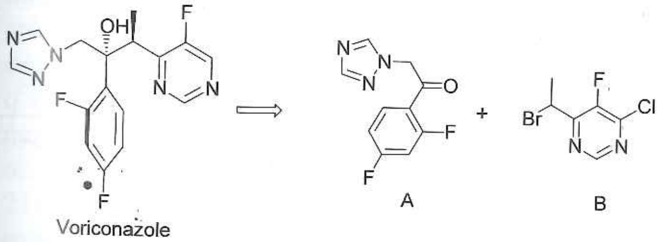
4 ORGANIC CHEMISTRY

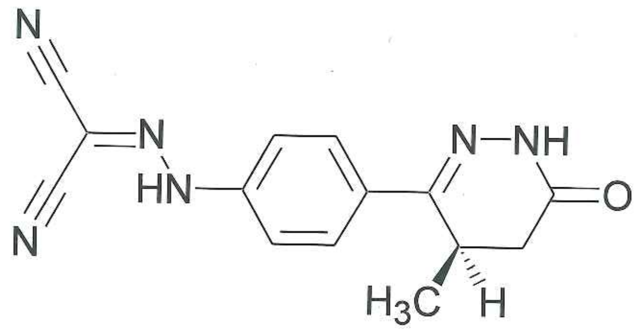
4.1 Process chemistry

Voriconazole (UK-109496) is one of the azole derivatives structurally related to fluconazole which is used as antifungal agent. Voriconazole is referred to as a second generation triazole. Clinical use of voriconazole was approved by FDA in May 2002. It was approved for primary treatment of acute invasive aspergillosis and salvage therapy for rare but serious fungal infections caused by the pathogens *Scedosporium apiospermum* and *Fusarium* spp. Unlike other agents, voriconazole has been approved in both oral and intravenous formulations. The trade name of voriconazole is Vfend™ developed by Pfizer Pharmaceuticals. Selected synthetic strategy involved bromination of 4-chloro-6-ethyl-5-fluoropyrimidine to yield 6-(1-bromoethyl)-4-chloro-5-fluoropyrimidine B which is further treated with intermediate A by the Reformatsky method to yield voriconazole. Simultaneously, efforts are in progress to synthesize voriconazole by a non-infringing route starting from readily available 5-fluorouracil.


Voriconazole
A
B

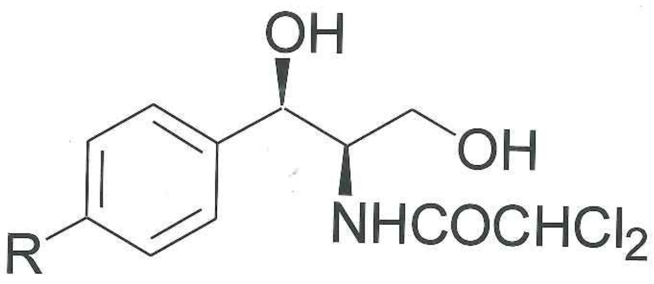
Levasimendan

Levosimendan, (*R*)-(-)-2-[4(4–methyl–6–oxo-1,4,5,6-4H-3pyridazinyl) phenylhydrazono] malononitrile, is an acute heart - failure agent. This medicine has the function of forward-direction adjustment of shrinkage force. It may improve the sensitivity of muscle fiber to calcium through the combination with troponin C. A laboratory process for Levosimendan was developed under sponsorship of M/s CIPLA Ltd., Mumbai. The process for the synthesis of levosimendan starts from acetanilide through the Friedel-Crafts acylation, diethylmalonate alkylation reaction, hydrolysis, decarboxylation and cyclization with hydrazine. The resolution of pyridazine derivative was studied, and levosimendan was prepared from the resolution through two reactions, nitrosation and the reaction with malononitrile.


Levasimendan

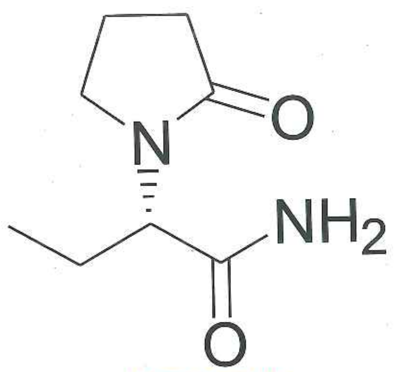
(–)-Chloramphenicol and (+)-thiamphenicol

An efficient enantioselective synthesis of (–)-chloramphenicol (1) and (+)-thiamphenicol (2) is described. These antibiotics have been synthesized from commercially available 4-nitrobenzaldehyde and 4-(methylthio)benzaldehyde, respectively using tethered aminohydroxylation and Sharpless asymmetric epoxidation as the chirality inducing steps.


R = NO_2; Chloramphenicol
R = SO_2Me; Thiamphenicol

Levetiracetam

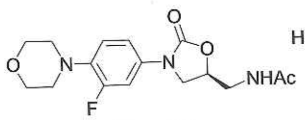
An efficient enantioselective synthesis of a new antiepileptic drug, levetiracetam is described, in high optical purity (>99.5% ee), using proline-catalyzed α-aminooxylation of *n*-butyraldehyde as the key step.



Levetiracetam
(> 99.5% ee)

Linezolid and eperezolid

An efficient enantioselective synthesis of the antibacterials, linezolid (U-100766), and eperezolid (U-100592) using proline-catalyzed asymmetric α-aminooxylation of aldehydes as the key step is described. This is the first report on the enantioselective synthesis of linezolid and eperezolid using asymmetric catalysis.

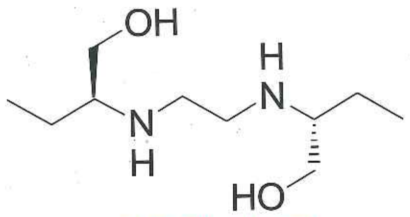


Linezolid

Eperezolid

(S,S)-Ethambutol

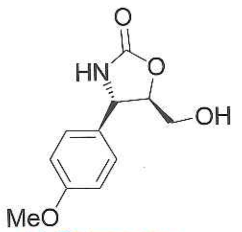
An efficient enantioselective synthesis of (S,S)-ethambutol, a tuberculostatic antibiotic, has been achieved in 99% ee via both proline-catalyzed α-aminooxylation and α-amination of butyraldehyde as the key step.



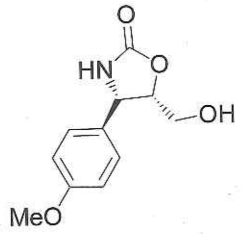
(S,S)-Ethambutol
(99% ee)

(-)-Cytoxazone and (+)-epi-cytoxazone

A short and efficient enantioselective synthesis of (–)-cytoxazone and its stereoisomer (+)-*epi*-cytoxazone, novel cytokine modulators, is described. Ti-catalyzed Sharpless asymmetric epoxidation of allyl alcohol and L-proline catalyzed three-component Mannich reaction constitute the key steps in introducing stereogenicity into the molecule.



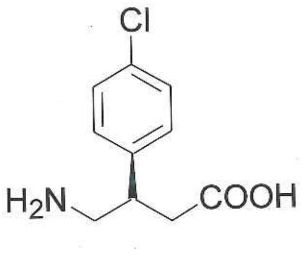
(-)-Cytoxazone



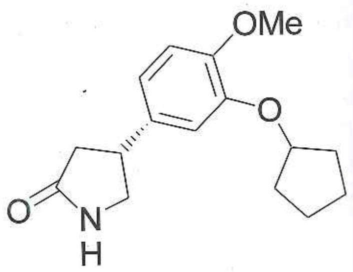
(+)-epi-Cytoxazone

(R)-Baclofen and (R)-rolipram

Sodium borohydride in combination with a catalytic amount of CoCl$_2$ has been found to be an excellent catalytic system in reductive cyclizations of suitably substituted azido and cyano groups of α,β-unsaturated esters to afford γ- and δ-lactams in high yields. The process has been demonstrated for the enantioselective synthesis of (*R*)-baclofen, (*R*)-rolipram, and (*R*)-4-fluorophenylpiperidinone, a key intermediate for (–)-paroxetine.



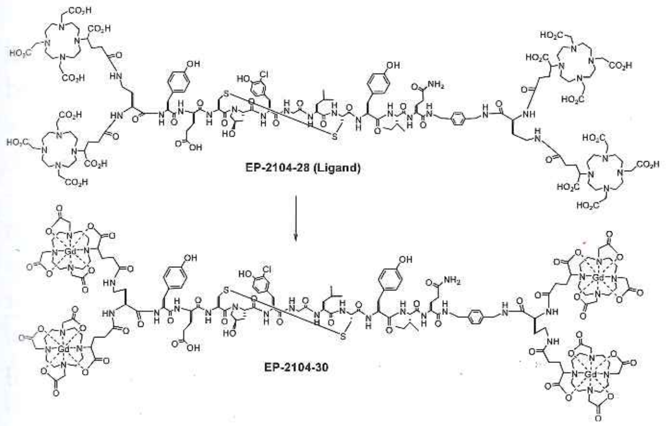
R-(-)-Baclofen



R-(+)-Rolipram

Magnetic resonance contrast agent

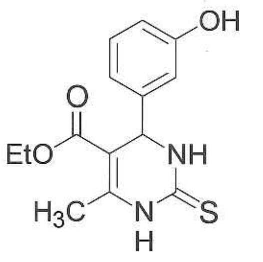
One of the most challenging areas of research in cell biology is tracking cell signaling pathway to understand mechanisms. The most popular and general method for imaging cell signaling is light microscopy, which employs the use of organic dyes or fluorescent receptor proteins. However, these techniques are limited by light scattering, frequently produce photo bleaching byproducts, and require invasive data collection. Magnetic resonance imaging (MRI) can overcome these problems which visualize intact opaque organisms in three dimensions and, therefore, provide an alternative to light microscopy and radiopharmaceutical methods. MRI is a powerful noninvasive technique for the visualization of soft tissue anatomy and for the diagnosis of diseases. Some phenomena of interest, such as angiogenesis (the formation of new blood vessels), are difficult to image with MRI. Therefore, target specific MRI contrast agents designed to bind to proteins, expressed by the cells involved in angiogenesis, could improve the imaging of this process drastically due to the accumulation of contrast agents around these cells.



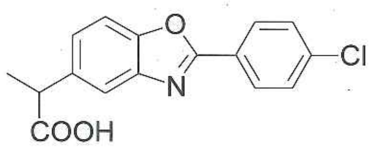
Chelates of gadolinium act as the efficient contrast agents for MRI by shortening bulk water proton relaxation times through rapid exchange of an inner-sphere bound water molecule with bulk solvent. NCL along with D & O Pharmachem Inc. and EPIX Pharmaceuticals, USA jointly developed a solution phase synthesis and characterization of new type of MRI contrast agent (EP-2104-30) based on optically pure organic chelating ligand (EP-2104-28). So far this molecule was synthesized by solid phase synthesis. However due to limitations of a scalable process, it was decided to devise a solution phase synthesis of this tetradecapeptide. The tetradecapeptide was synthesized for the first time by solution phase chemistry and viability of solution phase chemistry was established for scale up studies. The multistep synthesis was achieved in better chemical and optical purity than the one by solid phase synthesis (>99.5% purity).

4.1.2 Achiral drugs

Several ionic liquids (ILs) based on 1 3-di-*n*-butyl and 1-nbutylimidazolium salts with varying anions were synthesized and evaluated. Various biologically active heterocycles such as substituted 1,5-benzodiazepines, quinolines, benzimidazoles, benzoxazoles, benzthiazoles, triarylimidazoles, 2-aryl quinazolinones and 1,2,4-triaryl triazines were synthesized using the prepared ILs under mild conditions in excellent isolated yields without the need for any additional catalyst. Few commercial drugs incorporating some of the heterocycles indicated above were also synthesized using the methodologies developed. Examples are as shown below:



Monastrol

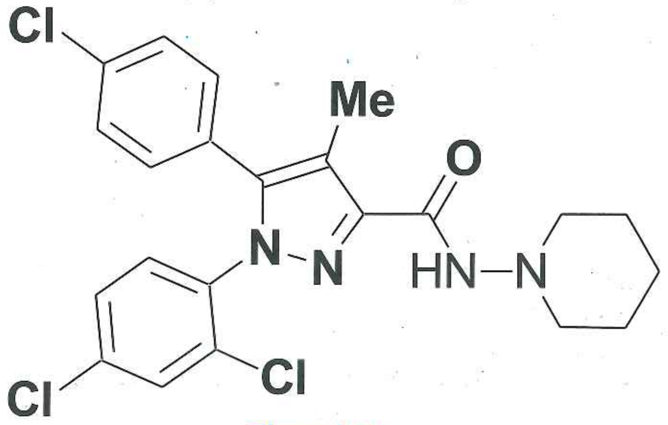


Coxigen
(Benoxaprofeneroidal)
Nonsteroidal anti-inflamma-tory and analgesis

The efficacy of these ILs to promote the heterocyclization reaction was correlated to the basicity of anions. It was observed that with increasing basicity of the anions there was a progressive increase in the yield. Evidence based on ^{1}H and ^{13}C-NMR chemical shift values indicating the hydrogen-bonded interaction of functional groups with IL to generate reactive species was obtained.

Rimonabant

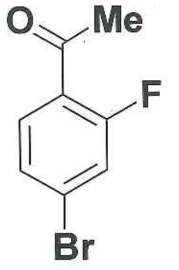
Rimonabant is a drug used for the treatment of obesity and as a potential agent for cessation of smoking. A laboratory process for rimonabant was developed under sponsorship of M/s CIPLA Ltd., Mumbai. The process for the synthesis of rimonabant involves six steps using chlorobenzene, propionyl chloride, 2,4-dichlorophenylhydrazine and N-amino-piperidine as starting materials.

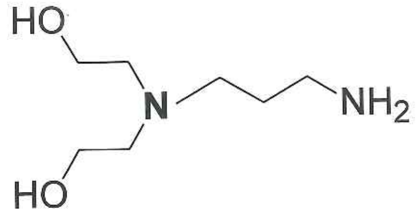


Rimonabant

Intermediates for anti-obesity drug

4-Bromo-2-fluoroacetophenone and N,N-Bis-(2-hydroxyethyl)-1,3-diaminopropane





4-Bromo-2-fluoroacetophenone is a key intermediate for the synthesis of anti-obesity drugs. The known processes for its synthesis involve cryogenic reactions and are not amenable for scale up on a large scale. A convenient new process for the synthesis of the key intermediate was developed using modified Weinreb reaction. The process developed is simple, involves use of cheap raw materials and easy to scale-up. The know-how has been transferred to M/s Peptimmune Inc., USA. A two-step convenient laboratory process for the title compound was developed by condensation of bis-ethanolamine and acrylonitrile followed by catalytic hydrogenation. The advantages of the process are reaction conditions are mild, does not require high hydrogen pressure and the reactions can be scaled-up easily.

An improved process for the preparation of cycloalkylphenols

An improved process for the preparation of cycloalkylphenols which comprises (i) reacting phenolic or substituted phenolic compound with alkylating agent in the mole ratio of 1:10 to 1:1.25 in presence of known catalyst such as montmorillonite K-10 clay in the range of 90-200 °C for a period of 2 to 20 h, (ii) cooling the reaction mixture to ambient temp., filtering the catalyst to obtain crude reaction mixture containing product, and (iii) isolating the product from reaction mixture by known methods, is provided. Thus, reacting 4-chlorophenol with cyclohexanol in the presence of montmorillonite K-10 clay at 120°C for 12 hr afforded 75% 4-chloro-2-cyclohexylphenol.

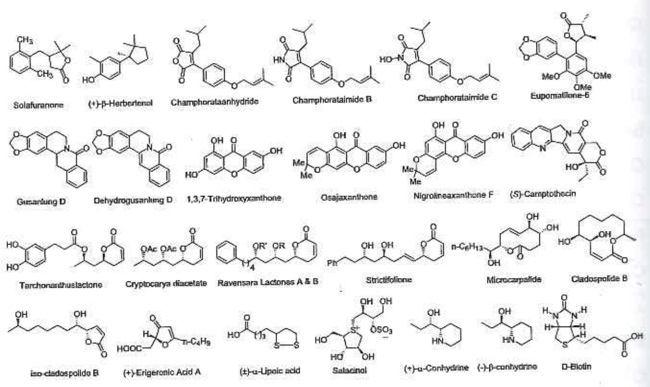
Synthesis of substituted isoxazole

Substituted isoxazoles are important intermediates in the synthesis of tetracycline derivatives (capable of killing bacteria resistant to other antibiotics). A facile synthesis of these derivatives was unveiled.

4.2 Organic synthesis

4.2.1 Total synthesis

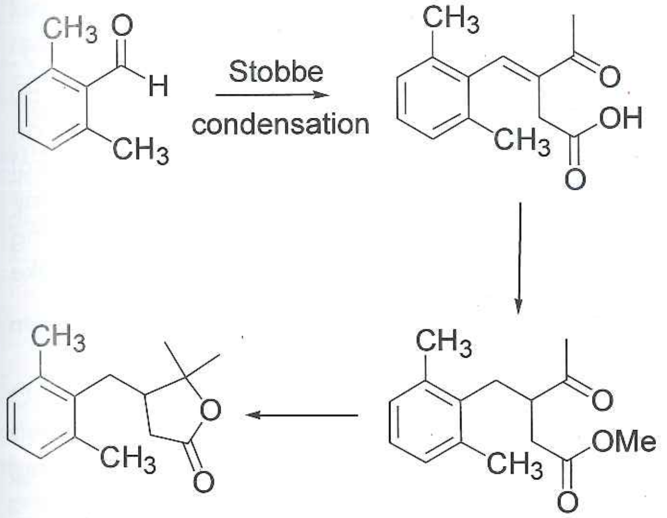
The field of discovery and synthesis of biological active natural products represents a dynamic and largely growing research area. By the use of new strategies to discover natural products of interest, many molecules with novel structural features have been isolated and their structures have been elucidated.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



Representative natural products synthesised

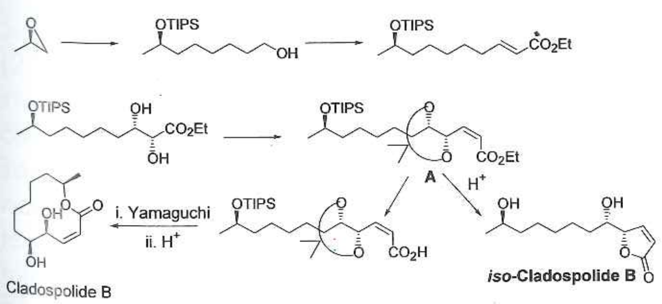
Synthesis of solafuranone

Syntheses of solafuranone, combretastatin analogues and designed benzylidene teralones were completed using Stobbe condensation as the key C-C bond making reaction. Thus, Stobbe condensation of 2,6-dimethyl benzaldehyde with ethyl levulinate afforded the arylidenelevulinic acid as a major component along with the minor regioisomer which was esterified with diazomethane to give the corresponding ester in quantitative yield. This ester was hydrogenated and reacted with methylmagnesium iodide in presence of anhydrous cerium chloride to afford the natural product solafuranone in racemic form.

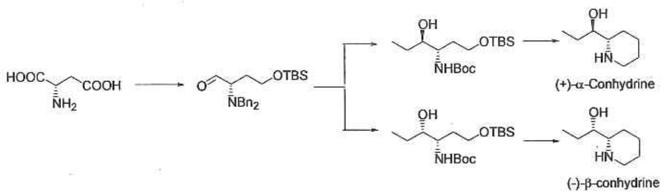


Solafuranone

Cladospolide: The novel hexaketide compounds *iso*-cladospolide B and cladospolide B were isolated from the fungal isolate I96S215. Cladospolide B is inhibitory to shoot elongation of rice seedlings (*Oryza sativa* L.) without damaging the cells. An efficient synthesis of *iso*-cladospolide B and cladospolide B has been achieved using Jacobsen's hydrolytic kinetic resolution (HKR), Sharpless asymmetric dihydroxylation and Yamaguchi macrolactonization as the key steps. As shown below, chiral propylene oxide prepared by using Jacobsen's hydrolytic kinetic resolution was manipulated using simple synthetic transformations and Sharpless asymmetric dihydroxylation to obtain the key intermediate A. The utility of A synthesize either *iso*-cladospolide B and cladospolide B by simple selective deprotection and subsequent lactonisations was demonstrated.



Conhydrine: Biologically active alkaloids containing a 2-(1-hydroxyalkyl)piperidine unit are abundant in nature. (+)-α-conhydrine and (-)-β-conhydrine, are two such alkaloids isolated from the seeds and leaves of the poisonous plant *Conium maculatum* L.

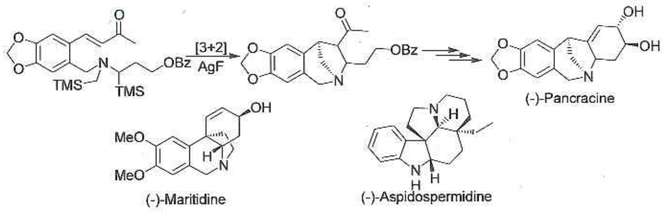


An efficient synthesis of (+)-α-conhydrine and (–)-β-conhydrine was achieved starting from L-aspartic acid by diastereoselective alkylation of an amino aldehyde derivative with ethylmagnesium bromide or diethylzinc and subsequent cyclizations.

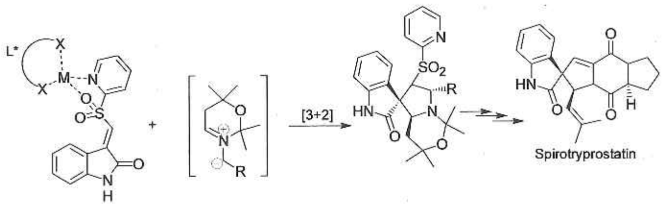
Alkaloids via [3+2] cycloadditions of nonstabilied AMY

A conceptually new synthetic route for the construction of structurally complex pentacyclic 5,11-methanomorphanthridine core structure in one step employing an intramolecular 1,3-dipolar cycloaddition of nonstabilzed azomethine ylide (AMY) generated in situ by sequential double desilylation approach was developed. This strategy is further demonstrated for the formal total synthesis of Pancracine, an important member of montanine type of Amaryllidaceae alkaloid. The crinine class of alkaloids like maritidine, oxomaritidine and vittatine possessing immumo-stimulatory, cytotoxic and anti-cancer activities are being synthesized using similar strategy. A new route was designed for the synthesis of optically active indole alkaloid aspidospermidine, having pentacyclic framework with quaternary and tertiary stereo centers from cheaply available 2-bromopyridine utilizing asymmetric birch reduction and intramolecular 1,3-dipolar [3+2] cycloaddition of nonstabilized AMY. After successful asymmetric Birch reduction, the synthesis is marching now towards an advanced intermediate of aspidospermidine.

ORGANIC CHEMISTRY

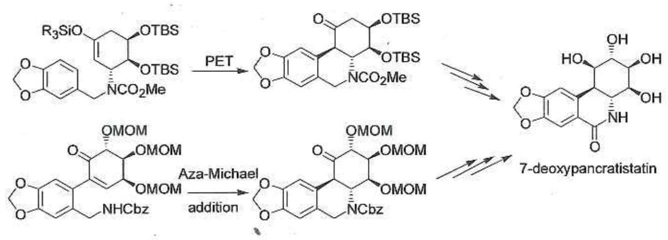


A catalytic asymmetric [3+2] cycloaddition strategy of masked cyclic nonstabilized AMY is developed to build optically pure pyrrolidines. This strategy has been applied to synthesize (+) and (-) elacomine and spirotryprostatin B and biologically important spiro oxindole alkaloids. The evaluation of chiral induction in catalytic asymmetric 1,3-dipolar cycloaddition is ongoing at present.



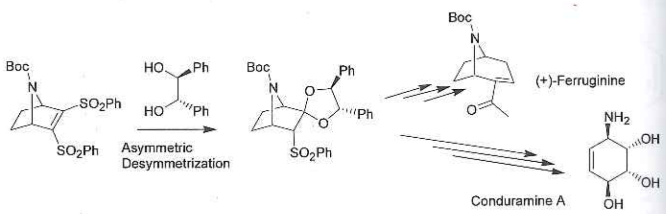
Synthetic studies towards an amaryllidaceae alkaloid, 7-deoxypancratistatin

A synthetic route based on the intramolecular cyclization of silylenol ethers to PET initiated arene radical cations has been demonstrated for the total synthesis of 7-deoxypancratistatin, an anti-cancer and anti-viral agent belonging to amaryllidaceae alkaloids. The synthesis has utilized versatile chiral pool D-(-)-quinic acid as the chiral source to build the highly oxygenated C-ring of the target molecule. The methodological diversity of our group is also demonstrated by the synthetic design to the 7-deoxypancratistatin using an intramolecular aza-Michael addition approach. The phenanthridone skeleton has been effectively constructed via intramolecular aza-Michael addition of carbamate tethered α-aryl enone. A suitably substituted chiral enone, derived from D-(-)-quinic acid undergoes similar transformation to yield analogue of 7-deoxypancratistatin.



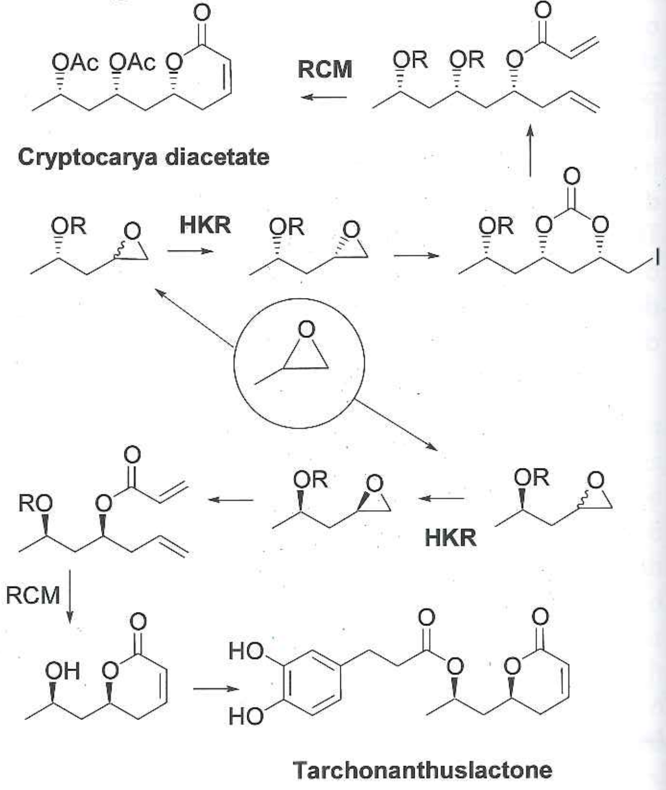
Asymmetric Desymmetrization: An efficient way of making enantiopure entities

Asymmetric desymmetrization of enantiopure 7-azabicyclo [2.2.1] heptane skeleton by enantiotopic discrimination between carbon atoms of a double bond in a reaction of chiral alcoholates with *meso*-bis (phenyl sulfonyl) alkene was studied earlier. Currently the skeleton is being exercised for the synthesis of natural products like Ferruginine, Conduramine A, etc.



Tarchonanthuslactone and cryptocarya diacetate

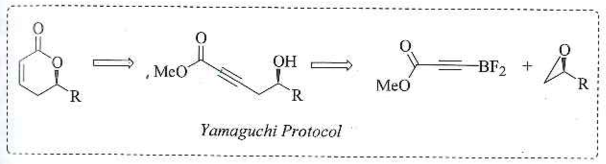
Optically active *syn*-and *anti*-1,3-polyols/5,6-dihydropyran-2-ones are ubiquitous structural motifs in various biologically active compounds. Such compounds are endowed with broad range of biological activities.

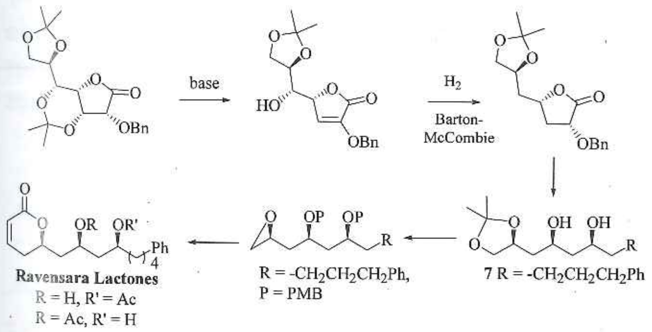


ORGANIC CHEMISTRY

A simple and efficient approach to 1,3-polyols in desired *syn-* or *anti-* fashion by iterative hydrolytic kinetic resolution of an epoxide and vinyl Grignard reaction has been successfully applied for the synthesis of some biologically active products. Thus, a short and practical enantioselective synthesis of tarchonanthuslactone and cryptocarya diacetate have been achieved in high diastereomeric excess using Jacobsen's hydrolytic kinetic resolution, diastereoselective iodine induced electrophilic cyclization and ring closing metathesis as the key steps.

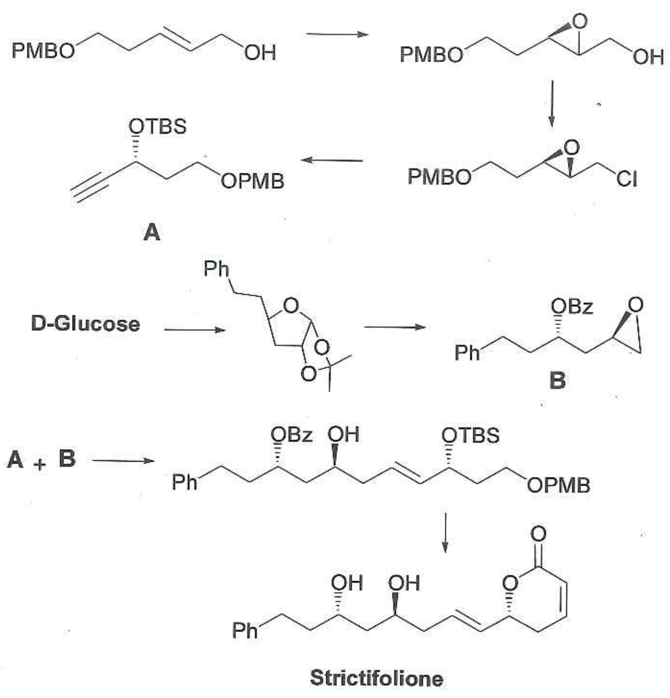
On the other hand, a novel elimination and stereoselective hydrogenaton on a sugar derived heptonolactone has been amply applied to prepare *syn-* and *anti-*configured 1,3-polyols in less than 5 steps and one of the intermediate has been amply applied to address the first total synthesis of naturally occurring enantiomers of ravensara lactones A and B.





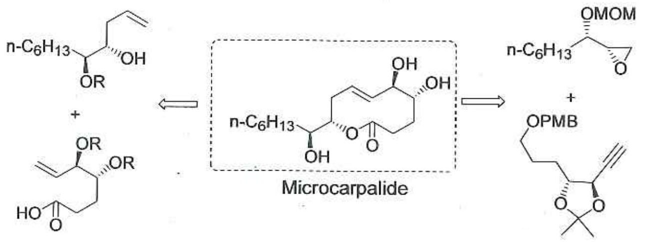
Strictifolione

Strictifolione was isolated by Aimi and co-workers (2000) from the stem bark of *Cryptocarya strictifolia*. The relative and the absolute configuration of strictifolione were revised by the same group. The broad range of biological natural products was ascribed to their inherent tendency to act as good Michael acceptors. The total synthesis of strictifolione using a combination of chiral pool approach and an asymmetric epoxidation reaction has been accomplished.



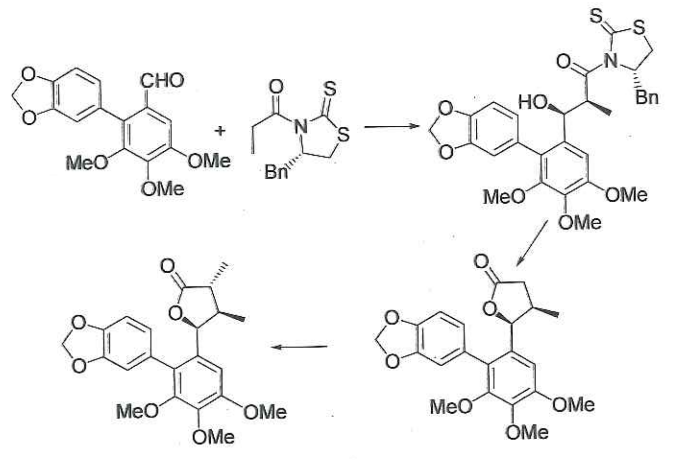
Microcarpalide

Microcarpalide, a new alkyl-substituted nonenolide, was isolated by Hemscheidt and co-workers in 2001 from fermentation broths of an unidentified endophytic fungus growing on the bark of *Ficus microcarpa* L. This compound acts as a strong antimicrofilament disrupting agent and displayed a weak cytotoxicity to mammalian cells, thus making it an attractive tool for studying cell motility and metastasis, and a potential lead structure to develop new anti cancer drugs. Microcarpalide belongs to a class of cyclic 10-membered macrolactones and posses an internal Z-configured olefin. Its structure and the promising biological activity have stimulated substantial synthetic work, culminating in several total syntheses. Three different approaches for the total synthesis of microcarpalide have been reported from NCL. Amongst the three approaches, two are convergent and use RCM as key reaction. The other linear approach use opening of an exoxide with an alkyne to form the requisite central carbon followed by Yamguchi macrolactonization.



Eupomatilone 6

In the process of establishing the relative configuration of eupomatilone-6, the proposed/ possible diasteromers of eupomatilone-6 were synthesized. The center of the synthesis is the stereoselective methylation at C-3 of a 4,5-disubstituted γ–butyrolactone to address the requisite 3,4,5-*trans-cis* and *trans-trans-* relative configuration. This synthetic exercise has been further extended by completing the first synthesis of optically active (3*R*,4*R*,5*S*)-eupomatilone-6 and established the absolute configuration of naturally occurring eupomatilone-6 as (3*S*,4*S*,5*R*).



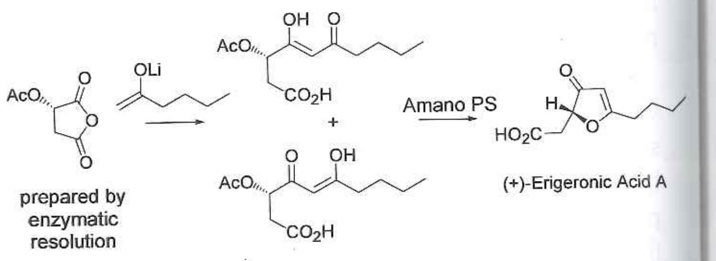
(-)-Eupomatilone 6

Cyclic anhydrides as versatile starting points

Use of cyclic anhydrides as potential precursors in total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids, employing variety of new synthetic strategies is an active area at NCL for several years. A few natural products were synthesized during this year using these precursors which include, camphorataanhydride, camphorataimide B, camphorataimide C, (+)-erigeronic acid A, gusanlung Dehydrogusanlung D and nuevamine skeleton.

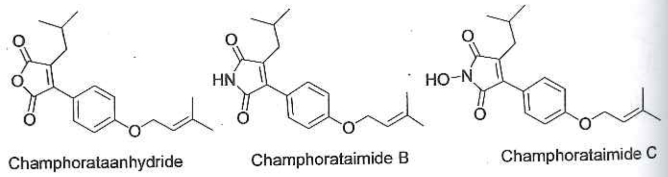
(+)-Erigeronic acid A

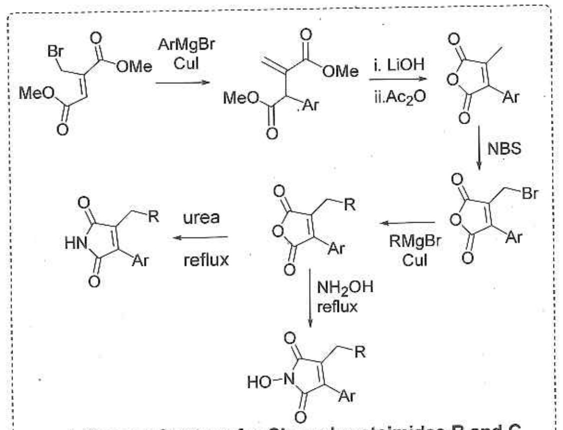
Starting from (*R*)-acetoxysuccinic anhydride, an elegant first synthesis of natural germination inhibitor (+)-erigeronic acid has been demonstrated using chiral pool strategy and an enzymatic hydrolysis pathway, which helped to assign (*R*)-configuration to the C-2 chiral centre. In the present synthesis of (+)-erigeronic acid, the highly regioselective ring opening of anhydride with the primary enolate of butyl methyl ketone and an enzymatic hydrolysis of intermediate keto-enol mixture and subsequent *in situ* dehydrative cyclization to form (+)-erigeronic acid are noteworthy.



Champhorataanhydride and champhorataimides B and C

The first synthetic approach to natural camphorataanhydride and bioactive camphorataimides B and C was reported. As depicted below, in the approach developed, the stepwise functionalization and generation of anhydride moiety with a variety of alkyl/ allyl/ benzyl/ aryl groups and conversion of anhydride to a variety of N-substituted maleimides provides sufficient flexibility to synthesize various analogues of camphorataimides.

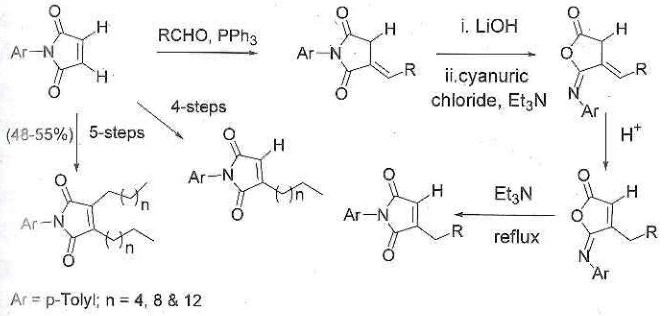




A General Strategy for Champhorataimides B and C

Bioactive natural products synthesized from cyclic anhydrides

A simple and efficient approach to alkylmaleimides and dialkylmaleimides via the two Wittig coupling reactions, taking advantage for the first time of kinetically controlled isoimides as intermediates to enforce the difficult migration of exocyclic carbon–carbon double bonds to the endocyclic position is demonstrated. A small library of compounds synthesized by using this contrathermodynamic rearrangement containing several alkyl and dialkyl substituted maleimides was synthesized.

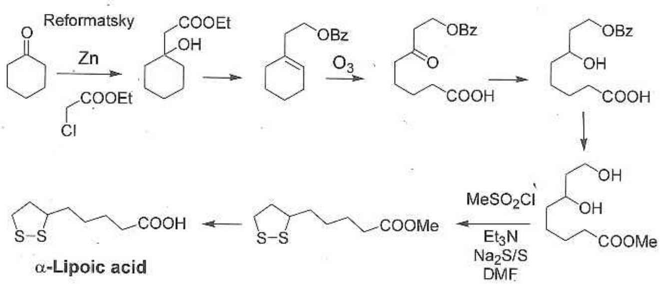


Synthesis of naturally occurring xanthones

A facile five-step synthesis of naturally occurring 1,3,7-trihydroxyxanthone has been described starting from 1,3,5-trimethoxybenzene via NBS-induced nuclear bromination, lithiation followed by an in situ benzoylation with methyl-2,5-dibenzyloxybenzoate, selective deprotection of the two benzyl groups, base-catalyzed intramolecular cyclization, and demethylations pathway. The regioselective coupling reactions of 1,3,7-trihydroxyxanthone with prenal in the presence of calcium hydroxide at room temperature and under thermal conditions at 140-150 °C have been demonstrated to exclusively obtain the natural products osajaxanthone and nigrolineaxanthone F, respectively.

α-Lipoic acid

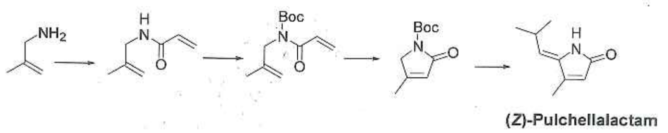
α-Lipoic acid has been shown to possess antioxidant abilities against attack by free radical as well as an inhibitory effect against HIV replication. Interplay between lipoic acid and glutathione in the guardianship against lipid peroxidation and metal toxicity has also been demonstrated. Moreover, lipoic acid is used to a great extent in the treatment of various diseases such as alcoholic liver diseases, mushroom poisoning, metal poisoning, diabetes, and neurodegenerative disorders. A simple nine-step synthesis of α-lipoic acid has been documented. Synthetic sequence with some of the key intermediates is given below:



Synthesis of α-lipoic acid

(Z)-Pulchellalactam

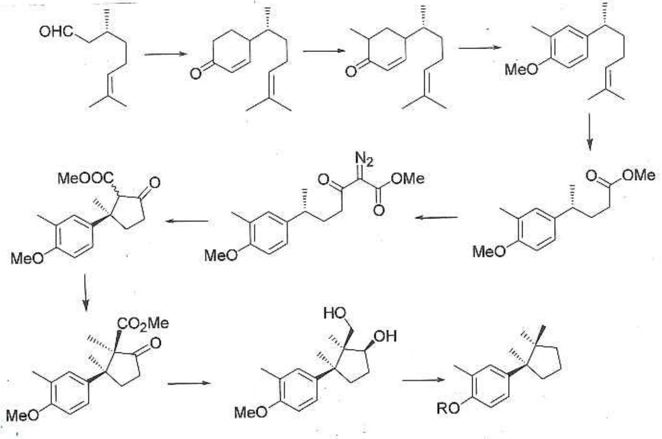
(Z)-Pulchellalactam, a pyrrolidinone, isolated in 1997 from the marine fungus *Corollospora pulchella* by Alvi *et al.* has been in focus due to its potent inhibitory action against protein tyrosine phosphatase, (PTP) CD45, which in turn activates B and T cells. Protein tyrosine phosphatase has been a target implicated in autoimmune and anti-inflammatory diseases. Employing RCM as the key step, a four-step synthesis of (Z)-pulchellalactam has been accomplished from acrylamide in an overall of yield of 54%.



Synthesis of (*Z*)-pulchellalactam

(+)-β-Herbertenol

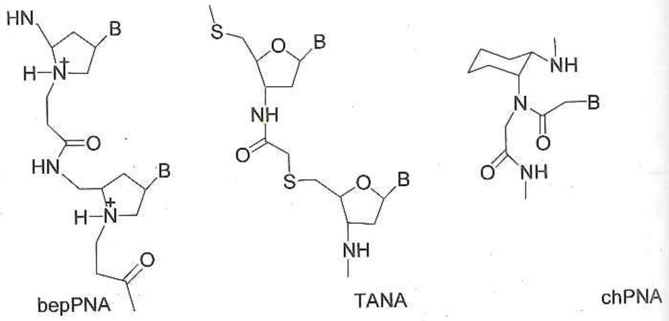
β-Herbertenol is a sesquiterpenoid, possessing 3-methyl-1-(1,2,2-trimethylcyclopentyl) cyclohexane skeleton, isolated from the herbertous species and other liverworts. It contains an oxygenated aromatic six membered ring and shows a wide spectrum of biological properties, which include potent antifungal, neurotrophic and anti-lipid peroxidation activities. Because of the difficulties associated with the construction of the vicinal quaternary carbons in the cyclopentane ring, herbertanes and cuparanes have become popular synthetic targets in recent years. Although, there are synthetic strategies reported towards (±)-β-herbertenol, not a single asymmetric synthesis is reported. The first enantiospecific synthesis of (+)-β-herbertenol was reported starting with R-citronellal and using rhodium mediated carbene insertion as the key step for the central cyclopentane ring formation.



Enantiospecific synthesis of β-herbertenol

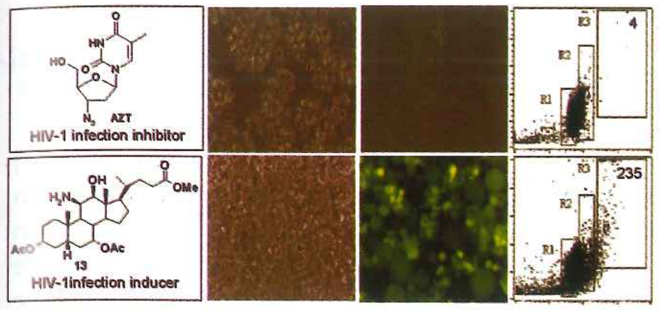
4.2.2. Organic biomolecular chemistry

Development of molecular entities that specifically bind to complementary RNA sequences is gaining importance in last 3-4 years after the development of RNA interference, miRA, steric blocking splice correction and exon skipping as offshoots of antisense therapeutics. These techniques require highly stable sequence specific RNA complexation for steric blocking of cellular enzyme functions. Sequences that bind to RNA usually bind also to DNA because of the flexibility of DNA backbone to conformationally adapt to be like RNA backbone. However, there are some examples in the literature such as 2′,5′-RNA, 2′,5′,3′-deoxy NA, and TNA that bind specifically to RNA over DNA. The 5-atom internucleotide linkers in amide-sugar backbone also are known to show better binding to RNA over DNA. Our recent research efforts that include the synthesis of a 5-atom amide linker in pyrrolidinyl PNA (bepPNA) showed sequence specific recognition of complementary RNA sequences. The homogeneous pyrrolidinyl PNA, being positively charged was less efficient in binding in triplex mode due to charge aggregation. The pyrrolidine ring geometry is flexible and is known to show base-dependent effects of nucleic acid affinities. To circumvent these problems, we chose to synthesize 5-atom sugar-thioacetamide linked oligomers (TANA). The homogeneous sequences exhibited excellent RNA selectivity over DNA and also over single base mismatched RNA. The cyclohexyl-PNA, a rationally designed PNA analog also was synthesized that showed RNA selectivity in both duplex and triplex modes. A six membered piperidinyl PNA was synthesized that showed selectivity of binding to RNA over DNA.



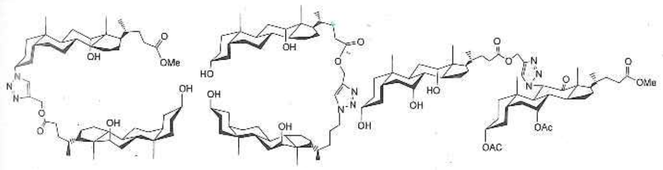
Amino functionalized novel cholic acid derivatives induce HIV-1 replication and syncytia formation in T cells

C-11 Azido/ amino functionalized cholic acid derivatives were synthesized in excellent yields. Contrary to the previous prediction of such analogous compounds to be HIV-1 protease inhibitors, surprisingly these compounds were found to enhance HIV-1 replication with induction of syncytia formation. The syncytia inducing property of cholic acid analogues may also be useful for screening the efficacy of compounds which inhibit syncytia induction and also for screening the efficacy of the existing and novel anti-retroviral drugs by artificial enhancement of HIV-1 replication and syncytia formation. This is the first report of syncytia induction and enhancement of viral replication in HIV-1 infected T cells by cholic acid derivatives.



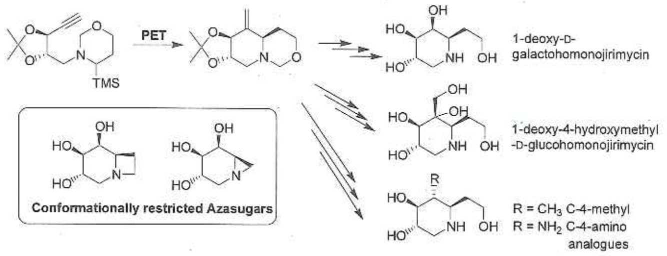
Synthesis of bile acid dimers linked with 1,2,3-triazole ring at C-3, C-11 and C-24 positions

New bile acid dimers containing 1,2,3-triazole as linker at C-3 and C-24 positions in high yield by [2 + 3] cycloaddition reaction have been synthesized. A highly hindered azido group at C-11 also has been converted to triazole using click chemistry to get dimer at C-11 position of cholic acid in high yield. These new molecules may find applications in molecular recognition, supra-molecular chemistry and pharmacology. This is the first report of use of click chemistry in bile acid chemistry.



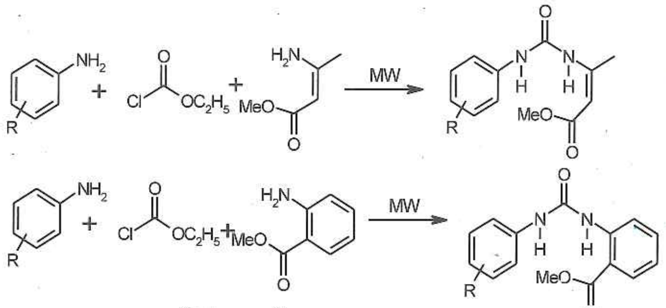
Synthesis and Evaluation of Azasugars as Glycosidase inhibitors

New and stereoselective strategy to synthesize an appropriate common template to obtain C-6 homologues of 1-deoxy-D-galactohomonojirimycin, 1-deoxy-4-hydroxymethyl-D-glucohomonojirimycin and their enantiomers by the cyclization of photoinduced electron transfer (PET) generated α-trimethylsilylmethylamine radical cation to the tethered alkyne functionality. The same template is also efficiently used to obtain neutral non-basic pseudo-glyconolactam, C-4 amino and methyl analogues of 1-deoxy-homonojirimycin as new analogues of 1-deoxyhomoazasugars. Some of these azsugars have shown specific enzyme inhibition. The conformationally restricted polyhydroxy azabicyclo [4.1.0] and azabicyclo [4.2.0] sugars are also being studied in our laboratory.



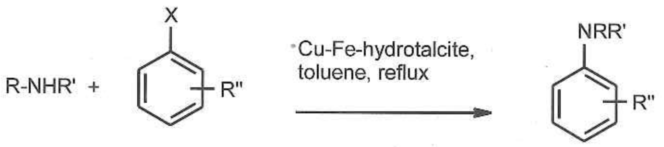
4.2.3. New synthetic methods

1. **An efficient one-pot synthesis of N,N′-disubstituted urea derivatives** from substituted anilines, ethyl chloroformate and methyl anthranilate or methyl 3-amino-2-butenoate under microwave irradiation has been reported.



Scheme-1

2. **An efficient N-arylation of amines with aryl halides in presence of heterogeneous recyclable Cu-Fe-hydrotalcite catalyst has been developed.**



R-NHR'=Substituted aniline, indole, cyclohexyl amine, benzyl amine

X=Br, I

R"=H, OMe, NO$_2$, Cl, CHO

3. A simple method for deprotection of *tert*-butyldimethylsilyl ethers by using stannous chloride under microwave irradiation

A facile regeneration of hydroxy compounds from their *tert*-butyldimethylsilyl ethers in presence of stannous chloride under solvent free conditions using domestic microwave oven has been performed efficiently in a short period (5-6 min). The conversion using stannous chloride in ethanol or water for comparison of the efficiency has been described. The generality of the transformation is confirmed using several examples.

$$\text{R-OTBDMS} \xrightarrow[\text{MW irradiation OR}]{SnCl_2} \text{R-OH}$$

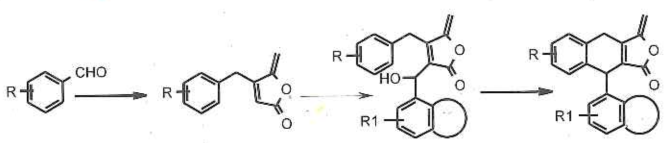
Ethanol or water
r.t. or reflux

R= alkyl, phenyl, naphthyl *etc*

4. Synthesis of 5-methylene –4-substituted-2(5H)-furanones

was achieved in two steps from ethyl levulinate and aryl aldehyde. The generality of the methodology was exhibited by several examples which provided a library of novel molecules for cytotoxic activity.

5. An efficient synthesis of novel 1,4-dihydronaphthalene lignans from 5-methylene-4-substituted-2(5*H*)-furanones



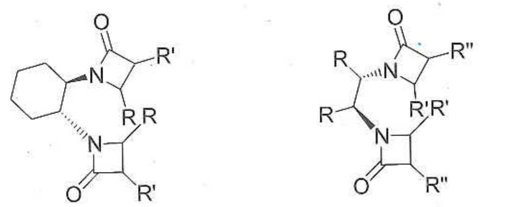
A number of novel lignan analogues have been synthesized in good yields by a short synthetic strategy involving preparation of 5-methylene-4-substituted-2(5*H*)-furanones followed by reaction with various substituted aldehydes in presence of LDA and subsequent cyclization with TFA.

6. 2-Benzylidene-tetralones were subjected to magnesium directed addition of benzyl bromides when unexpected conjugate addition products predominated as against the expected 1,2-addition products. A library of 30 novel compounds was generated.

7. Synthesis of C2-symmetric β-lactams:

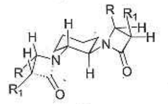
Synthesis of β-lactams using Staudinger's [2+2] cycloaddition reaction of ketenes with imines is an active area of our research. This has been successfully demonstrated by the synthesis of large number of substituted β-lactams. A synthetic method has been developed for bis-β-lactams from vicinal bisimines. The C_2-symmetric bis-imines on cycloaddition reaction with ketenes give C_2-symmetric bis-β-lactams in very good yields.

C_2-Symmetric bis β-lactam

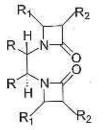


R = Aryl, R' = O-Aryl/alkyl

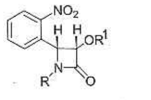
R = CH_3, Ph
R' = Alkyl, Aryl
R" = O-Alkyl, O-Aryl



1



2



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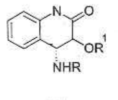


4

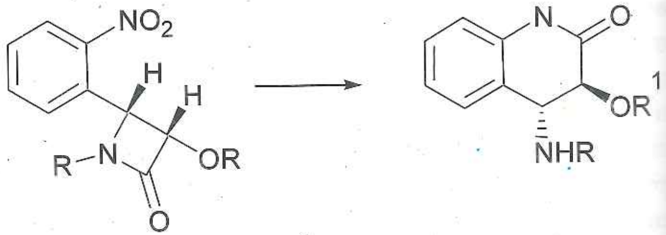
C_2-Symmetric bis betalactam
R = Aryl, R1 = O-Aryl/alkyl

R = CH_3, Ph
R_1 = Alkyl, Aryl
R_2 = O-Alkyl, O-Aryl

R, R^1 = Alkyl, Aryl etc

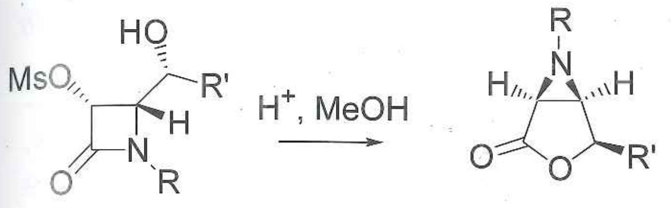
R, R^1 = Alkyl, Aryl etc

8. A methodology using β-lactams as synthons for the synthesis of various biologically important dihydroquinolinones compounds was developed.



R, R^1 = Alkyl, Aryl etc

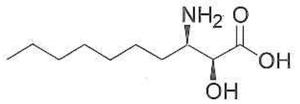
9. Synthesis of (2*R*,3*S*) and (2*S*,3*R*)-3-amino-2-hydroxydecanoic acid (AHDA), which is an important part structure of natural product microginin is accomplished.



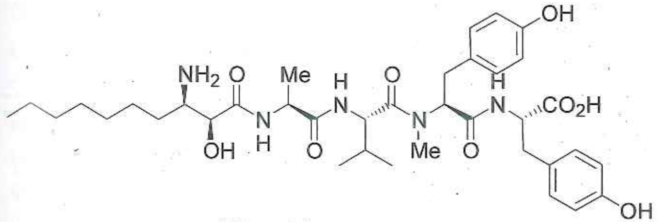
R = aryl
R' = H or CH_2OH
R" =

10. 2,3-Aziridinolactones from β-lactams

A small library of 2,3-aziridino-γ-lactones, *trans* C-3-Alkyl/ Aryl azetidin-2-ones an important precursors for biologically important glutamic acid derivatives was synthesized from β-lactams.



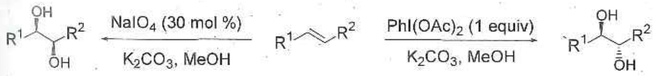
(2S,3R)-3-Amino-2-hydroxydecanoic acid



Microginin

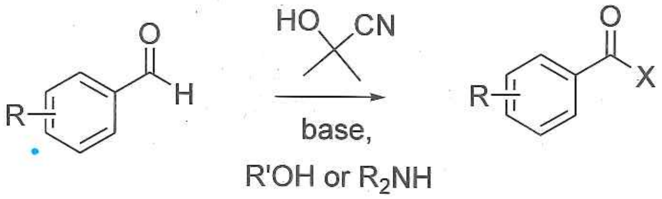
11. $NaIO_4$/LiBr-mediated diastereoselective dihydroxylation of olefins: A catalytic approach to the Prevost-Woodward reaction

LiBr catalyzes efficiently the dihydroxylation of alkenes to afford syn and anti diols with excellent diastereoselectivity depending upon the use of $NaIO_4$ (30 mol %) or $PhI(OAc)_2$ (1 equiv), respectively, as the oxidizing agents. The oxidation of non-benzylic halides has been achieved for the first time to afford the corresponding diols in excellent yields.



12. A facile direct conversion of aldehydes to esters and amides using acetone cyanohydrin

Aromatic aldehydes with electron-withdrawing groups undergo rapid reactions with a variety of alcohols and secondary amines to afford the corresponding esters and amides, respectively, in high yields, when treated with NaCN or $Me_2C(OH)CN$ and base under ambient reaction conditions. In case of α,β-unsaturated aldehydes, simultaneous reduction of the C:C bond along with esterification occurred to produce the saturated esters in high yields.



X = OR' or NR'_2

13. Green protocol for the synthesis of N-oxides from secondary amines using vanadium silicate molecular sieve catalyst

Vanadium silicate molecular sieve catalyst VS-1 was found to promote efficiently the oxidation of αα,α'α'-tetrasubstituted secondary amines with 30% aqueous hydrogen peroxide as oxidant. In comparison to other catalysts reported to date, this heterogeneous catalyst offers a remarkably simple workup procedure and is reusable without any appreciable loss of activity.

14. A novel $Cu(OTf)_2$ mediated three component high yield synthesis of α-aminophosphonates

Copper(II) triflate catalyzes efficiently the three-component condensation reaction of an aldehyde, amine and $P(OMe)_3$ in acetonitrile at room temperature to afford the corresponding α-aminophosphonates in high yields.

15. Natural kaolinitic clay: A remarkable catalyst for highly regioselective chlorination of arenes with Cl_2 or SO_2Cl_2

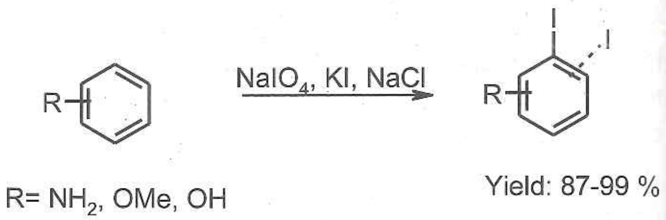
Natural kaolinitic clay containing transition metals such as Fe and Ti in its lattice has been found to exhibit unusual regioselectivity in the liquid-phase chlorination of arenes with either Cl_2 or SO_2Cl_2 as the chlorinating agent para-chlorinated products are predominant for most of the substrates with an exceptional case of ortho-selectivity for the chlorination of aniline.

16. NaIO$_4$-Mediated selective oxidation of alkylarenes and benzylic bromides/ alcohols to carbonyl derivatives using water as solvent

A new transition-metal-free, sodium metaperiodate (NaIO$_4$)-mediated direct oxidation of methylarenes and benzylic bromides to the corresponding aromatic carboxylic acids is described. Under the same reaction conditions, benzylic alcohols are selectively oxidized to afford the corresponding aldehydes in good yields without undergoing over oxidation. Unprecedentedly, oxidation of benzyl bromide, toluene, or benzyl alcohol with NaIO$_4$ underwent nuclear bromination followed by oxidation to give 4-bromobenzoic acid in 60-79% yields.

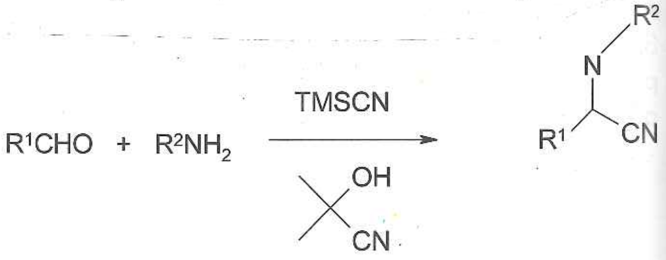
17. NaIO$_4$/KI/NaCl: A new reagent system for iodination of activated aromatics through in situ generation of iodine monochloride

A new reagent system consisting of NaIO$_4$/KI/NaCl in aqueous AcOH was found to be effective in iodinating a variety of activated aromatic substrates via in situ-generated iodine monochloride, to furnish iodo-aromatics in excellent yields. This iodination procedure was applied successfully for a cost-effective synthesis of 3,3'-diaminobenzidine, a key intermediate for preparation proton conducting membranes for fuel cell applications, with high yield and a purity of 99.7%.



18. Cu(OTf)$_2$ or Et$_3$N-catalyzed three-component condensation of aldehydes, amines, and cyanides: a high yielding synthesis of α-amino nitriles

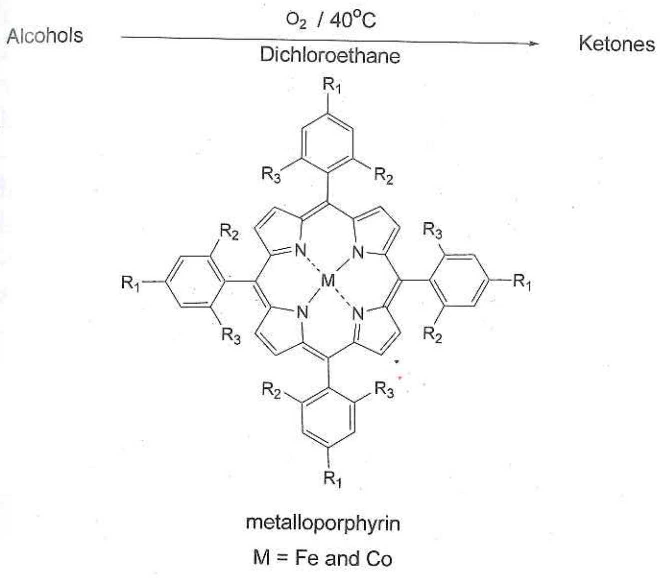
Copper(II) triflate or Et$_3$N were found to catalyze, under ambient conditions, the addition of a cyanide anion, such as trimethylsilyl cyanide or acetone cyanohydrin, onto in-situ generated imines, furnishing α-amino nitriles in excellent yields.



19. Immobilization of metallporphyrins on polystyrene: Efficient catalysts for aerobic oxidation of alcohols

Metalloporphyrins of iron and cobalt have been successfully encapsulated for the first time using polystyrene matrix, exhibiting high activity for ecologically benign aerobic oxidation of alcohols mimicking cytochrome P-450 dependent mono oxygenases. This methodology provides a simple and environmentally friendly protocol for immobilization of metalloporphyrins on to polystyrenes in general, which gives stable, reusable and efficient catalysts for aerobic oxidation of alcohols. These catalysts not only have high turnover frequencies but also could be recovered quantitatively by simple filtration and reused without loss of activity.

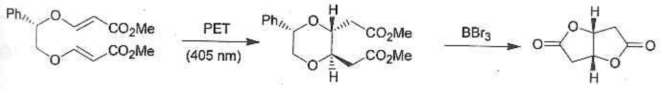
The simplicity and extended scope of the system, the non-hazardous nature of the catalyst and the versatility of the method towards a wide range of activated and non-activated alcohols makes these polymer supported metalloporphyrins catalyzed oxidation an attractive, environmentally friendly synthetic tool for the oxidation of alcohols to ketones by molecular oxygen. The combination of polymer supported MPs and molecular oxygen, as sole oxidant constitutes an excellent example of clean technology process for the oxidation of alcohols.



metalloporphyrin
M = Fe and Co

20. An efficient and short synthesis of a Designer Synthon

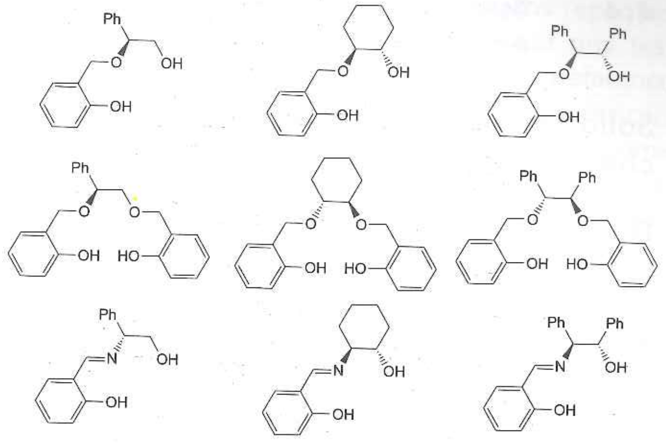
Chiral 6-phenyl-2,3-bismethylenemethoxy carbonyl [1,4] dioxane is synthesized by PET cyclization of a diene as an optically pure multitalented compound for the synthesis of many natural product intermediates such as 2,6-dioxabicyclo[3.3.0]octane-3,7-dione and chiral 1,2-*trans* diols.



4.2.4 Organometallic chemistry

Asymmetric catalysis

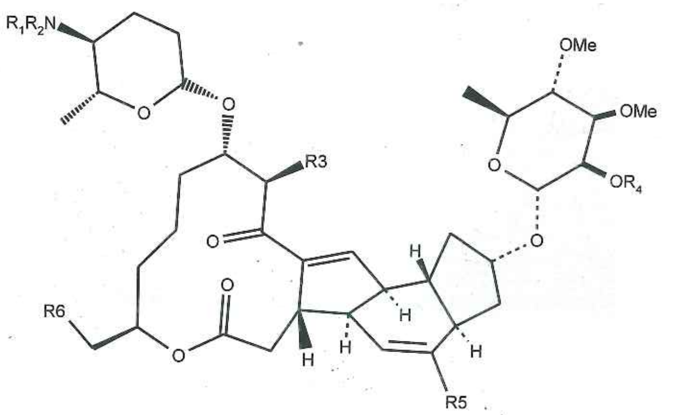
In continuation of our efforts in the area of asymmetric catalysis, attempts were made to develop new chiral ligands with defined properties. These were then used to prepare metal complexes, which in turn were examined as catalysts for selected reactions. This year we studied salen and hemi salen-type ligands. These are multidentate ligands with logically designed architecture suitable for steric and electronic tuning. Additionally, tridentate and tetradentate ligand function renders them useful for a variety of metal complexes.



We have so far examined these as titanium complexes for pinacol coupling. Efforts are underway to prepare other metal complexes suitable for asymmetric reduction, alkylation and aldol reaction.

4.3 Natural products chemistry

A mixture of spinosyns produced by fermentation process was received from industry for identification of the compounds present in the mixture. Column chromatography using silica gel could not separate the mixture satisfactorily, which on HPLC analysis showed presence of one major and four minor components. Therefore, preparative HPLC method was used for separation of the components. The purified compounds were identified on the basis of ^{1}H and ^{13}C NMR, IR and mass spectra and were found to be spinosyn A, spinosyn B, spinosyn D, spinosyn E and spinosyn H.



All the purified compounds (20 to 100 mg.) with their spectral data have been sent to the company along with the report.

4.4 Supramolecular crystal engineering

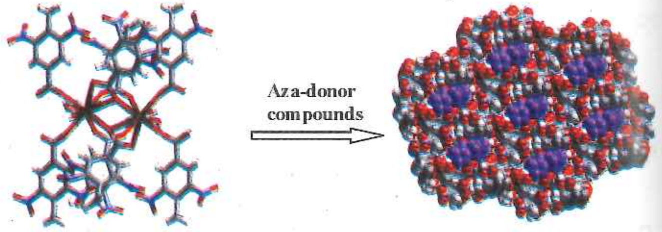
Solid state and supramolecular structural chemistry

Design and synthesis of novel supramolecular assemblies of tailor-made properties governed by the three-dimensional arrangement of molecular entities into distinct architectures such as lamellar sheets, hexagonal networks, cavity and channels structures etc. utilizing non-covalent interactions such as hydrogen bonds, coordination bonds, etc. is the focus of the research themes carried out in solid state and supramolecular structural chemistry laboratory and some successful examples are listed below:

Molecular ladders: Utilization of O-H···N hydrogen bonds, that are generally formed between –COOH and aza-donor moieties, for the construction of the molecular ladders have been demonstrated through supramolecular synthesis of 3,5-dihydroxybenzoic acid with 4,4'-bipyridine/ 1,2-bis(4-pyridyl)ethane/ ethene and analyzing the resulting assemblies with the aid of single crystal x-ray diffraction methods. A typical structural outcome along with an analogy of natural process is represented.

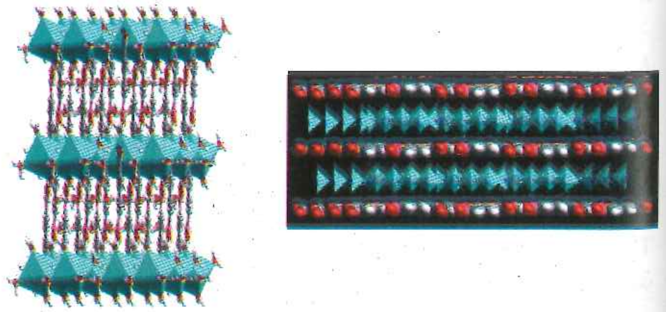
Representation of molecular ladders, mimicking the natural ladders, through ensemble of molecules of dihydroxybenzoic acid and aza-donor compounds

Channel structures: Synthesis of zeolite mimicking structures by coordination bonds was successfully demonstrated through organic-inorganic hybrids and well explored for the application of such systems in catalysis, guest-exchange processes, etc. However, a combination of hydrogen bonds and coordination bondsas design elements were not well known and for this purpose, we synthesized supramolecular Assemblies of 3,5-dinitro-4-methylbenzoic acid and aza-donor compounds (4,4'-bipyridine, 1,2-bis(4-pryidyl)ethane/ethene in the presence of Pr(III). The resultant assemblies formed channel structures such yhat the coordination polymers self-assembled through C-H···O hydrogen bonds yielding channels that are being filled with aza-donor compounds as shown below:



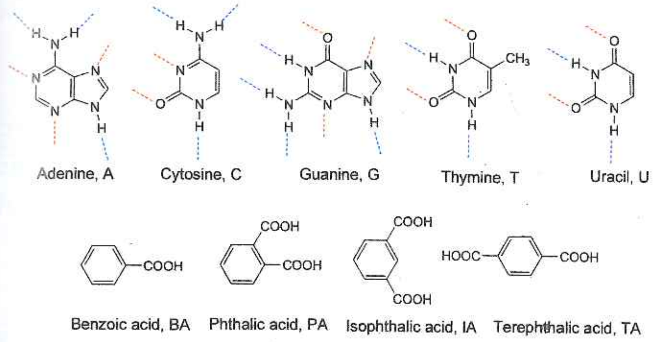
Coordination polymer of 3,5-dinitro-4-methylbenzoic acid forming channels filled with aza-donor compounds (shown in purple)

Lamellar structures: Organic-inorganic hybrid complexes are well known not only for the creation of void structures but also lamellar type of structures to evaluate for conductivity, magnetic studies. In this direction, our endeavor with novel functional group, boronic acid, gave lamellar, structures through secondary coordination networks of metal ions separated by organic entities. In a typical example, reaction between 4-carboxyphenylboronic acid and cobalt nitrate gave a structure as depicted below:



Left: lamellar structure formed between Co(II) and 4-carboxyphenylboronic acid, right: similar structure along with 1,2-bis(4-pyridyl)ethane

Selective molecular recognition: Elucidation of DNA structure in the form of double helix through the formation of hydrogen bonds by nucleobases in the form of AT and GC base pairs is the inspiration for the evolution of the studies related to the synthesis of molecular complexes through noncovalent interactions. Thus, selective molecular recognition studies employing native nucleobases would be of high value to further understand role of the nucleobases in the physiological process. For this purpose, experiments through co-crystallization of the nucleobases with various –COOH moieties revealed that adenine and cytosine only recognize –COOH.



4.5 Entomology

4.5.1 Basic entomology

Learning in insects

Learning behavior in insects if understood properly would be of much help in devising strategies for their effective control. Keeping this in view, NCL initiated the work to determine whether the presence of a deleterious chemical in a preferred host plant could alter the feeding preference of a notorious polyphagous insect pest, Asian armyworm (*Spodoptera litura*), which has been reported to have developed resistance against most of the conventionally used pesticides. The preference of the Asian armyworm, for castor (*Ricinus communis*) relative to cabbage (*Brassica oleracea*) was quantified by two separate two-way choice tests (without treatment and with treatment of the test chemicals used in the present study) with naïve third instar larvae each time. This was followed, by continuous feeding (48h) on the preferred host treated with the test chemicals and using naïve third instar larvae for conditioning. Each treatment consisted of one of nine compounds, including seven naturally occurring allelochemicals [(viz. (-)-α-pinene, (-)-β-pinene, β-myrcene, d-limonene, cineole, rutin, and ajwain oil)] and two synthetic insecticides (viz. alphamethrin and malathion). Following this, a two-way choice test was repeated with the same batch of larvae without any test chemical. Larvae continued to maintain preference for castor despite exposure to the deleterious chemicals. Preference for castor was not overcome by exposure to novel deleterious chemicals, suggesting that aversion, though experienced is not learned.

Third instar larva of *Spodoptera litura*

Adults of *Spodoptera litura* (Left: Female; Right: Male)

Sub-lethal effect of IGR on certain biochemical parameters in insect

The effect of sublethal concentrations, LC$_{20}$, LC$_{30}$ and LC$_{40}$ of a dispersible formulation of an acylurea insect growth regulator, flufenoxuron (Cascade™) on certain biochemical parameters in the larvae of *Tribolium castaneum* was investigated. When neonates were fed on diet treated with sublethal concentrations for 24 h, it was observed that at all concentrations tested, there was a significant reduction in chitin content on the 15th day of development. Total soluble protein content at LC$_{20}$ and LC$_{30}$ decreased with increasing age of the larvae. At LC_{20} and LC_{40} concentrations there was a progressive increase in the protein: chitin ratio as a function of increase in age of the larvae. SDS-PAGE analysis of the larval tissue extracts indicated gross quantitative changes in some of the protein bands (MW 50-97 kDa). Western blot analysis revealed significant increase in the level of HSP70 in the extracts of larvae fed on LC_{30} treated diet, on the 7th and 10th day of development in the decreasing order. Conversely, a significant decrease in the hyper-phosphorylated form of $p34^{cdc2}$ kinase due to flufenoxuron treatment indicating modulation of cell cycle regulation was observed. Thus, sublethal concentrations of flufenoxuron alter expression of developmentally regulated proteins, HSP70 and $p34^{cdc2}$ and chitin formation in a stage-specific manner thereby resulting developmental abnormalities in *T. castaneum*.

Electrophysiological studies

Electrophysiological studies with adult males and females of *T. chilonis* and *C. carnea* to a wide group of volatile chemicals from plants were carried out. EAG results indicated that some of the volatiles act as orientation cues thereby enhancing parasitization / predation efficiency. GC-EAD studies are under progress.

Responses of maxillary galeal sensilla of *S. litura* and *H. armigera* to salts, amino acids and sugar were examined and dose-response relationships established. Unique responses to castor plant saps in both the species were observed which are similar to their response to 5mM inositol thereby suggesting that the sensillum provides a labeled line patterning of response to the insect, indicating it as an acceptable plant. Such a response was not observed with cotton leaf sap.

Further electrophysiological observations include the increase in spike responses to sucrose when chloride salts of monovalent cations are used while bivalent cations suppressed the responses.

Electrophysiological responses in both *S. litura* and *H. armigera* to a compound belonging to a novel group of secondary plant metabolites were obtained. Insects fed on diet spiked with this compound show latency in their response. Efforts are underway to study the existence of such a relationship, if any, in other insect species representing different insect orders.

4.5.2 Applied Entomology

Studies on the interaction and performance of *Antheraea mylitta* on its host plants with special reference to *Shorea robusta*

In our continuing efforts to document the annual cycle of changes in primary and secondary metabolites in the three host plants (*sal*, *arjun* and *asan*) with a view to correlate it with feeding preferences of the tasar silkworm, *Antheraea mylitta* are being pursued. Extraction and quantification of phenolics from *asan*, *sal* and *arjun* has been completed from leaves collected at weekly intervals. Flavonoids with respect to *arjun* and *asan* have also been completed.

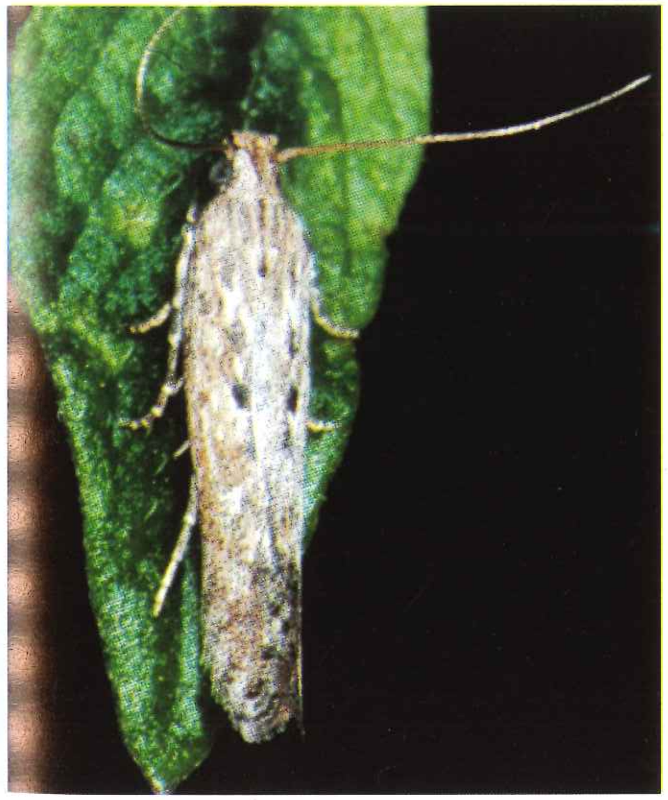
Discovery, development and commercialization of bioactive substances and traditional preparations from plant sources

Under this CSIR coordinated project, this year NCL screened around 1500 plant extracts against three lepidopteran insect pests viz. *H. armigera* (cotton bollworm), *S. litura* (Asian armyworm) and *P. operculella* (potato tubermoth) against the insecticidal, feeding deterrence, oviposition deterrence and insect growth regulation activities. The leads obtained are being confirmed at different concentrations at the respective participating laboratories including NCL.

Utility of sex pheromones in IPM

Under this CSIR-NETWORK project, work was carried out with *P. operculella* to understand the response of this insect (using EAG techniques) to green leaf volatiles, since these green odor components and their blends are utilized to locate host plants for suitable feeding and oviposition sites. The wide spectrum of responses of both males and females of *P. operculella* to different compounds belonging to diverse chemical classes reflects differential tuning of receptors on the antennae suggesting a species specific adaptation of the set of olfactory receptors to the particular green odor components of potato leaves. Current research focuses on identifying relevant odorants using single-sensillum recordings from olfactory receptor neurons. Such studies linked to a gas chromatograph would further help in determining the molecular receptive range of the receptor neurons.

Potato tuber moth larva mining into potato leaf

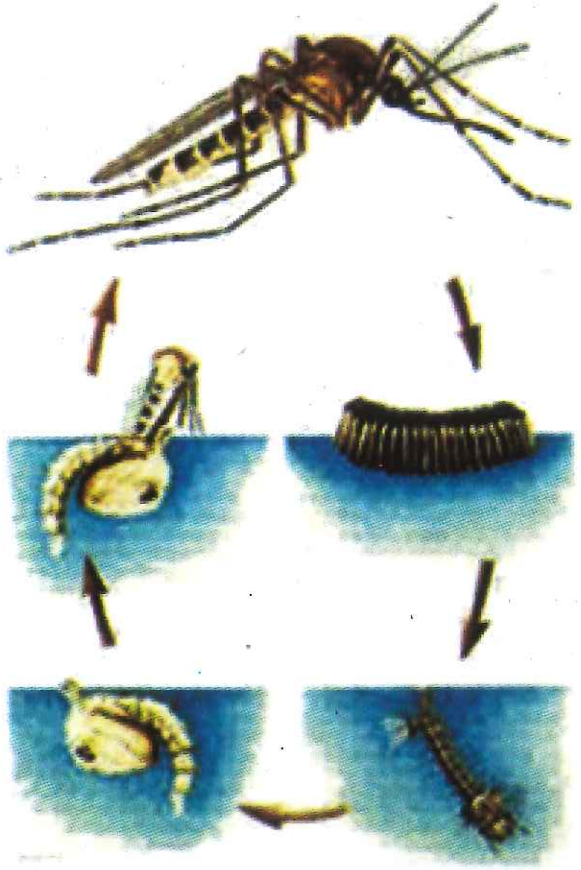


Adult potato tuber moth

4.5.3 Medical entomology

For identifying chemicals with larvicidal repellent activities various terpenoids and oils from plants of the Himalayan region for their mosquito repellent activity either singly or in combination were evaluated. The combinations which showed biological activities are being pursued to improve upon their performance.

Potency of various fractions of hexane extracts of seeds of *Sterculia guttata* were evaluated against the larvae of *Aedes aegypti* and *Culex quinquefasciatus*. Bis(2-ethylhexyl)benzene 1,2-dicarboxylate was found to have chronic toxicity against the larvae of both the species. This work was done in collaboration with Bhide Foundation for Research & Education in Chemistry and S.P. College, Pune.



Life cycle of mosquito

5. PHYSICAL AND MATERIALS CHEMISTRY

5.1 Theoretical chemistry

5.1.1 Fock space coupled-cluster linear response approach

The constrained variational approach for linear response of a specific state in Fock space multi-reference coupled-cluster (FSMRCC) approach was developed. In the last year, significant advancements to coding of polarizability of one valence problems have augmented the efforts of calculation of electric first-order response properties. The code was tested with small molecules, where benchmark results are available.

5.1.2 Density functional response approach or molecular properties

A computationally viable alternative to full analytic response to Kohn-Sham density functional theoretic (DFT) approach, which solves coupled-perturbed Kohn-Sham (CPKS) procedure in non-iteratively was formulated. In the above procedure, the derivative of KS matrix was obtained using finite field and then the density matrix derivative was obtained by single-step CPKS solution followed by analytic evaluation of properties. This was implemented in deMON2K software and used for calculation of electric properties.

5.1.3 CIP based coupled-cluster method for electron-molecule resonance

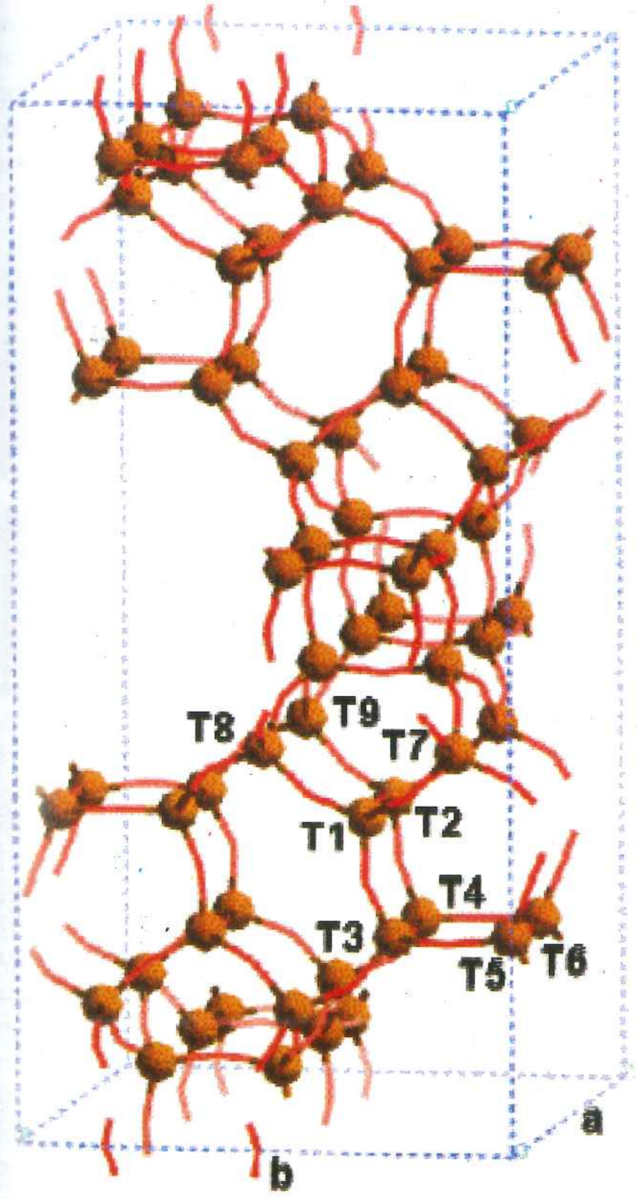
An approximation to the earlier complex absorption potential based multi-reference coupled-cluster method to calculate resonance of molecular anions was developed. The procedure is based on the analytical continuation method. The advantage of analytical continuation of the Hamiltonian in the complex plane giving the direct access to the resonances parameters is that they can be represented by using L^2 wave function. The essential idea underlying the complex absorbing potentials to calculate the resonances is to introduce an absorbing boundary condition in the exterior region of the molecular scattered target which results in a non-Hermitian Hamiltonian, one of the square integrable eigenfunctions of which corresponds to the resonant state. The associated complex Eigen-value then gives the position and width of the resonance or the auto-ionizing state. The important relaxation and correlation effects are included in the coupled-cluster method. The approximation developed in this year involves use of complex correlated independent particle (CIP) potential, which simplifies the computation scheme. In the CIP –FSMRCC method, the analytical continuation over an already correlated effective Fock space Hamiltonian was applied. This procedure was tested to shape resonance in C_2H_4, CO and Mg.

5.1.4 Study of reactivity descriptors for interaction-induced OH shift

First-principle study of interaction-induced OH frequency shift in halide ion-water clusters was made. New reactivity descriptor bond deformation kernel (BDK) based on conceptual density functional theory has been introduced to describe OH frequency shifts in fluoride ion- water clusters. Central to our model is the use of local polarization, which can be described by Normalized-Atom-Condensed Fukui Functions (NFF), which is the normal condensed Fukui Function, multiplied by number of atoms. Using the NFF and charge transferred to water from halide ion, a BDK has been defined, which appropriately describes the shift in OH frequency.

5.1.5 Study of zeolite Sn-beta using periodic density functional theoretic study

Sn-beta zeolite has attracted recent interest due to better catalytic behaviour compared to Ti-Beta zeolite. Al-free Sn-beta zeolite was recently synthesized and it was shown by another group to have efficient catalytic activity in Beyer-Villeger oxidation reactions in presence of H_2O_2. At NCL, the structure, bonding and acidity of Sn-beta zeolite was studied using periodic DFT and it was demonstrated that incorporation of Sn in BEA framework reduces the cohesive energy and is an endothermic process. It was also shown that among the T-sites, T2 site is the most probable site for Sn- incorporation. T2 site is also higher Lewis acid site in comparison to other T-sites. Theoretical analysis done at NCL also showed that Sn atom polarizes the orbitals of oxygen atoms.



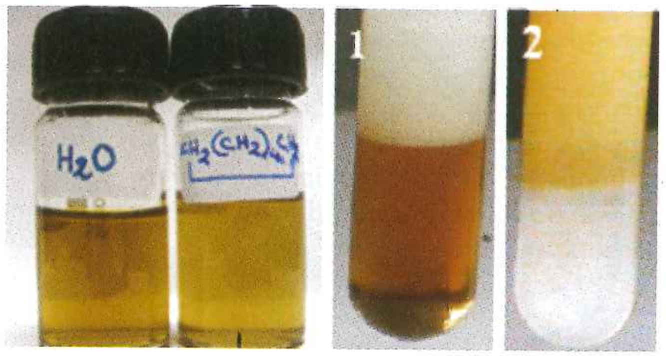
5.2 Materials chemistry

5.2.1 Biological synthesis of nanoparticles

The exciting new repertoire of bio-inspired methods for nanoparticle synthesis have been extended to other chemical compositions such as oxides, etc. apart from simple metals and metal sulphides and it was shown that some of the biosynthetic methods lead to excellent shape control in the nanoparticles. Methods like leaching silica nanoparticles from abundantly available materials like sand and rice husk have been developed and may lead to finding greater applications of these materials that are cost effective.

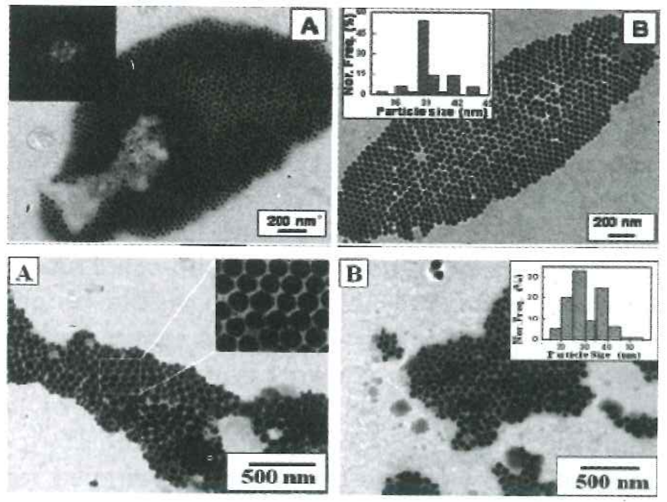
5.2.2 Chemical synthesis of nanoparticles

There is a growing interest in the ability to direct nanoparticles into various physicochemical environments (different liquid phase) for possible catalytic and sensor applications. To this effect, a simple and efficient way of obtaining silver nanoparticles that are dispersible both in organic and aqueous solvents using a single capping agent was demonstrated. Efficient methods for the phase transfer of $Ni_{core}Ag_{shell}$ again utilizing a single capping agent were developed.



$Ni_{core}Ag_{shell}$ (sample vials) and Ag nanoparticles (test tubes) in water and organic solvents

Highly monodisperse nickel and cobalt nanoparticles were synthesized by a simple wet chemical reduction technique in the presence of a surfactant sodium dodecyl sulfate (SDS) and a capping agent oleic acid.

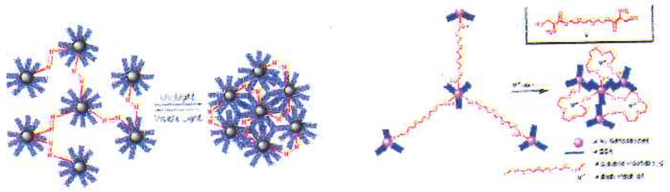


Ni (top frames) and Co (bottom frames) nanoparticles prepared by aqueous solution routes

The foam based technique that has been shown to be a convenient method for the preparation of metal, metal oxide and metal carbonate nanoparticles was extended to prepare multicomponent oxides like $CoFe_2O_4$ and $MgFe_2O_4$.

5.2.3 Organic-nanoparticles functional hybrids

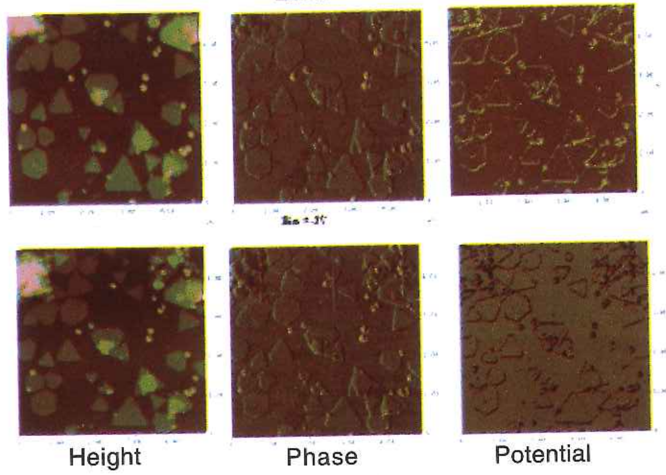
Functional materials fabricated from nanoparticle building blocks are evincing great curiosity among researchers keeping future technological needs in mind. At NCL photo-responsive gold nanoparticle networks by linking them with ligands bearing azo-benzene moieties were prepared. As a novel extension of the above work the ligands that can sense and phase transfer alkali metal ions in aqueous media to organic media were devised. These approaches could find applications in sensors and drug delivery systems.



Photoresponsive and ion sensing gold nanoparticle networks

5.2.4 Nanoparticle applications

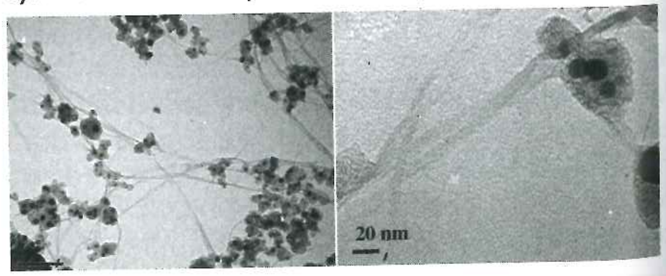
Various applications of the nanomaterials such as gas-sensors (using anisotropic Au and Ag nanostructures), dielectric- nanodevices and electro-rheological devices (using $BaTiO_3$ nanoparticles), magneto-caloric refrigeration devices (using magnetic-metal core-shell nanoparticles) for MEMS applications (cooler-on-a-chip) are being explored. The photocatalytic activity of TiO_2 nanoparticles and their composite structures has also been explored and initial results indicate photocatalytic activity in visible range. Recently, the magnetocaloric refrigeration measurements have shown observation of giant magnetocaloric effect in core-shell magnetic nanoparticles. The composites of dielectric-magnetic nanoparticle are being investigated for the multiferroic applications. The electric field near metal nanoparticles can be enhanced by plasmon resonances as well as sharp edges. Initial measurements on gold nanotriangles using the surface potential microscopy (SPM) studies have shown accumulation of charges on the edges. This effect can be used for applications such as guiding electromagnetic energy in subwavelength-sized optoelectronic devices, enhanced fluorescence spectroscopy, Raman spectroscopy, near-field imaging, etc.



Surface potential imaging of Au nanotriangles

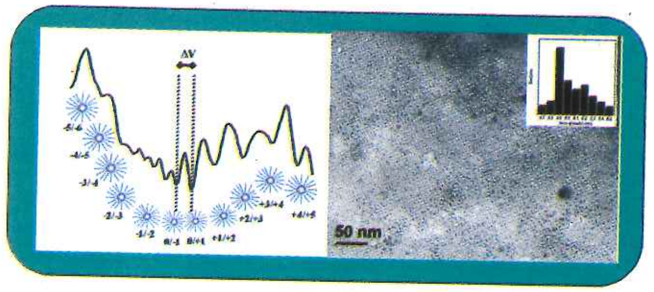
5.2.5 Synthesis of SWNTs by chemical vapour deposition

Single walled carbon nanotubes (SWNT) are the most promising of all nanomaterials, with unique electronic and mechanical properties which lend themselves to a variety of applications, such as FE displays, nanostructured composite materials, nanoscale sensors, and elements of new nanoscale logic circuits. In all cases the quality of the SWNT material is important, and for some applications it is paramount. Despite sustained efforts, all currently known SWNT synthetic techniques generate significant quantities of impurities, such as amorphous and graphitic forms of carbon and encapsulated catalytic metal nanoparticles. SWNTs were grown by using CH_4 as a carbon source in presence of a catalyst FeCo supported on MgO or Al_2O_3. The quality obtained by this synthetic route is quite well despites its low yield.



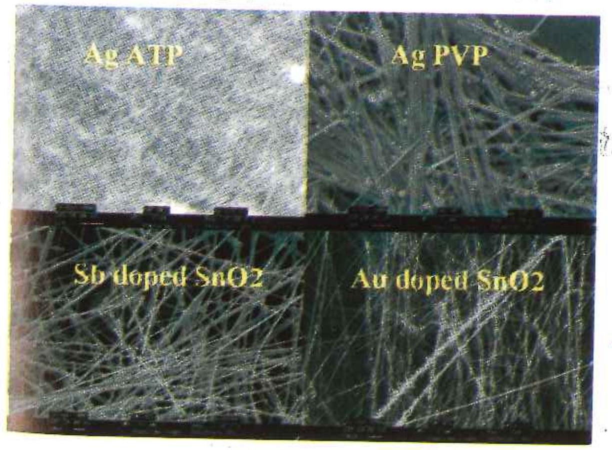
5.2.6 Quantized double layer charging of Rh_{2051} $(TDA)_{321}$ nanoparticles

Solution phase voltammetry (DPV and CV) of Rh_{2051} $(TDA)_{321}$ nanoclusters (4.9±0.2 nm) shows an interesting single electron behavior at room temperature exhibiting thirteen consecutive peaks.



5.2.7 High aspect ratio materials

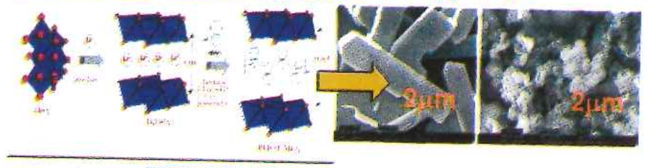
The main focus of this project was to develop metal nanowires (specifically, silver) and metal oxide nanowires in high aspect ratio and to make polymer-nanowire composites. Silver nanowires (60nmX40μm) were synthesized with two different capping agents, PVP and ATP. Tin oxide nanowires were synthesized by vapor deposition method using different dopants such as ruthenium, antimony and gold. These tin oxide nanowires were tested for gas sensing; preliminary experimental results showed sensitivity towards NO_2 and CO and it was observed that the sensing ability of tin oxide varies with the dopant used. Template directed synthesis is another kind of method that represents a straight forward route for the synthesis of 1D nanostructure. It was used in several different ways to synthesize nanorods, nanowires and nanodots with varying size. Porous anodic alumina membrane was used as the template for the synthesis of RuO_2 and Ru nanorods by using potentiostatic method.



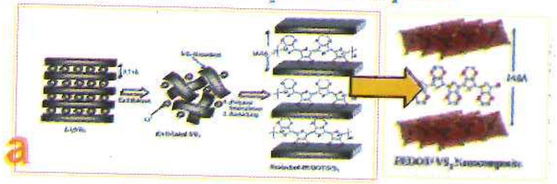
5.2.8 Hybrid nano-structured materials

Inorganic host and organic guest nano-composites have been considered as promising candidates for power source devices due to their abnormal high supercapacitor behavior and interest for applications like LEDs, supercapacitors, electrochromic and antistatic coating. Various metal oxides viz. V_2O_5, MoO_3, VS_2, etc have been analysed after making their nanocomposites with organic conducting polymer Poly(3,4-Ethylenedioxythiophene) [PEDOT] due to its enhanced stability compared to polyaniline and polypyrrole. The improved electrochemical performance observed with the intercalation of electronically conductive PEDOT is due to the expansion of the interlayer distance and electronic conductivity of the V2O5 and MoO3 oxide hosts. Thus, the intercalation of PEDOT in V2O5 and MoO3 produces a new functional hybrid nanocomposite as promising cathode for high-energy rechargeable lithium batteries and supercapacitors, respectively.

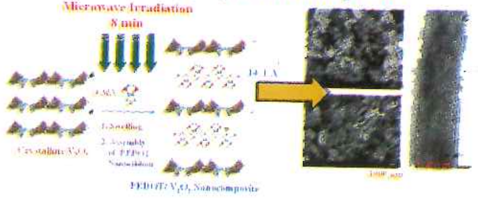
PEDOT / MoO_3 Nanocomposite



PEDOT / VS_2 Nanocomposite

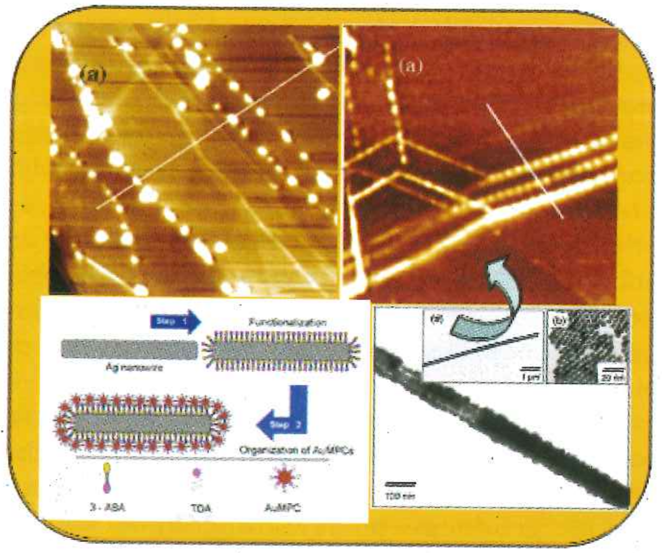


PEDOT/ V_2O_5 Nanocomposite



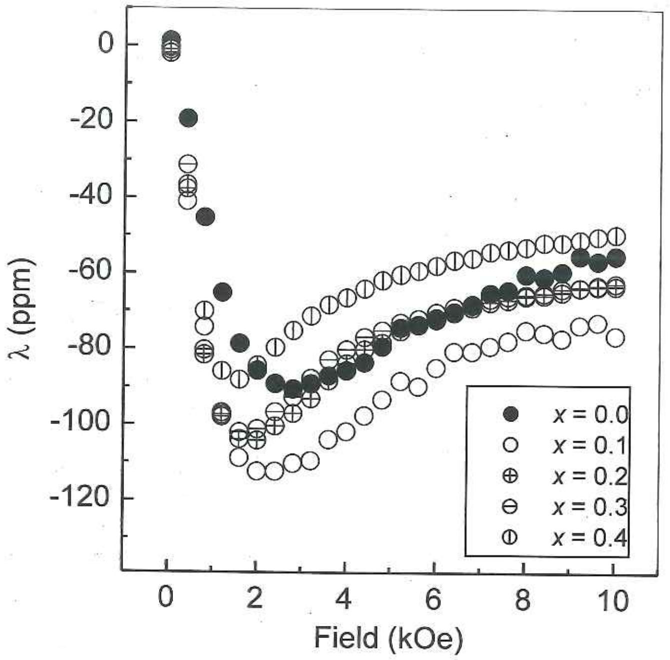
5.2.9 Heterostructure assembly

The directional integration of tridecylamine protected gold (Au-TDA) nanoclusters on silver nanowires (AgNWs) forming a hybrid structure with exceptional electron transfer properties using transmission electron microscope (TEM), noncontact atomic force microscopy (NcAFM), and scanning tunnelling microscopy (STM)/ spectroscopy (STS) was achieved by simple chemical route.



5.2.10 Magnetostrictive smart materials

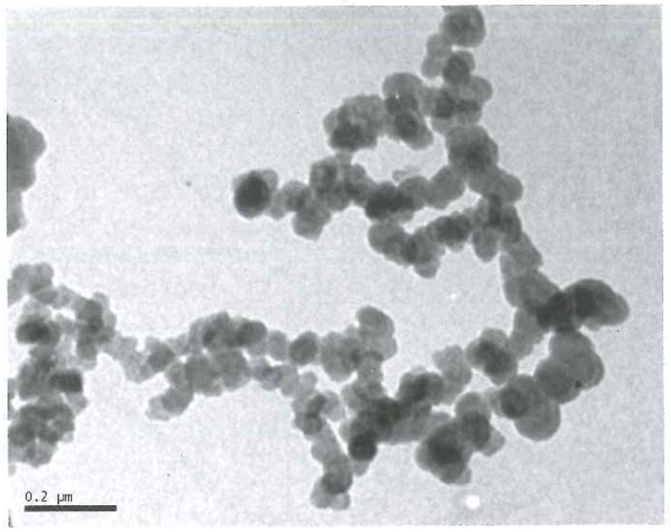
Magnetostrictive smart materials are useful for various technological applications. Attempts are being made at NCL to develop suitable ceramic oxide magnetic materials as a substitute for currently available alloy based materials, for use as magnetostrictive smart materials. Different oxide based magnetic materials such as ferrites, perovskite type oxides, etc. are being studied for identifying suitable materials with high magnetostriction at low magnetic fields. From the studies on different spinel cobalt ferrites, it was found that small amounts of manganese when substituted for cobalt enhances the magnetostriction at low magnetic fields. More than 25% increase in the magnetostriction at relatively low magnetic fields is obtained for 8% substitution of Mn for Co in $Co_{1.2-x}Mn_xFe_{1.8}O_4$.



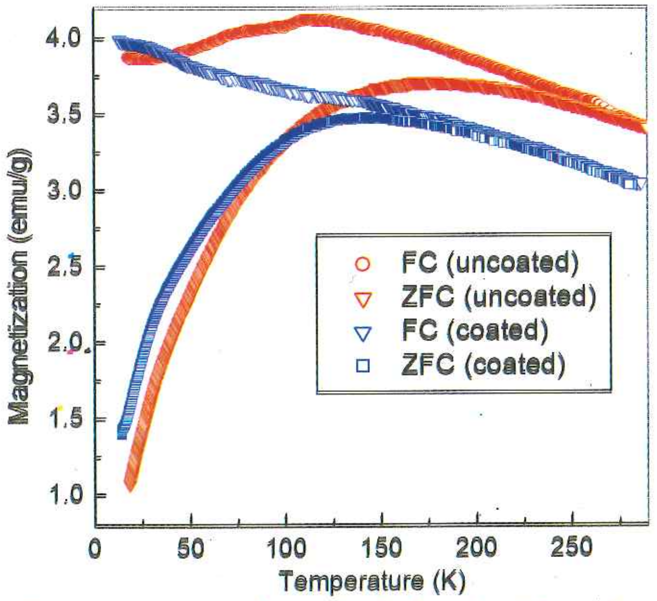
Enhanced magnetostriction at low magnetic fields in manganese doped cobalt ferrite

5.2.11 Nano-magnetic materials

Nanomagnetic materials are useful for a variety of applications such as biomedical applications, magnetic storage, ferrofluids, etc. Currently nanosized oxide based magnetic materials and ferrofluids are being synthesised at NCL to study the magnetic properties of these nanosized magnetic materials and to understand their magnetic behaviour required for various applications. The emphasis of the work is to understand the magnetic properties of the nanoparticles when coated with suitable surfactants. This information is highly desirable for many of the applications. Figures below show the transition electron micrograph of Fe_3O_4 (magnetite) nanoparticles of almost uniform particle size and the difference between the magnetic characteristics of the uncoated and surfactant coated nanoparticles. After coating with a surfactant, there are considerable changes in the magnetic characteristics due to decreased inter particle magnetic interactions.



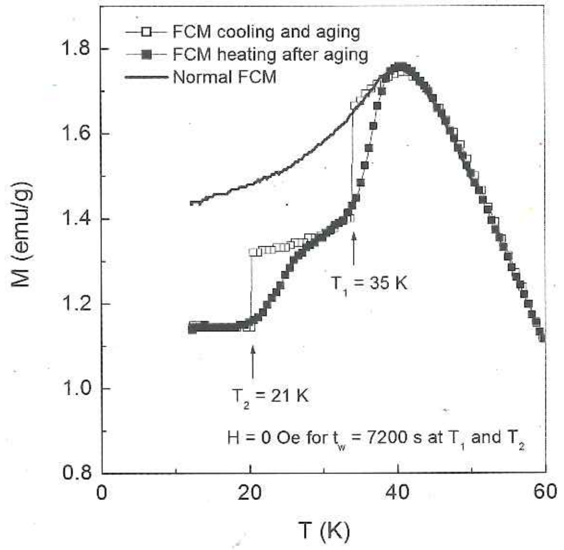
TEM of magnetite nanoparticles



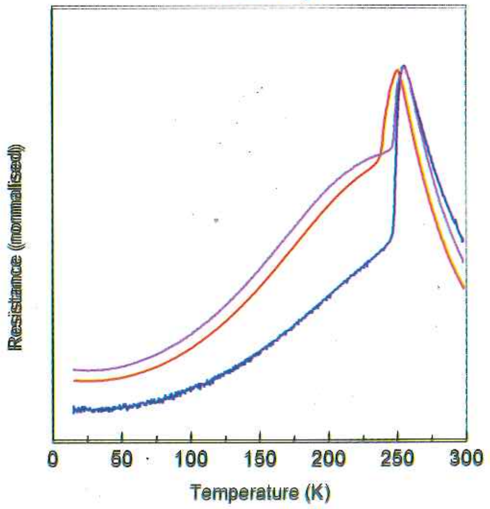
Magnetic characteristics of uncoated and surfactant coated magnetite nanoparticles

5.2.12 Magnetoresistive oxides and related systems

Perovskite type manganese oxides exhibiting colossal magnetoresistive properties are fruitful candidates for future technological applications. Our emphasis is to understand the magnetic and electrical properties and processing-structure-property correlation of different types of perovskite type ferromagnetic materials as well as to look for new related ferromagnetic oxides with interesting properties. For example, by controlling the oxygen stoichiometry in $LaMnO_3$, one can get antiferromagnetic, ferromagnetic or spin glass characteristics. The spin glass characteristics are similar to that of magnetic nanoparticles showing aging and relaxation effects, as shown below, indicating confinement of magnetic clusters in a non-magnetic like environment within the perovskite lattice. The electrical characteristics of the colossal magnetoresistive manganite, $La_{2/3}Ca_{1/3}MnO_3$, is found to be highly dependent on the processing conditions. Figure below shows the variation of the electrical resistance of the material as a function of temperature, processed under different conditions. Metal-insulator transition as well as the electrical resistance in the ferromagnetic state is highly dependent on how the material is processed. These results give crucial information on the characteristics of the specific materials.



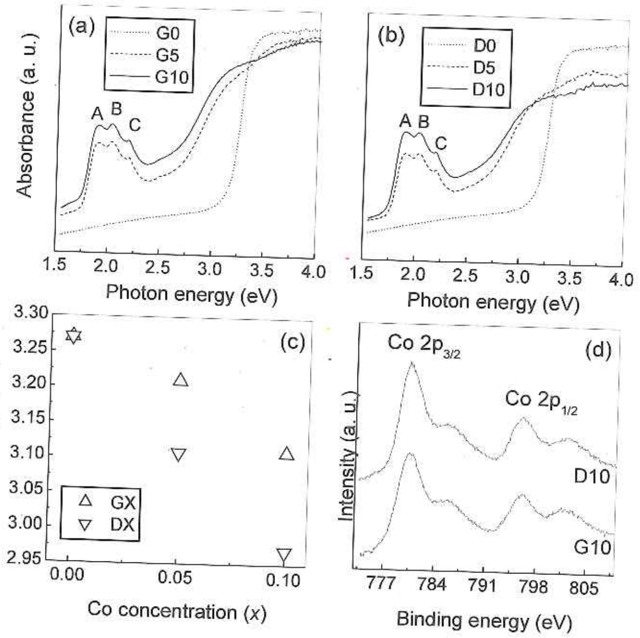
Aging and relaxation in non-stoichiometric $LaMnO_3$



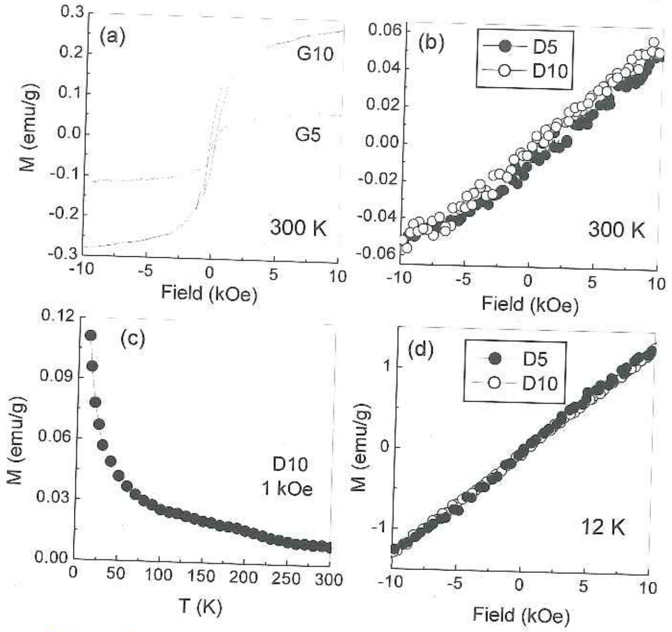
Processing dependent electrical resistance behavior of $La_{2/3}Ca_{1/3}MnO_3$

5.2.13 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. The transition metal doped ZnO is found to be either magnetic or non-magnetic depending on the particular synthesis conditions. However, the electronic and optical properties are almost identical irrespective of their magnetic characteristics. Our detailed studies showed that ferromagnetism is not an intrinsic property of the transition metal (Co) doped zinc oxide.



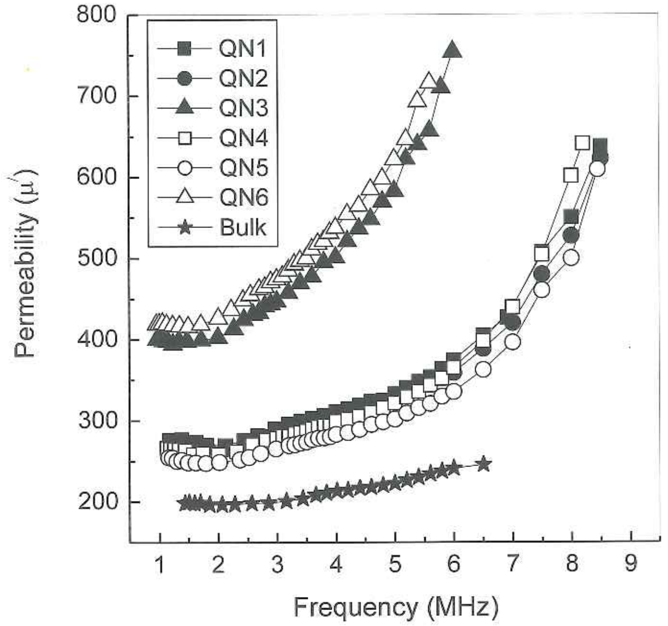
Electronic properties of ferromagnetic (G series) and paramagnetic (D series) Co doped ZnO



Magnetic properties of ferromagnetic (G series) and paramagnetic (D series) Co doped ZnO

5.2.14 Low temperature synthesis and processing of advanced ceramics

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, citrate -gel, 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, ii) the increased reactivity due to high surface area, iii) low sintering temperatures, iv) homogeneity in chemical composition, cost reduction, etc. Moreover, the nanoparticles can be sintered at relatively lower temperatures, with enhanced performances, in the case of functional materials like ferrites, ferroelectric materials such as barium titanate, etc. Figure below shows the enhanced permeability of a nickel-zinc ferrite, synthesized by a low temperature method and sintered at relatively low temperatures. Large enhance in the permeability is obtained compared to the bulk samples and such higher values are highlydesirable for many technological applications. Our emphasis is on the synthesis of different functional oxides at low temperatures by following different routes and studies on thephysical properties of the functional materials such as I-V measurements, impedance analysis and C-V relations, magnetic characteristics, etc. The physico-chemical characterization techniques such as XRD, SEM/TEM and TGA are also being carried out to understand and compare the different materials obtained following various synthetic strategies.



Comparison of the permeability spectra of NiZn ferrite synthesized at low temperatures and processed under different conditions.

5.3 Rate governing forces for organic reactions in ionic liquids and in water

An experimental study of physical-organic chemistry of Diels-Alder reactions has revealed that hydrophobic packing is dominant over secondary orbital interactions in transition state structures of simple Diels-Alder reactions carried out in water and salt solutions. Anomalous salt patterns in Diels-Alder reactions were observed that are against the established definitions of salting-out and –in phenomena. Also, a thermodynamic method was developed to separate and quantify different ionic interactions in ionic solutes possessing hydrophobic characteristics.

5.4 Instrumentation

The group has expertise in the area of instrument development for scientific applications, PC based instrumentation, embedded instrumentation along with the maintenance of sophisticated instruments. The group had completed the major development of the scientific instrument known as Brewster Angle Microscope (BAM) coupled with Langmuir trough. During year 2003-2004. The development of BAM – Image2K was completed using horizontal set up of laser collimator and software development was done using VC++. The instrument was again redesigned during 2005-2006 using laser diodes and vertical set up to make instrument compact. This instrument allows user to plot real time pressure area isotherm while simultaneously viewing the Langmuir monolayers.

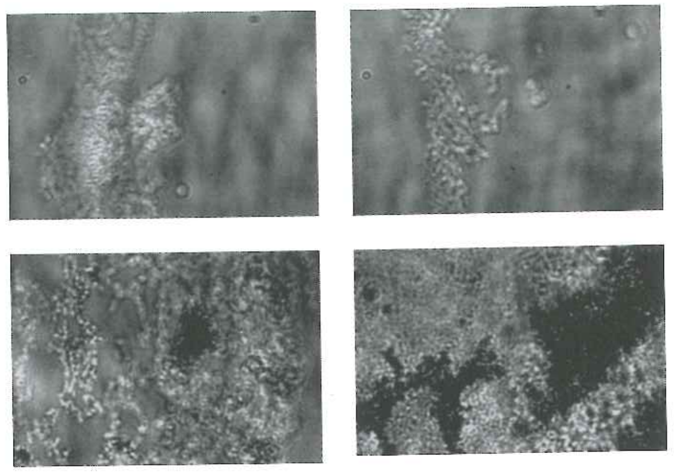
The developed instrument is PC based solution in which all the parameters and controls are passed through the Graphical User Interface (GUI) developed in LabVIEW. For measuring the surface pressure, AD/DA card (NI6014) from National Instrument is used. The parameters like molecular weight, volume inserted on subphase and concentration of the monolayer and control for barrier direction and speed has been passed through the developed controlled software.

Brewster Angle Microscope set up consists of a small laser diode which emits 25mW at 650nm. The emitted beam passes through a polarizer and then illuminates a spot of about 2 mm² on the surface. The reflected light passes an objective (specially constructed) and is finally detected by a charge coupled device (CCD) camera. The lateral resolution of the microscope is ~ 1μm· The camera is coupled to the frame grabber card by National Instruments for real time capturing of the compressed monolayer. The developed software has a facility to record the video while monolayer is being compressed by the barrier. The file is stored in the form of .avi extension. Some image processing features like histogram calculation, changing brightness, contrast values and measuring the area of interested domains by mouse dragging are also included for post processing. The real time system software was developed using LabVIEW (Professional Development System PDS 7.0).

The instrument is being used by Nanoscience Group at NCL. Following are the systems for which BAM results have been obtained:

1. *Time dependent complexation of sodium borohydrate reduced gold nanoparticles with octadecylamine Langmuir monolayers*: The system was studied and BAM images clearly indicated that the density of particles increases at the surface as a function of time of complexation.

2. *Assembly of hydrophobized Ni nano particles as a function of surface pressure*: Brewster Angle Microscopy and pressure area isotherm measurements have been employed for this study.



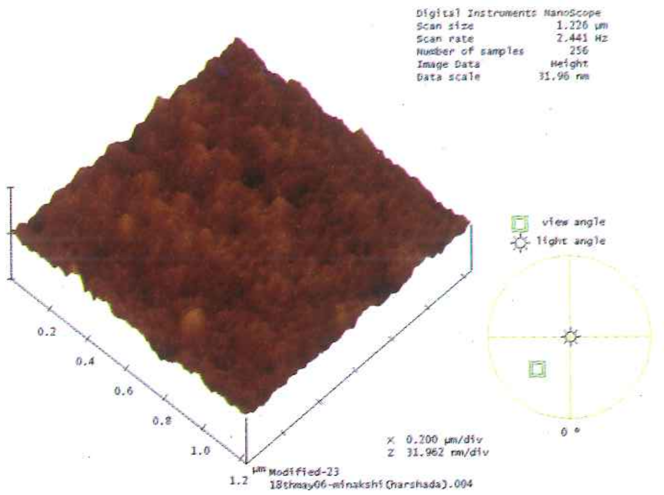
BAM images of Ni nano particles at different concentration

6. POLYMER SCIENCE AND ENGINEERING

6.1 Membrane science and technology

6.1.1 Proton exchange membrane for fuel cell application

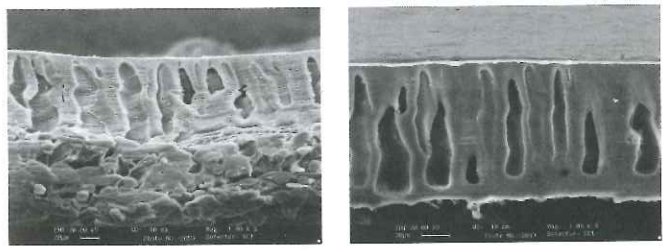
Polybenzimidazole is being evaluated as proton exchange membrane (PEM) material owing to its various advantages such as high thermo-chemical stability, high CO tolerance and low fuel cross-over. The polymer synthesis and membrane preparation were standardised (1 sq.ft). The membranes are being evaluated for electrochemical performance.



AFM of modified membrane

6.1.2 Ultrafiltration

The arsenic (As) rejection using membranes is restricted to reverse osmosis (RO), nanofiltration (NF) and microfiltration (MF) processes. RO and NF need high pressure for their operation, while MF, though can be operated at low pressure, leads to sludge formation since the coagulation of As into bigger size molecules is required using additional chemicals. The charged ultrafiltration membranes were demonstrated that would reject As(V) at low pressure (> 1 bar) based on Donnan exclusion principle. These membranes were prepared by modifying membrane surface that leads to lowering of pore size while inducing the charge on the surface.

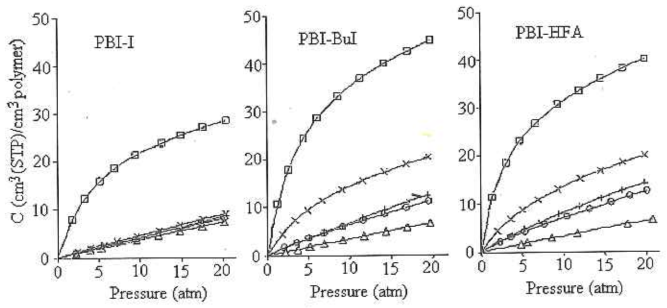


SEM of unmodified and modified membrane

The pore smoothening of the modified membrane was confirmed by AFM analysis. The mean surface roughness analyzed by AFM showed 3.196 nm for unmodified membrane, which reduced to 1.901 nm for the modified membrane.

6.1.3 Gas permeation

Improvements in intrinsic gas permeation properties by suitable structural modification in promising polymer families (polybenzimidazole, polyphenylene oxide and polyarylates) are being attempted. Basic understanding of gas solubility and diffusivity in polymer matrix resulting from structural variation was obtained by performing sorption and pure gas permeation studies. The figure shows the sorption of various gases in unsubstituted polybenzimidazole (PBI-I), PBI based on tert-butyl isophthalic acid (PBI-BuI) and hexafluoroisopropylidene bis(benzoic acid) (PBI-HFA). As a result of these structural modifications the PBI membranes lie above Robeson's upper bound.

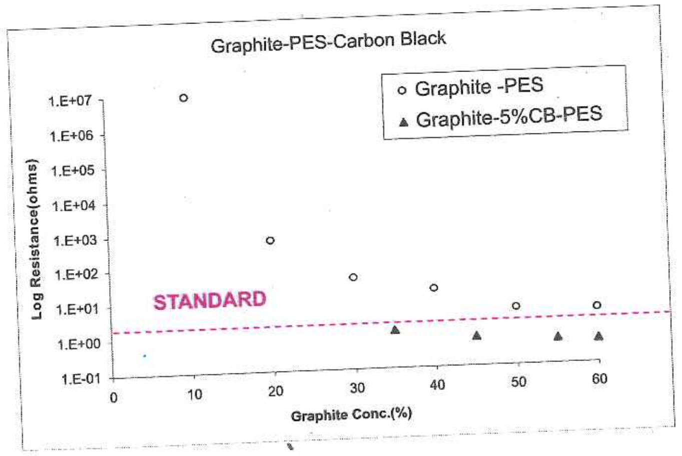


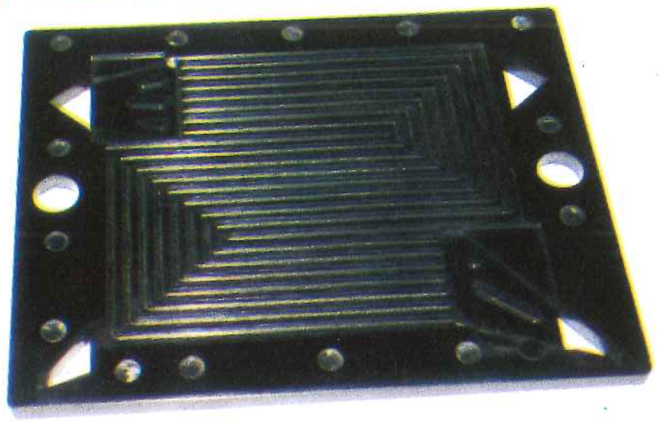
Sorption properties of polybenzimidazoles

6.2 Electroactive polymers

6.2.1 Conducting polymer hybrid composites bipolar plates for fuel cells

Amongst the fuel cells, viz. proton exchange membrane (PEMFC), direct methanol (DMFC), phosphoric acid (PAFC), molten carbonate (MCFC) and solid oxide (SOFC), the PEMFC and DMFC are being investigated extensively since these have much greater advantages such as better efficiency, light weight, less operating cost, etc. Bipolar plates constitute the major component, conventionally made from sintered and machined graphite, contributing to its total weight, size, and cost. The bipolar plate acts as collector for the charge / electrons generated and transfer the same to external circuit. Additionally, these plates also provide the channels for the flow of the fuel (hydrogen or methanol) as well as the oxygen or air in the cell on either side of the membrane separator. Further, the plates provide a path for heat dissipation and maintenance of the operating temperature of the fuel cell stack. In order to reduce the cost and weight of the fuel cells, it is essential to fabricate these plates by alternative routes such as injection molding, compression molding, etc. A novel method of mixing natural graphite with high temperature thermoplastics and another conducting component has been evolved which leads to low percolation threshold and moldable conducting compound. The target value of conductivity (indicated by dotted line) was achieved even at low additive concentration.

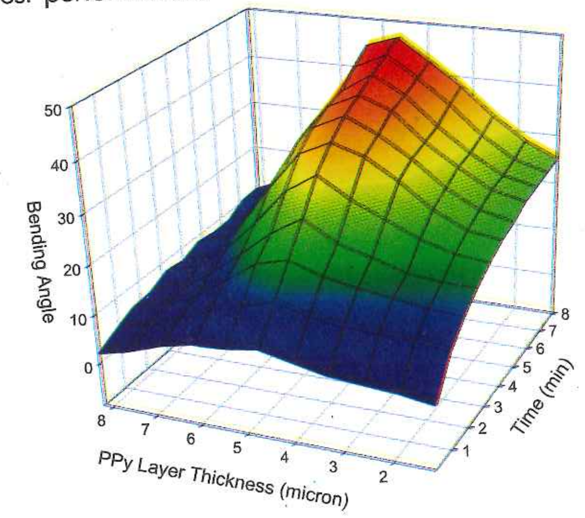




Complex design of the injection molded bipolar plate made from conducting hybrid composite

6.2.2 Conducting polymer bi-layer actuators

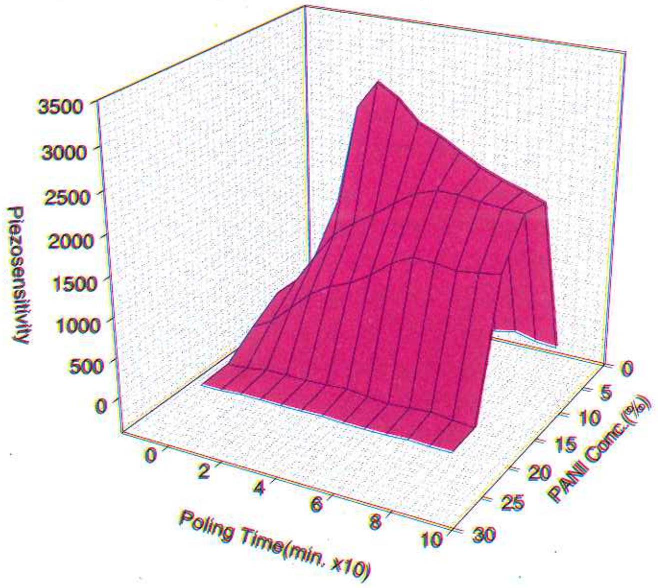
Actuators are important in various areas such as remote control systems, robotics, biomedical devices, automobiles, etc. The polymeric actuators exhibit usually large strains but have low load bearing capacity. In order to improve the latter, the electroactive polymers are coupled with strong insulating backing layers. From the point of view of device applications, extensive studies were carried out on conducting polypyrrole based bi-layer actuators in order to maximize their actuation efficiency with respect to various geometric parameters, backing layer modulus, preparation conditions, etc. A phenomenological model has been proposed for the same which gives good control of these parameters for best performance.

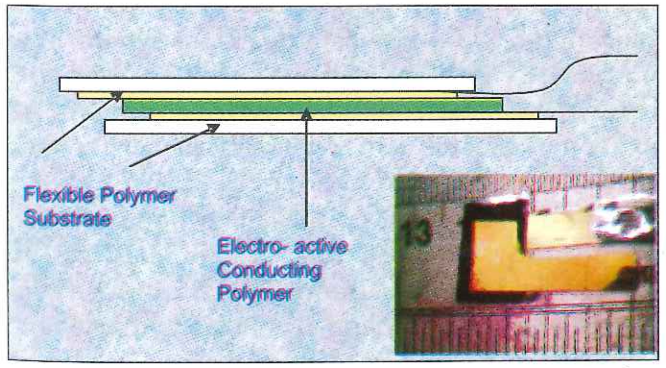


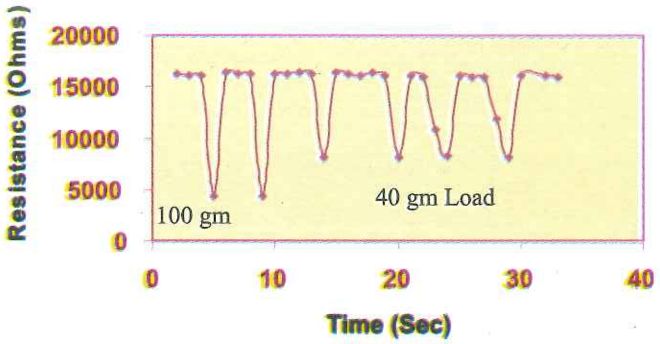
Effect of PPy layer on the time dependence of the actuator response in PPy / polypropylene bi-layer actuator. Backing layer thickness 40 μm, applied potential 1.0 V, 0.1M $LiClO_4$ in CH_3CN

6.2.3 Enhanced piezo-sensitivity in polyvinylidene fluoride / conducting polymer composites

The application of electroactive polymers such as polyvinylidene fluoride (PVDF) as piezo-sensor in robotics has limitations due to its insulating nature. Attempts to make semi-conducting piezo-resistive sensors, PVDF have been combined with conducting polyaniline and its electrical resistivity was studied with application of different mechanical loads. Such materials showed fairly high levels of piezo-sensitivity which depended on the composition, the dopant used during preparation, the particle size of the conducting phase, etc. Recently, it has been possible to enhance the piezo-sensitivity of these composites even further by electrical poling. The sensitivity factor was enhanced 100 folds by application of electrical potential for certain duration at appropriate temperature. The effect of this poling treatment on the piezo-sensitivity of these composites is depicted in the figure.







The touch sensitive device made from such films is shown in figure together with the response characteristics at low mechanical pressures.

6.3 Polymerisation and polymer materials

6.3.1 Super-absorbing materials by HIPE polymerization

Macroporous polymers by suspension polymerization (50% pore volume) are commercially used in superabsorbent materials, sanitary napkins, ion exchange applications, liquid chromatography, metal recovery, cell immobilization, tissue engineering and cosmetics. High internal phase emulsion (HIPE) polymerization (water-in-oil and water-in-oil-in-water) enables the synthesis of porous, cross-linked polymeric networks with more than 95% internal phase pore volume. HIPE systems possess an open-cellular morphology and secondary pore structure within the polymer walls.

Research at NCL has shown that normal aqueous redox polymerisation does not always work in HIPE methodlogy. Thus, use of vinyl acetate and acrylic acid has no effect on polymerisation rate; silver-persulphate does not act as a redox pair. A number of new redox systems have been established. The polymerization is effectively inhibited by phenothiazine in a manner akin to suspension and emulsion polymerization. The pore structure is dictated by a number of parameters, including the cation of the redox initiators, as seen in figure.

glass transition temperature of pendant pentadecyl chain containing polyesters and polyimides demonstrated the "plasticizing" ability of pentadecyl chain. Encouraged by the results of homopolymers, it was of interest to synthesize copolymers with a systematic variation of pentadecyl substituted cyclohexylidene containing monomers and study the effect of comonomer content on the final copolymer properties. High molecular weight copolyesters and copolyimides containing pentadecyl substituted cyclohexylidene moiety were synthesized. All of the (co)polyesters and (co)polyimides exhibited high thermal stabilities.

A series of new polyesters with a systematic variation of methyl and /or bromo substituent on phenyl rings was synthesized from bisphenols containing bulky perhydrocumyl cyclohexylidene "cardo" group by two-phase interfacial polycondensation technique. Moderate to high molecular weight polyesters soluble in common organic solvents were obtained. The presence of constitutional isomerism in polyesters containing substituted cyclohexylidene moieties was established by detailed NMR spectral analysis. All the polyesters were amorphous in nature as indicated by their wide-angle X-ray diffraction patterns. The polyesters indicated high thermal stabilities.

The utility of perhydrocumyl cyclohexylidene containing polyesters as membrane materials for gas separation was demonstrated. Polyesters derived from isophthalic acid chloride exhibited lower permeabilities and higher permselectivities than their terephthalic acid chloride derived analogues. The systematic variation of methyl and bromo substituent on phenyl rings revealed that the incorporation of polar groups within polymer structures which inhibit free volume collapse help in increasing gas permeability and permselectivity.

6.4.3 Synthesis of polyimides

A series of polyimides was synthesized from perhydrocumyl cyclohexylidene containing diamine and commercial dianhydrides by one-step high temperature solution polycondensation in *m*-cresol. All the polyimides were amorphous in nature as indicated by their wide-angle X-ray diffraction patterns. Polyimides exhibited high thermal stabilities.

6.4.4 New dicarbanionic initiator for the synthesis of poly(styrene-b-butadiene-b-styrene)

A new dicarbanionic initiator has been developed 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 was 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.

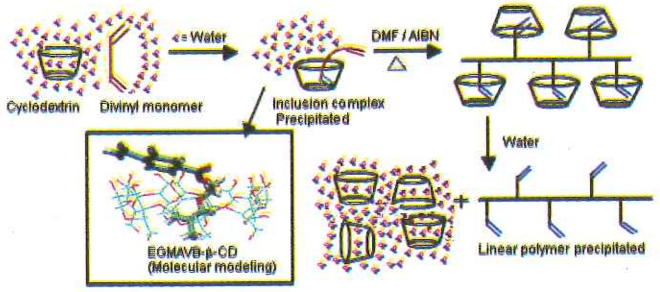
This is the first example of a dicarbanionic initiator totally soluble in non-polar media without any additives, which allowed us to synthesize well-defined polybutadiene telechelics with a high percentage of 1,4-PB units (91%). This initiator has proved to be very efficient in providing SBS triblock 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%. Thus, a long-standing issue faced by the industry of styrenic thermoplastic elastomers could be sorted out. This project is in collaboration with University of Bordeaux, France

6.4.5 Functional polymers from divinyl monomers via cyclodextrin host guest chemistry

Crosslinked polymers find a wide range of applications such as ion exchange resins, adsorbents, molecularly imprinted polymers, supports for reagents in organic synthesis, enzyme immobilization and drug delivery systems. A sequential multistep approach wherein a soluble linear polymer is first synthesized isolated and then crosslinked offers significant advantages in most applications. Recent approaches to synthesize soluble polymers from divinyl monomers have led to hyperbranched structures. Therefore there is a need to devise a one step methodology for the synthesis of solvent soluble, linear and crosslinkable polymers.

In the methodology developed at NCL, the insoluble divinyl monomers form an inclusion complex with â-cyclodextrin and its derivatives such as dimethyl â-cyclodextrin. The vinyl group included in the cavity of â-cyclodextrin does not participate in polymerization. As a result, a divinyl monomer behaves as a monovinyl monomer. The polymerization results in a solvent soluble linear polymer containing a vinyl double bond per repeat unit.

This polymer can subsequently be cross-linked by free radical initiator or by UV irradiation, to yield films, micro, and nanoparticles and graft copolymers. The material has potential to find application in various fields such as coating, microelectronics, photoresists, molecularly imprinted polymers, ion exchange resins, as chromatography support, reagent in organic synthesis, drug delivery systems and other biomedical applications.

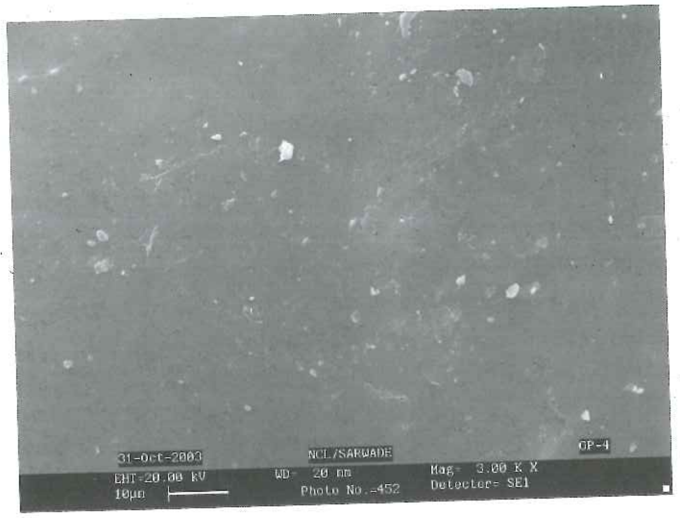


6.4.6 Structural and functional mimicry of bio-systems - carbohydrate - laced synthetic polymers as microbe nutrient source

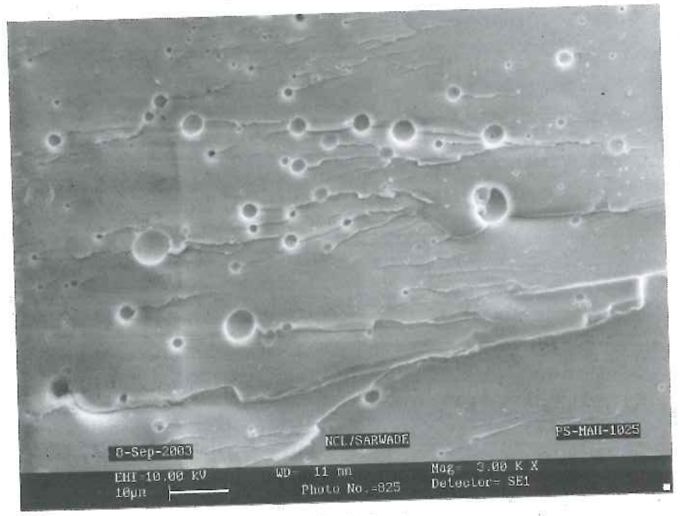
The objectives of this project were to investigate synthesis of mono- and disaccharide (sucrose, lactose and glucose) anchored polyolefins onto functionalized polystyrene and polyethylene, and controlling the extent of saccharide linked to the polymer. This is followed by a study of interactions of pure bacterial cultures such as *Pseudomonas sp.* (NCIM 2220), *Serratia sp.* (NCIM 5061), *Bacillus sp.* (NCIM 2812), etc. and pure fungal cultures such as *Aspergillus niger* NCIM 1025 (ATCC 9642), etc., with the new carbohydrate linked polymers for use as nutrient sources for the microbial cultures. The ultimate goal is to establish the relationships of "polymer structure"-"polymer property"-"microorganism specificity" to arrive at the mechanism of polymer biodegradation.

The saccharides are food sources for microorganisms. In an aqueous environment, the hydrophobic polymer chain is in a tightly coiled conformation with all the hydrophobic groups in the centre of the coil and the hydrophilic carbohydrate groups on the exterior of the coiled polymer chain. This feature can allow microorganisms to adhere to the polymer surface.

The project activities included: i) synthesis of glucose-linked polyethylenes and glucose, lactose and sucrose linked polystyrenes, ii) biodegradation studies by fungal cultures *A. niger* and *Trichoderma* (including isolates), bacterial cultures serratia, bacillus, and pseudomonas, iii) fungal degradation studies completed (including isolates) including weight loss studies, protein weight studies. These studies showed the extent of biodegradation that occurred, iv) bacterial degradation studies completed including weight loss studies, protein weight studies. These studies showed the extent of biodegradation that occurred, and v) atomic force microscope and scanning electro microscope methods to understand the adherence of microorganisms onto the polymers has been carried out in some specific cases.



Sugar linked polystyrene film in un-degraded form

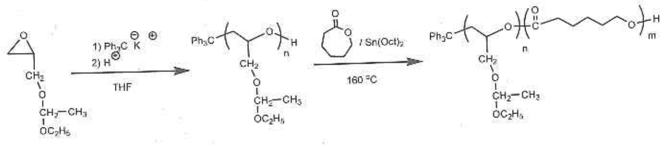


SEM of commencement of biodegradation by bacteria on sugar-linked polystyrene film

6.4.7 Amphiphilic copolymer micelles for a sustained delivery of actives

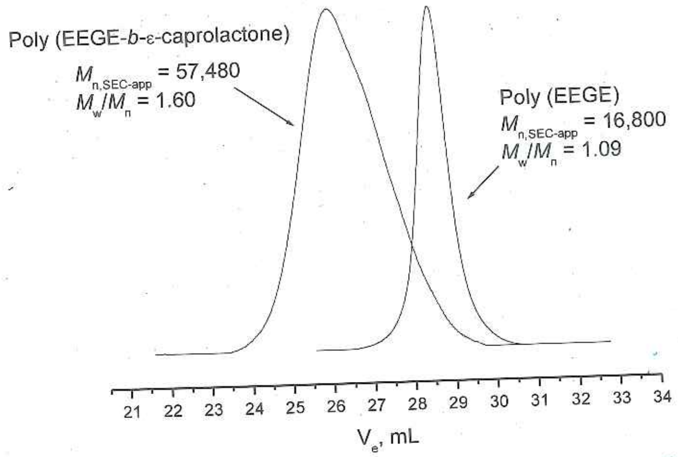
Amphiphilic block copolymer micelles can hold hydrophobic agents in its miceller core and deliver the reagents slowly into an aqueous environment through diffusion. New amphiphilic block copolymers for oral formulation to deliver flavor components, antimicrobials were proposed. The advantage of the tailor-made block copolymers is that it is possible to control the association of amphiphilic diblock copolymer in solution in a definite manner in to micelles, lamella or vesicles depending on its segmental block lengths and concentration. The assemblies of diblock copolymers can be used as vehicle to deliver hydrophobic actives in oral care products such as toothpaste.

Poly(ethoxyethylglycidol ether-*b*-ε-caprolactone) was synthesized and evaluated its micellar characteristics and antimicrobial agent loading capability. The synthesis of block copolymer was accomplished through anionic and ring opening coordinative polymerizations.



Synthesis of poly(ethoxyethylglycidol ether-*b*-ε caprolactone) through anionic and ring opening coordinative polymerizations.

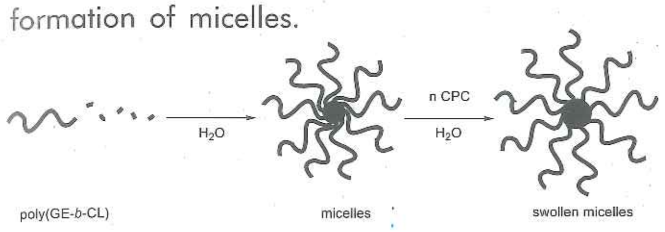
The polymerization of protected glycidol, ethoxyethylglycidyl (EEGE) ether was performed using various potassium alkoxides and triphenylmethanide as initiators in THF at 50 °C for 24 h. The homopoly(EEGE) was recovered and characterized using ^{1}H NMR and SEC. The chain-ends of poly(EEGE) were used to polymerize ε caprolactone, CL at 150 °C in bulk for 24h in the presence of catalyst. The progress of the polymerization can be seen in figure.



SEC eluogram of poly(ethoxyethyl glycidyl ether-*b*-ε caprolactone) diblock copolymer formation

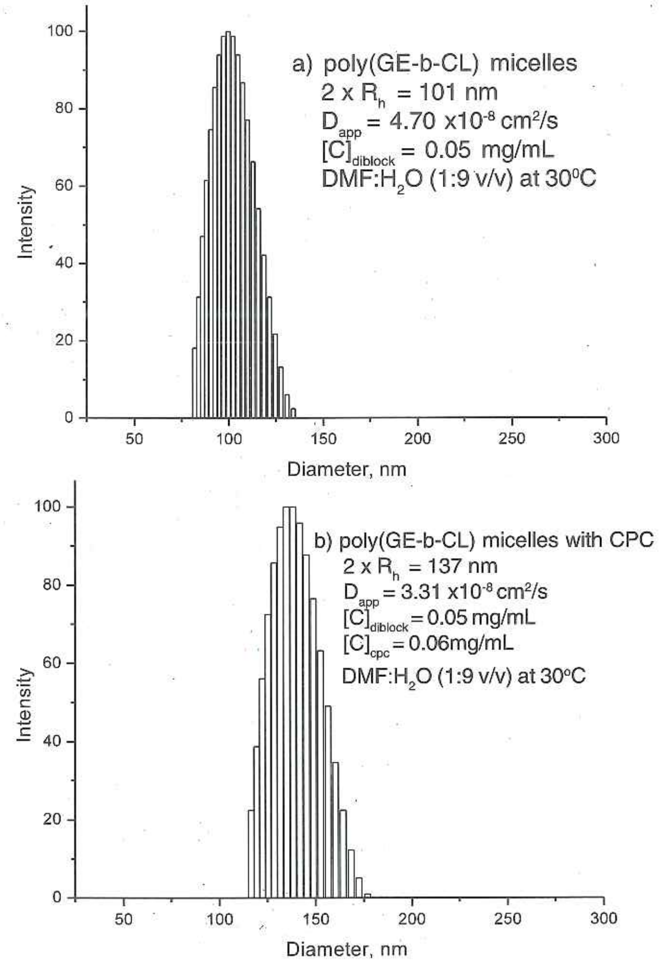
6.4.8 Oral active swollen micelles of amphiphilic diblock copolymers

The synthesized diblock copolymers were used to form micelles in aqueous solution. The diblock copolymers were dissolved in a small amount of dimethylformamide (DMF) and diluted with water to form micelles. The aqueous solution of diblock copolymer in the presence of a small amount of DMF shows slight blue coloration indicating the formation of micelles.



CPC swollen micelles of poly(glycidol-*b*-ε-caprolactone) and poly(ε-caprolactone-*b*-acrylic acid)

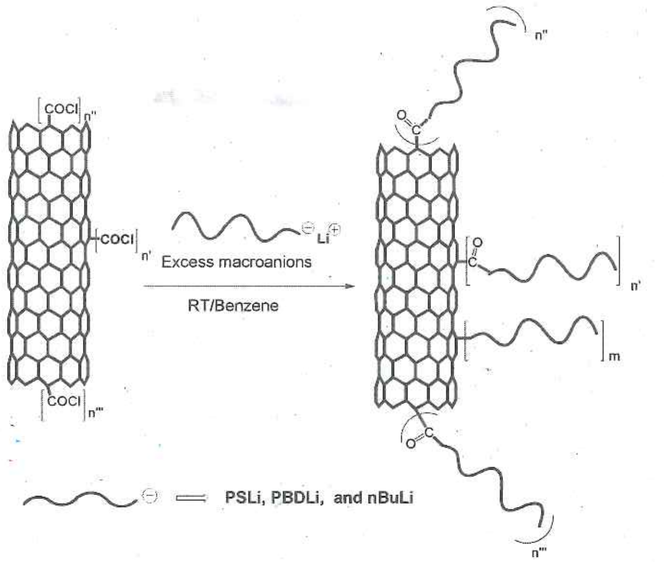
Dynamic light scattering studies of the poly(glycidol-*b*-ε-caprolactone) in water:DMF (9:1 v/v) solution show the presence of micelles with diameter around $\sim$100 nm. The polydispersity of micelles is moderately narrow. Upon addition of an active such as cetylpyridinium chloride (CPC) (reagent for oral formulation), the size of the micelles increased to 137 nm. The size of micelles increases up to $\sim$37 nm in the presence of CPC which indicates inclusion of considerable amount of CPC into the hydrophobic core of the micelles.



Dynamic light scattering studies of a) the poly(glycidol-*b*-ε-caprolactone) micelles in water:DMF (9:1 v/v) solution b) swollen micelles in the presence of CPC

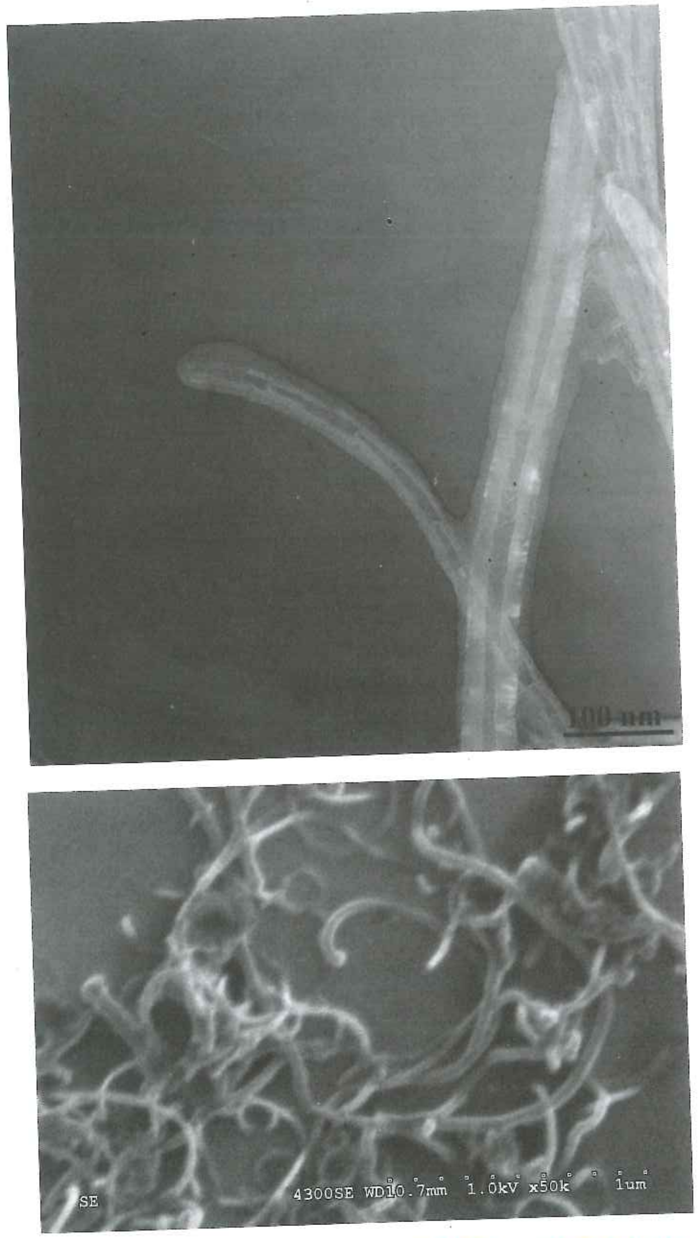
6.4.9 Grafting reactions of living macroanions with multi-walled carbon nanotubes

Grafting reactions of living polystyryllithium (PSLi) with acid chloride containing multi-walled carbon nanotubes (MWNTs-COCl) were performed under vacuum in benzene at room temperature. Covalent grafting of polystyrene (PS) was characterized using spectroscopic, microscopic and thermogravimetric analyses. Grafting at different ratios of macroanion to acylchloride concentration of the carbon nanotubes showed that the grafting efficiency was not dependent on the concentration of the macroanions. The mole percent of PS present in the MWNTs-*g*-PS samples was inversely proportional to the precursor molecular weight of PSLi.



Grafting reactions of living macroanions with MWNT-COCl in benzene at 30 °C for 15 h. A direct addition of macroanions with *sp*² network is also shown

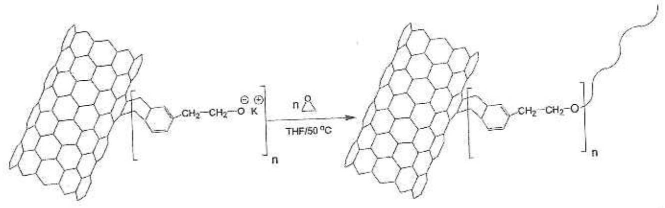
Direct reactions of PSLi, polybutadienyllithium and *n*-butyllithium with pristine MWNTs without any functional groups were also performed in the presence and in the absence of tetrahydrofuran in benzene. The grafting reactions of living macroanions either with MWNTs-COCl or with pristine MWNTs indicated a partial grafting of polymer with carbon nanotubes in benzene at room temperature.



TEM (A) and SEM (B) images of MWNTs-*g*-PS exhibiting presence of thin amorphous layers of PS

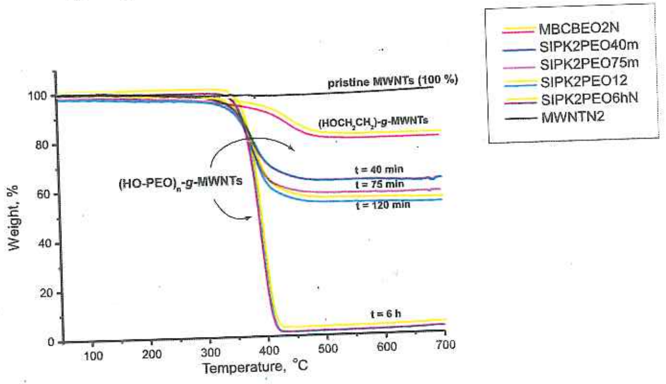
6.4.10 Surface initiate anionic from multi-walled carbon nanotubes

The surface of multi-wall carbon nanotubes (MWNTs) has been covalently functionalized with appropriate initiator moieties and used in anionic polymerization and atom-transfer radical polymerization (ATRP). Initiator grafted MWNTs were obtained by reacting hydroxyethyl-2-bromoisobutyrate with the surface bound carboxyl groups of MWNTs. Polymer grown MWNTs after washing and drying show the characteristic vibration bands in the IR spectrum and the corresponding polymer decomposition in the thermogravimetic analysis. The homo, block and copolymers consisting of polystyrene and poly(methyl methacrylate) brushes chemically bound to the surfaces of MWNTs up to 70 wt.% have been synthesized and characterized. However, the growth of high molecular weight polymer was difficult due to a low concentration of radical initiator on the surface. High concentration of initiator could be attached directly to the surfaces of nanotubes using functionalized benzocyclobutene compounds via o-quinodimethane intermediate at 200 °C. Anionic polymerization of ethylene oxide and ATRP of methyl methacrylate and styrene have been successfully carried out in high yield. Surface grown poly(ethylene oxide) containing < 1 wt. % MWNTs has been synthesized and characterized.

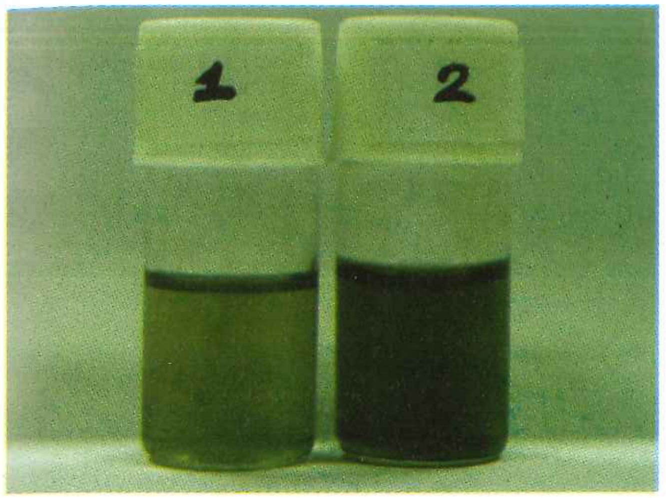


Anionic polymerization of ethyleneoxide from the surface of MWNTs

Anionic polymerization of ethylene oxide was performed under high vacuum. The polymerization proceeded smoothly to yield high conversion. The kinetics of the surface grown PEO is slow. However, the polymerization shows a linear time dependent growth of PEO. The recovered PEO grown from the surface of MWNTs contains only less than 1 wt. % carbon nanotubes indicating a large amount of polymer grafted to the tubes. High percentage of PEO on MWNTs (90-98 wt % of PEO) was observed by TGA. The obtained PEO-g-MWNTs are soluble in THF, $CHCl_3$, H_2O and other solvents.



TGA of MWNT-g-PEO during surface initiated polymerization at different time



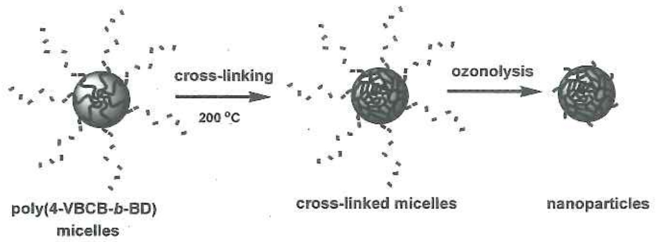
Vials of solutions of $(PEO)_{90}$-*g*-MWNTs. 1) $CHCl_3$, 1.25 mg/mL 2) H_2O, 3mg/mL

6.4.11 Living anionic polymerization of 4-vinylbenzocylcobutene and synthesis of nanoparticles from poly(4-vinylbenzocyclobutene-b-butadiene) micelles

Block copolymers obtained can be self-assembled in solution and in bulk to form micelles, vesicles, and microphase separated bulk morphologies with features on the nanoscale. Anionic polymerization of 4-vinylbenzocyclobutene has been initiated with the aim of making block copolymer assemblies that can be used to synthesize organic nanoparticles. The pendant benzocyclobutene groups of the homo or block copolymers can undergo radical crosslinking at 200 °C. Hawker and co-workers have elegantly exploited the thermally switchable cross-linking behavior of poly(4-vinylbenzocyclobutene) to synthesize polymeric nanoparticles through intramolecular crosslinking.

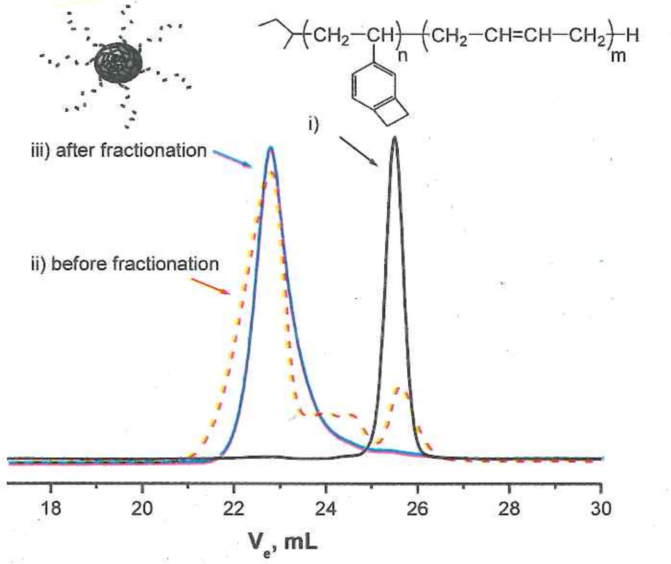
6.4.12 Synthesis of nanoparticles from diblock copolymer micelles as precursor

The objective is to make diblock copolymer of poly (4-vinylbenzocyclobutene) with 1,3-butadiene. Nanoparticles could be synthesized by cross-linking the benzocyclobutene pendants in the micelles at the core and cleaving the polybutadiene corona block via ozonolysis.



Synthesis of functional polymeric nanoparticles usingmicelles of poly (4-vinylbenzocyclobutene-b-butadiene)

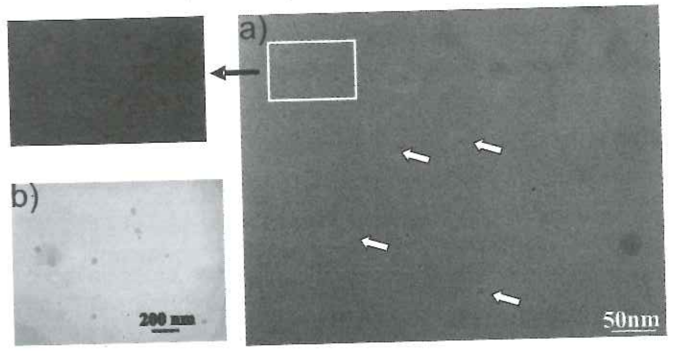
This micellar precursor strategy gives several advantages as 1) control of the size of the core through block length of diblock copolymer, 2) functional groups such as –OH or –CHO can be introduced through ozonolysis on the surface of the nanoparticles, and 3) it is possible to control the distribution and the density of nanoparticles as the extent of cross-linking at the core and the unimer formation strongly dependent on the temperature of micellar stabilization.



Size exclusion chromatography of core cross-linked micelles; i) poly(VBCB-b-BD) diblock copolymer, $M_{n,LS}$ = 33,000 g/mol, M_w/M_n = 1.02, ii) after cross-linking at 200 °C, and iii) after fractionation, $M_{n,LS}$ = 1,800,000 g/mol, M_w/M_n = 1.50

Several diblock copolymers were synthesized through sequential living anionic polymerization using high vacuum technique. The diblock copolymers exhibit stoichiometric molecular weights with narrow molecular weight distribution ($M_w/M_n<1.03$). The diblock copolymers were dissolved in decane which is a non-solvent for poly(VBCB) segments to form micelles. The solution of this diblock copolymer in decane showed a blue tint confirming the formation of micelles.

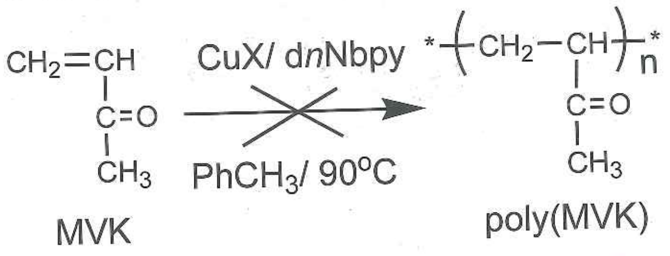
The static and dynamic light scattering (DLS) of the micelles indicated the existence of uniform spherical micelles with apparent aggregation numbers (N_w) in the range of 11-78. Thermal cross-linking of benzocyclobutene pendants in the micellar core was accomplished. The SEC traces of core cross-linked micelles indicate about 10-15 % unimer formation during cross-linking. DLS of core cross-linked micelles dissolved in THF, which is a good solvent for both blocks, indicated that the micelles remain intact due to cross-linking. In order to obtain functional nanoparticles, the core cross-linked micelles were subjected to ozonolysis to cleave the 1,4-polybutadiene corona segments in dichloromethane at -78 °C. The reaction was quenched with dimethylsulfide as a reducing agent to produce hydroxy functional groups on the surface of the nanoparticles. The insoluble nanoparticles were dispersed in methanol/ dimethylformamide mixed solvent under sonication and drop coated on a carbon grid for TEM characterization. TEM images show discrete nanoparticles ranging from 2-4 nm along with agglomerated nanoparticles ranging from 15-30 nm in diameter. The size of the nanoparticles is comparable to the size of the core in diblock copolymer micelles which corroborates the TEM results. Enlarged images of the agglomerated particles show clearly that they are composed of several discrete nanoparticles.



TEM of nanopartilces synthesized using poly(VBCB-*b*-BD) micelles as precursor. a) dispersed and b) agglomerated nanoparticles

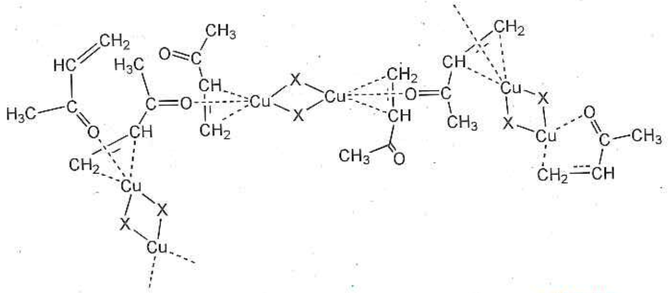
6.4.13 Coordination of copper with methyl vinyl ketone inhibits atom transfer radical polymerization

Polymerization of methyl vinyl ketone (MVK) via copper mediated ATRP using various initiator/CuX/ligand/solvent systems was investigated. The ligands such as N,N,N′,N′,N″ pentamethyldiethylene triamine (PMDETA), N-(*n*-propyl)-2-pyridylmethanimine (NPPI), 2,6-*bis*[1-(2,6-diisopropylphenylimino)ethyl]pyridine (BPIEP), 4,4′-di(*n*-nonyl)2,2′-bipyridine (d*n*Nbpy), and 2,2′-bipyridine (bpy) were used in the presence of CuX (X = Cl or Br) with [MVK]: [I]: [CuX]: [Ligand] = 127: 1: 1: 2. Experiments were conducted in different solvents such as diphenyl ether, THF, anisole, and also in bulk at 90 °C for several hours (3-24h).



Non-polymerizing nature of methyl vinylketone due to its strong coordination with copper

During the polymerization, the color of the reaction mixture changed to reddish-brown or green depending on the nature of ligands used for the reaction. However, no polymer was produced. GC studies demonstrated that the reaction mixture contained a large amount of unreacted MVK. The fact that the radical polymerization of MVK produces polymer and the copper mediated ATRP initiating system does not produce polymer indicates that the copper catalyst is the cause for the inhibition of polymerization. It was concluded that that there exists a strong coordination between MVK and copper that prevents polymerisation. The ^1H NMR spectrum of MVK-CuBr complex showed a huge up-field shift of vinyl and CH_3 protons of MVK indicating an enhanced pi-electron interaction of vinyl groups with copper.



The proposed extended-coordinative structure of $(MVK)_m$-$(CuBr)_n$ based on *X*-ray crystal structure of MVK-CuX. The structure shows both trans-confirmation, and inter/intra molecular MVK coordination with CuX dimer.

The coordination of copper with monomer would influence the equilibrium of activation and the deactivation processes in ATRP and, thus it could significantly alter the kinetics of polymerization. In the case of MVK, the coordination of copper appears to be very strong, extensive which completely inhibits the polymerization. The monomer coordination with copper catalyst in ATRP is very high in MVK than other monomers such as N,N-dimethylacrylamide and methyl (meth)acrylate monomers.

6.4.14 Visible light induced cationic polymerization of n-butyl vinyl ether

The cationic polymerization by harvesting visible light via photoinduced electron transfer reactions was intiated. n-Butyl vinyl ether (BE) has been polymerized using diphenyl diselenide (PhSeSePh) and 1,4-dicyanonaphthalene (DCN) where PhSeSePh acts as a cationic initiator and DCN as a light harvestor (≥ 300 nm). The polymer produced at –15 °C and –25 °C with different irradiation intervals exhibited different molecular weight and molecular weight distribution (MWD). The polymer was characterized by ^1H NMR spectroscopy. The polymerizations were found to be living, linearly increasing molecular weight and narrow MWD with conversion. The mechanism of cationic polymerization has also been proposed.

6.5 Polymer degradation and stabilisation

6.5.1 Hindered amine light stabilizers

A polymeric hindered amine light stabilizer (HALS), where HALS moiety was attached at the terminal end of the polypropylene chain via end-functionalized vinylidine PP through simple organic reactions was synthesized. It comprises the synthesis of vinylidine-terminated polypropylene by using Cp_2ZrCl_2/MAO as catalyst system and epoxidation of vinylidine polypropylene. The final product was synthesized by carrying out the reaction between epoxy end functionalized polypropylene and 4-amino-2,2,6,6-tetrametyl piperidine. The new formulations show very good stabilization performance in polyolefins and other polymers.

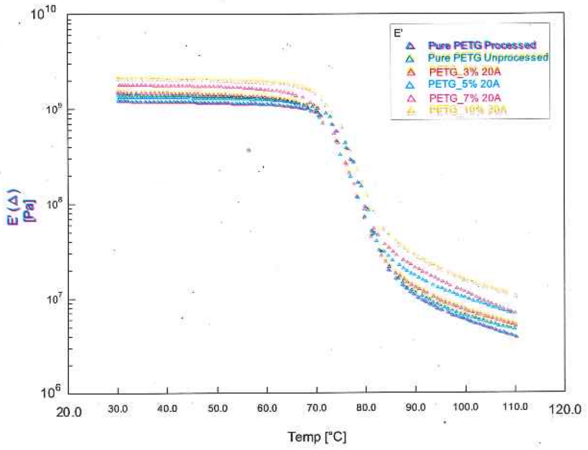
6.5.2 Durability of natural fiber reinforced composites

Polymer composites were prepared by melt mixing of ethylene propylene copolymer (EPC) with (i) 3% NaOH treated jute fiber, (ii) 17.5% NaOH treated jute fiber and (iii) commercial microcrystalline cellulose powder using maleated EP (MEP) copolymer as compatibilizer. The durability of the composites was evaluated under UV irradiation chamber supplying wavelength λ e″ 290 nm and composting conditions for different time intervals. Composites made from microcrystalline cellulose showed higher mechanical properties, biodisintegrability as well as photo-resistance whereas specimen containing 3% NaOH treated fiber exhibited lowest photo-resistance. The increasing quantity of MEP in composition decreases photo-stability. Neat EP copolymer was found highly stable than all the composites with increasing UV irradiation. It was found that the composites were less durable under both abiotic and biotic conditions in comparison of neat polymer.

6.6 Organic-inorganic hybrids

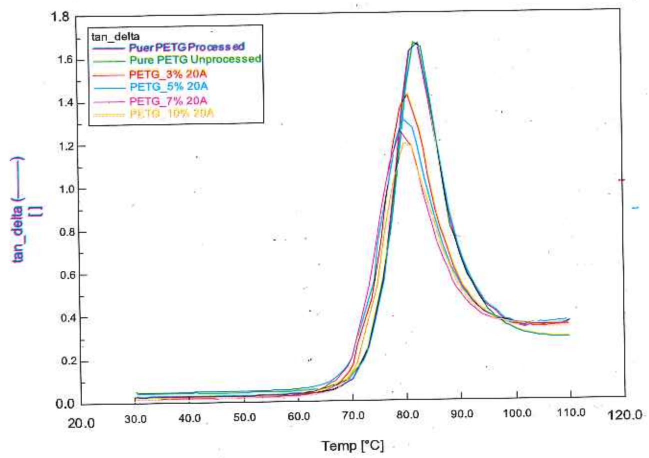
6.6.1 PETG/clay nanocomposites

The solid-state viscoelastic properties of poly (ethylene glycol-co-cyclohexane-1,4-dimethanol terephthalate) (PETG), 20A nanocomposites containing a series of 20A content were studied using dynamic mechanical analysis (DMA). The storage modulus of the nanocomposites shows an increase in the glassy state as compared to the pristine processed and unprocessed PETG as a function of 20A concentration. The unprocessed PETG has a higher storage modulus than that of processed PETG.



PETG 20A Nanocomposites

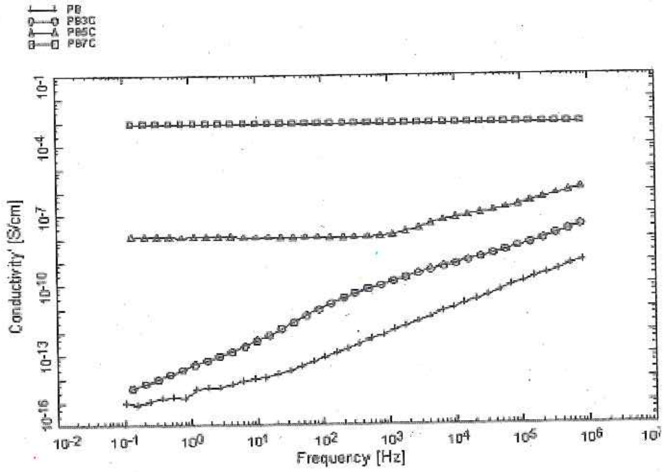
This has been attributed to a small amount of thermal degradation of the polyester during processing. The increase in the storage modulus of the nanocomposites suggests that amount of the undesired thermal degradation has been negated by the reinforcement effect of the clay nano-layers. The storage modulus of the nanocomposites in the rubbery regime increased by orders of magnitude over that of the pure PETG, which further corroborates the reinforcement effect of the clay nano particles. The temperature dependence of tan delta for PETG and its nanocomposites with 20A showed systematic reduction in damping with increasing 20A loading in the nanocomposites. Also there is a slight reduction in the T_g of the nanocomposites as compared to the pure PETG. This could be attributed to the plasticization effect of the low molecular weight dimethyldihydrogenated tallow compound used to render the clay organophillic for effective compatibilization with the polymer.



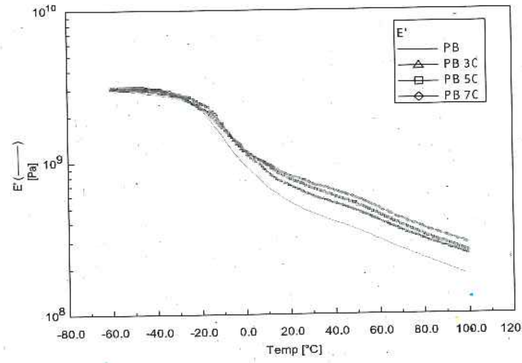
PET G 20A Nanocomposites

6.6.2 PB/MWCNT Nanocomposites

The effect of multiwalled carbon nanotubes (MWCNT) on the kinetics of crystallization and phase transformation of poly (1-butene) (PB) was studied using differential scanning calorimetry (DSC). The isothermal crystallization studies indicated that the crystallization rate was accelerated in nanocomposites as evidenced by the significant increase in crystallization temperatures and lower crystallization half time compared to pristine PB. The observed changes in the crystallization kinetics were ascribed to the enhanced nucleation of PB in presence of MWCNT. The nucleating activity calculated from the non-isothermal crystallization data confirmed that the MWCNT provide an active surface for nucleation of PB. The rate of phase transformation from kinetically favored tetragonal to thermodynamically stable hexagonal form was enhanced significantly due to incorporation of MWCNT. The half time for phase transformation for PB was about 58 hrs which remarkably reduced to 25 hrs for PB containing 7% MWCNT.

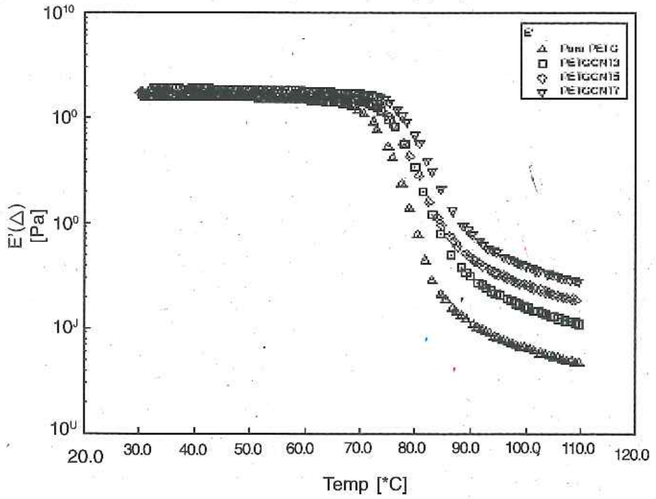


Linear viscoelastic properties and dielectric behavior of poly(1-butene)/ MWCNT nanocomposites were investigated. Dynamic mechanical analysis showed significant increase in storage modulus in the rubbery regime. The tan d peak temperature remained constant; however, the peak intensity was lowered for the nanocomposites. In melt rheological studies the nanocomposites showed a shift in crossover frequency to the lower side, suggesting delayed relaxation of the molecular chains in the presence of MWCNT and this shift was found to depend on the content of MWCNT. The dielectric constant increased from 2.2 to 70 for the nanocomposite with 7 wt. % MWCNT. The electrical conductivity increased significantly as shown in the figure. The results of rheology and dielectric studies indicated that a percolation network was formed that is responsible for the observed changes.

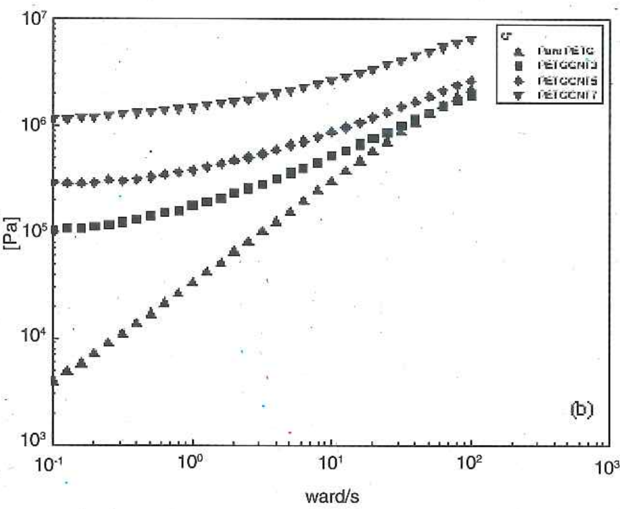


6.6.3 PETG/MWCNT nanocomposites

Amorphous copolyester, poly(ethylene glycol-co-cyclohexane-1,4-dimethanol terephthalate) (PETG), and carbon nanotube based nanocomposites were fabricated by using simple melt processing technique. The reinforcement effect of carbon nanotubes in the copolyester was investigated experimentally using different approaches based on dynamic mechanical analysis, rheology, and dielectric relaxation spectroscopy.



The nanocomposite hybrids showed a mechanical reinforcement effect with significant increase in the stiffness especially in the rubbery regime with increasing nanotube content. The nanocomposites showed an increase in their T_g as compared to the pure polymer and increase in damping, which is derived from the presence of a percolating superstructure of the filler. From the dynamic rheological experiments, up to four orders of magnitude increase in storage modulus of the nanocomposites was observed. The non-terminal behaviour observed for molten nanocomposites suggested a solid-like viscoelastic response, which increases with increasing nano-tube content. The results of the solid and melt – state viscolelastic characterization showed that the percolation threshold of these nanocomposites is below 3 % weight fraction of nanotubes. Additionally the results indicated that the solid-like response in the nanocomposites is due to lack of complete relaxation of the polymer chains, which originates predominantly due to the presence of an interconnected filler network rather than due to adsorption of polymer chains on nano-tube surface. Dielectric relaxation spectroscopy confirmed the presence of this percolating structure. The responses of both rheological and electrical properties were different although both were related to the formation of a percolating network superstructure of the filler.

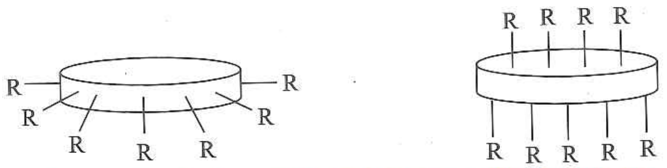


6.6.4 Novel hybrid of chitosan-g-lactic acid and montmorillonite

The utilization of biopolymers and the development of organic-inorganic hybrids are ever increasing interest of material science researchers around the globe for various applications. The present attempt was intended to prepare nanocomposites of lactic acid grafted chitosan and layered silicates. Nanocomposites were prepared by dissolving chitosan and dispersing Na^+-MMT (sodium montmorillonite) in aqueous solution of L- lactic acid with subsequent heating and film casting. The films have shown enhanced hydrophilicity as compared to PLA. It was observed that nanocomposites are exhibiting better thermal and physical properties than neat chitosan-g-LA and PLA.

6.6.5 Hybrid inorganic-organic nanoparticles

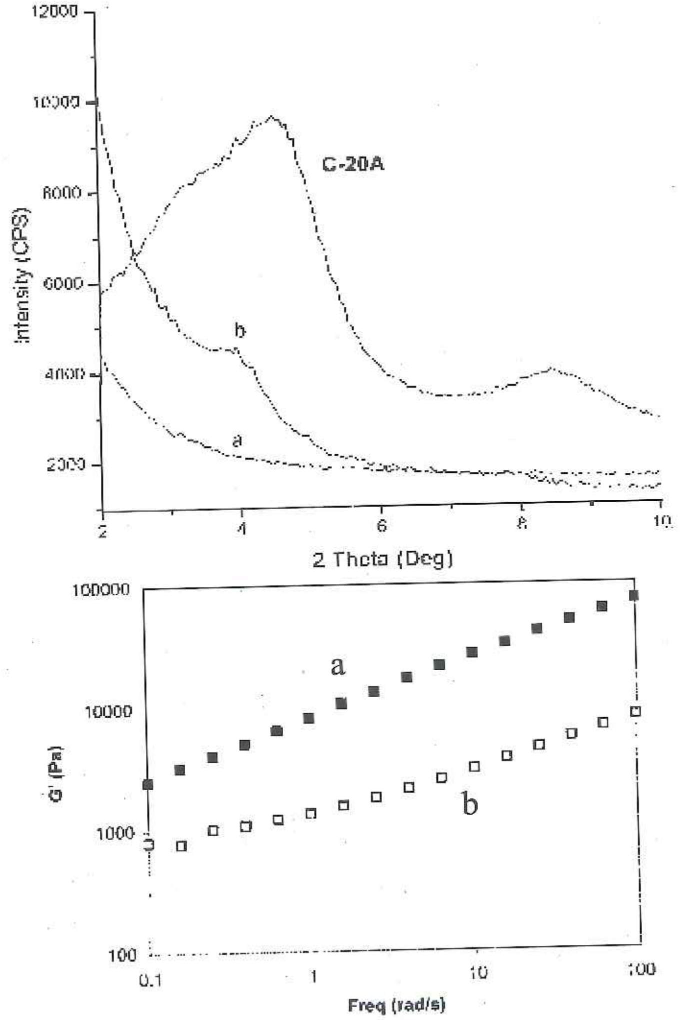
Methods to synthesize plate-like hybrid inorganic-organic nanomaterials that present covalently-bound organic functionalities specifically at either the basal surface or the edges have been developed. These organic groups can be used to tune nanoparticle interparticle interactions or their interactions with a matrix polymer. Thus, vinyl functionalized hybrid nanoparticles organize into networks in polyolefins, forming composites that show higher zero shear viscosity and increased shear thinning. Edge- functionalized nanoplates also showed qualitatively different gelation in water and water/alcohol mixtures.



Schematic of edge and basal plane modified synthetic organoclays

6.6.6 Rheology of in situ synthesized polyethylene-nanoclay composites

PE-MMT nanoclay composites were prepared by two different methods – (i) suspending the clay as such in a homogeneous Al/Fe catalysed polymerization process, and (ii) heterogenizing the Al/Fe catalyst on the MMT surface and polymerizing PE using this catalyst. The microstructure of these samples as probed by WZXD revealed the high degree of exfoliation for (ii) compared to (i). Rheological measurements on these samples showed a substantially higher storage modulus for sample (ii) than sample (i), which is easily explained based on the formation of a percolating network of clay particles due to exfoliation in the sample (ii).

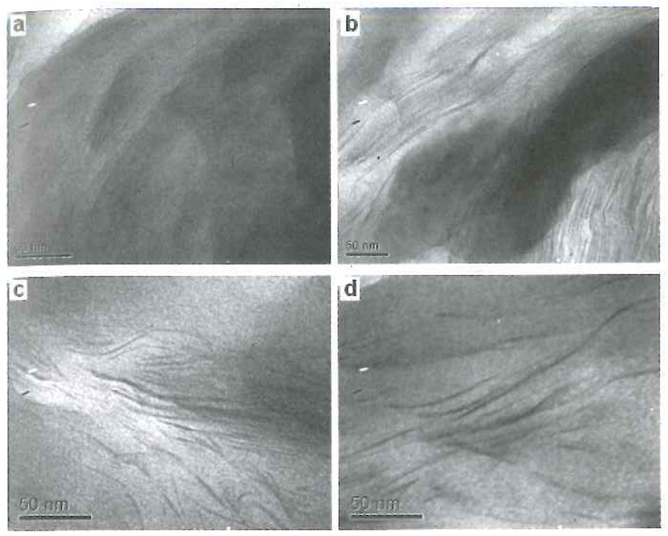


WAXD and rheology of samples (b) homogeneously catalysed and (a) heterogeneously catalysed PE-nanoclay composites

6.6.7 Preparation and characterization of sulfonated syndiotactic polystyrene ionomers / organoclay nanocomposites

Polymer/layered silicate nanocomposites often exhibit remarkable enhancement in material properties when compared with virgin polymers at very low filler loadings. Recently, to improve the surface energy of semicrystalline polymers in the preparation of nanocomposites, ionic groups were introduced on to the polymer chains. Nanocomposites prepared from ionomers of polypropylene, polyethylene and a variety of other nonpolar thermoplastics polymers also revealed good levels of organoclay exfoliation.

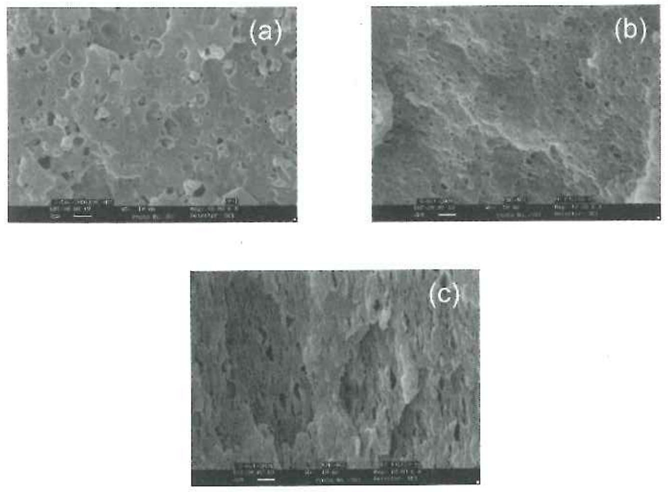
Nanocomposites of sulfonated syndiotactic polystyrene (SsPS) ionomers with organoclay, modified by 1-hexadecyl-2,3-dimethylimidazolium cation were prepared. The effect of ionomer content and cation type on the intercalation/exfoliation efficiency of the SsPS ionomer/organoclay nanocomposites were studied using wide-angle X-ray diffraction (WAXD) and transmission electron microscopy (TEM). The dispersion of the organoclay in the polymer matrix improved with an increase in the ionomer content. The efficiency of intercalation/exfoliation enhanced on changing the cations of the ionomers from H^+ to Rb^+ in the group I series of the periodic table. Ionomer-organoclay interaction enhanced the crystallization rate of nanocomposite compared to SsPS ionomer due to prevention of ionic aggregation by clay platelets.



TEM micrographs of SsPS ionomers 3.8 mole %/ organoclay nanocomposites (a) SsPS, (b) NaSsPS, (c) KSsPS and (d) RbSsPS

6.6.8 Controlling the properties of PP-EP using nanoclays and mixed compatiblizers

Polypropylene-ethylene/propylene rubber copolymers are widely used in load bearing applications for their good balance of flexural and impact properties. Attempts were made to improve the properties of PP-EP through the use of nanoclays that was dispersed in the matrix and dispersed phased through the use of mixed compatibilizers. The best balance of properties was obtained through the use of PP-MA + PE-MA compatibilizers.



SEM micrographs of PP-EP/nanoclay composites; native polymer (a); PP-EP/clay/PP-MA (b); PP-EP/clay/PP-MA+PE-MA (c)

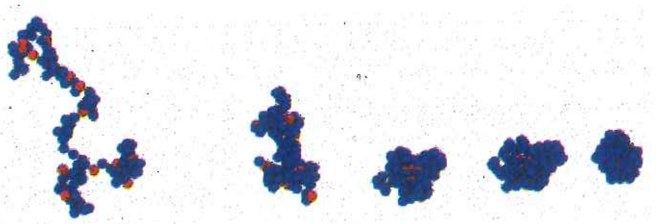
6.6.9 Nanocomposite hydrogel membranes

Nanocomposite hydrogels composed of specific polymers and water-swellable inorganic clay exhibit enhanced mechanical properties. The novel nanocomposite hydrogels can overcome some of the limitations in the conventional hydrogels. The study of laponite (inorganic clay) incorporated PVA-N-tertiary butyl acrylamide [NTBA] hydrogel membrane were undertaken. The incorporation of laponite in nanocomposite membranes was investigated by FT-IR spectroscopy and thermogravimetric analysis. The swelling ratio of membranes was determined as a function of temperature and laponite content. Swelling studies of nanocomposite membranes exhibited decrease in swelling with an increase in laponite content in the nanocomposite membranes. The swelling ratio of nanocomposite membrane with 20% laponite slightly increased with an increase in temperature. Dynamic mechanical analysis showed systematic increase in storage modulus with laponite content, which indicated enhancement of mechanical property upon laponite addition. There was also a decrease in the tan δ peak values of nanocomposite membranes with an increase in laponite content in nanocomposites. The permeabilities through nanocomposite membranes as a function of solute size and laponite content were studied and the results showed molecular screening based on size. The permeability of solute reduced due to presence of well-dispersed laponite in the nanocomposite.

6.7 Structure-property-performance correlation

6.7.1. Coil-globule transitions in copolymers

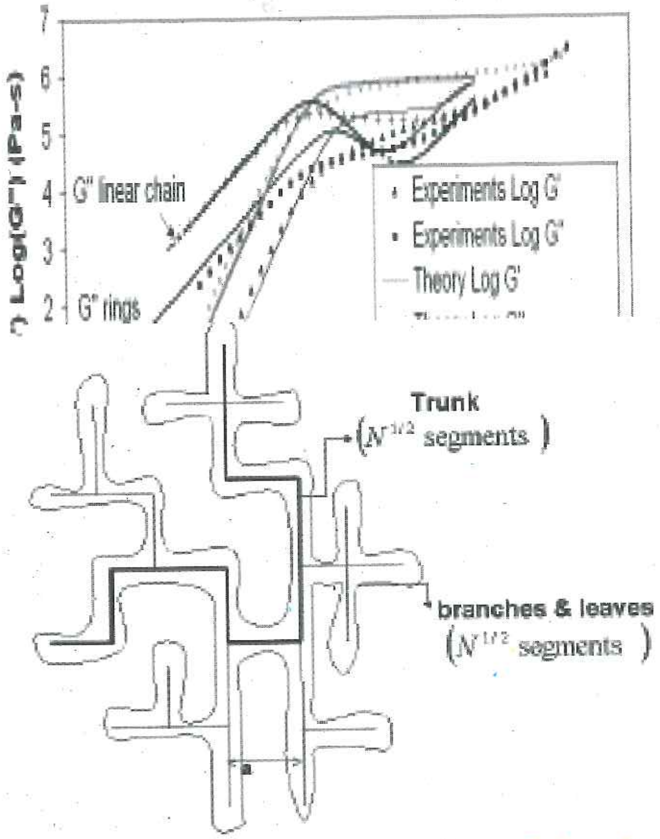
The influence of comonomers on single molecule collapse and on melt crystallization of polyolefins is being explored. The simulation results point to an interesting effect: copolymers with sticky comonomers collapse more abruptly than homopolymers, but only for a small percentage of comonomers. For increased comonomer contents, the normalized behaviour of the copolymers is qualitatively identical to that of homopolymers.



Monte Carlo simulation of collapse of single copolymer coil to a core-shell globular state

6.7.2 Dynamics of ring polymer melt

A mean field coarse grained model for predicting the thermal motions and the linear viscoelastic behaviour of flexible endless ring polymers in a given obstacle environment (fixed, melt) has been developed. The model predicts that the plateau modulus of a ring polymer melt would be substantially lower than that of a chemically identical linear polymer melt of the same molecular weight due to two effects – dilution caused by rapidly relaxing loops and a compact static structure. The predictions for linear viscoelastic behaviour compare semi-quantitatively with the experimental data available in the literature.

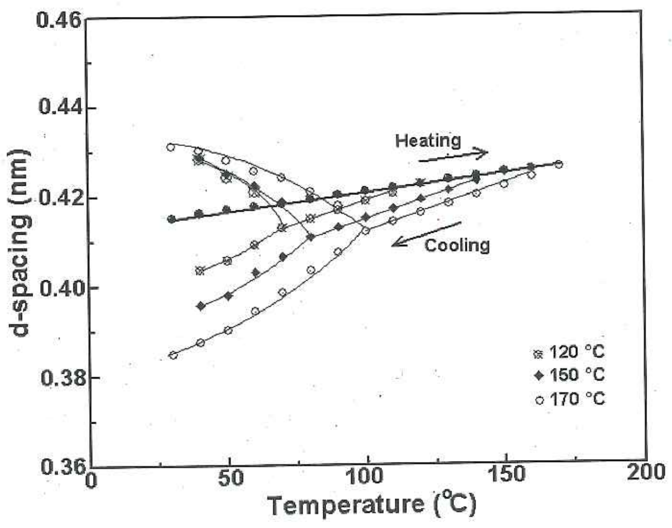


Model for a flexible ring polymer and its predictions of linear viscoelasticity as compared to experimental data

6.7.3 Crystalline phases in Nylon 11: Studies using HTWAXS and HTFTIR

Nylons, the first "engineering thermoplastics", are characterized by strength, elasticity, resistance to abrasion and chemicals, and capacity to be permanently set by heat. The properties are governed by the structure consisting of flexible methylene segments and rigid amide groups connected in an alternate manner along the chain axis. Among nylons, nylon-6,6 and nylon-6 are commercially successful and have been extensively explored scientifically. Nylon chains experience relatively large thermal motion even at room temperature due to the twisting motion around the CH_2–amide bonds. Increasing the temperature activates the thermal motion of the chains further and this results in the occurrence of crystalline transition and in the case of nylon-6,6 it is called the Brill transition.

In the odd nylons group, nylon-11 received considerable scientific attention because of its piezoelectric and ferroelectric properties. Nylon-11 exhibits polymorphism and several researchers have studied the polymorphism of nylon-11. For the first time we reported the observation of change in the 001 d-spacing during phase transition. The value and the variation of the *d* spacing of the 001 reflection is highly phase sensitive. The 001 *d* spacing showed a change in the value when α and α′ phase changed into the pseudohexagonal phase or vice versa. Similar changes were seen when the γ phase transformed in to pseudohexagonal phase on heating to melt. The above studies indicated that nylon-11 showed a change in the structural features above 110°C on heating which manifested as a change in the crystalline phase.



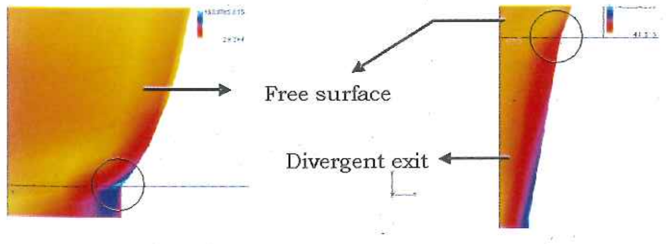
The behavior of the *d* spacings of the melt quenched sample on heating to 170 °C and on cooling from the holding temperatures 170 °C, 150 °C and 120 °C to room temperature. The arrows indicate the direction of heating/ cooling.

The variable temperature FTIR studies indicated that α and α′ phases had similar conformation in the crystalline phase. The γ phase showed characteristic infrared bands at different positions from those of α and α′ phase. It was speculated from the HTFTIR studies on TFA cast film with 5% TFA that the interaction of TFA with amide groups might be responsible for the formation of γ phase.

6.8 Rheological studies in polymers

6.8.1 Delaying sharkskin through the use of dies with divergent exits

The effect of a divergent exit on the occurrence of sharkskin distortions on extruded surfaces as a function of shear rates was investigated. It was noted that the sharkskin instability is delayed and/ or completely removed with increase in the length of the divergence exit of the die. The experimental studies were modelled using viscoelastic CFD. Simulations showed that the divergent exit causes a remarkable reduction in principle stresses along surface streamlines immediately upon exit of the die. Sharkskin may be eliminated when the principle stresses decrease below the critical rupture stress. Reduction in the velocity in the divergent exit also reduces the 'reconfiguration rate' of stretched polymer chains, thereby causing a reduction of the sharkskin distortions.



Stress concentration (blue coloured, marked with a circle) seen immediately after the die exit in the case of die with no divergent exit (a); the stress concentration dramatically reduces when a divergent exit is introduced in the die (b)

6.9 Polymer product development

6.9.1 Orbital implants

The porous polyethylene orbital implants developed in the laboratory were subjected to rigorous third party clinical trials for six months. The results of the trials were successful and paved the way for commercial introduction of the product in the market. It is expected that the product will be equivalent in all respects to an imported product and will be available at a substantially lower price in the Indian market. The process for making porous polyethylene orbital implant has been transferred to Biopore.

Commercially available Biopore orbital implants

6.10 Biomedical applications of polymers

6.10.1 Hydrogel membranes for bio separations

Recently, major attention has been focused towards developing stimuli-sensitive hydrogels and membranes for selective separations. Chitosan [CS] and poly(vinyl alcohol) [PVA] hydrogels were investigated to design and develop the thermosensitive membranes, which exhibit discontinuous volume transition in water as a function of temperature. Poly(N-isopropylacrylamide) [PNIPAm], is the most commonly used thermosensitive polymer exhibiting the lower critical solution temperature [LCST] in the range of 31-33°C. Thermo- and pH- sensitive hydrogel membranes were synthesized based on chitosan and PNIPAm. Thermosensitive membranes based on modified PVA polymer were also developed. Irreversible adsorption of PVA onto hydrophobic membranes such as poly(vinylidene fluoride) [PVDF] using XPS, water contact angle, etc was studied. The molecular origin of the wettability of PVDF surface by hydrophilic PVA has been deduced by XPS and EDAX measurements.

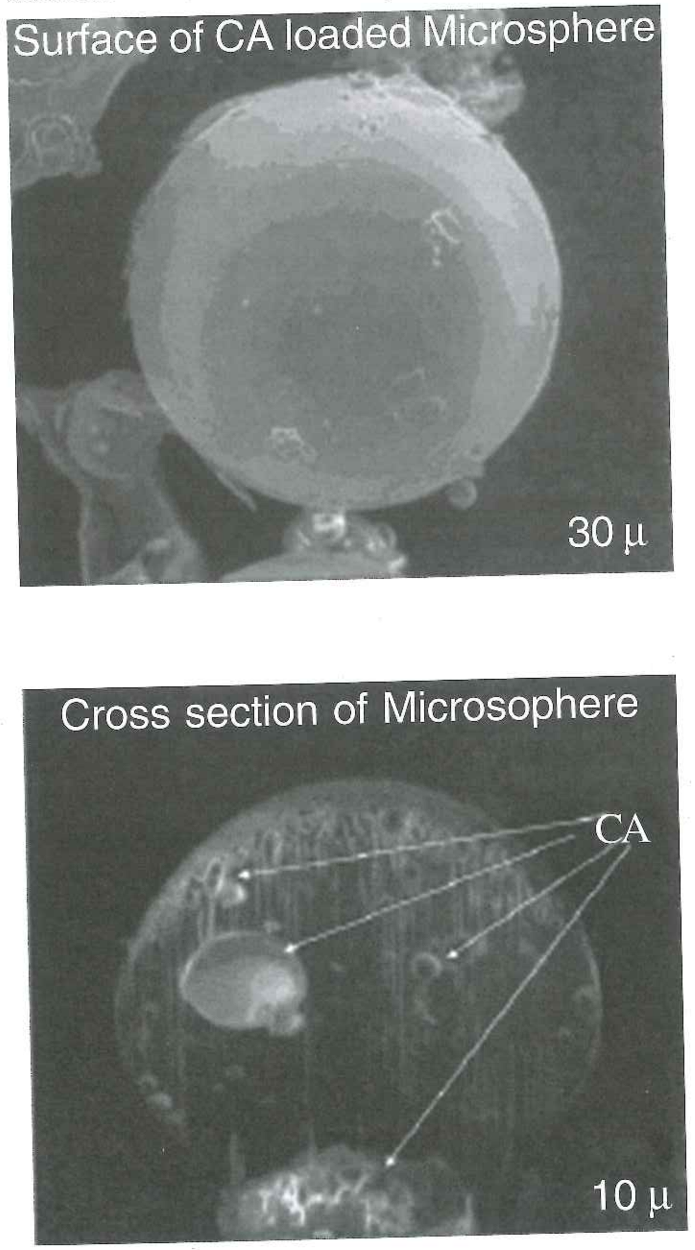
6.10.2 Enhancing bioavailability of drugs

To attain the desired therapeutic objective, the drug has to be delivered at an optimal rate and amount. The *pharmaceutic* approach which involves modification of the formulation, manufacturing process or physicochemical properties of drug without changing the chemical structure, is the most preferred approach to enhance bioavailability (the rate and extent of drug absorption). The primary concern for drugs exhibiting lower bioavailability and restricted absorption window is designing the delivery systems which release the drug at the desired site thus enhancing their absorption and in turn the bioavailability. A major consideration in use of polymers for drug delivery is drug-polymer interaction, drug transformation and its degradation. The drug-excipient interactions can result in complete loss of activity of drug or delayed release.

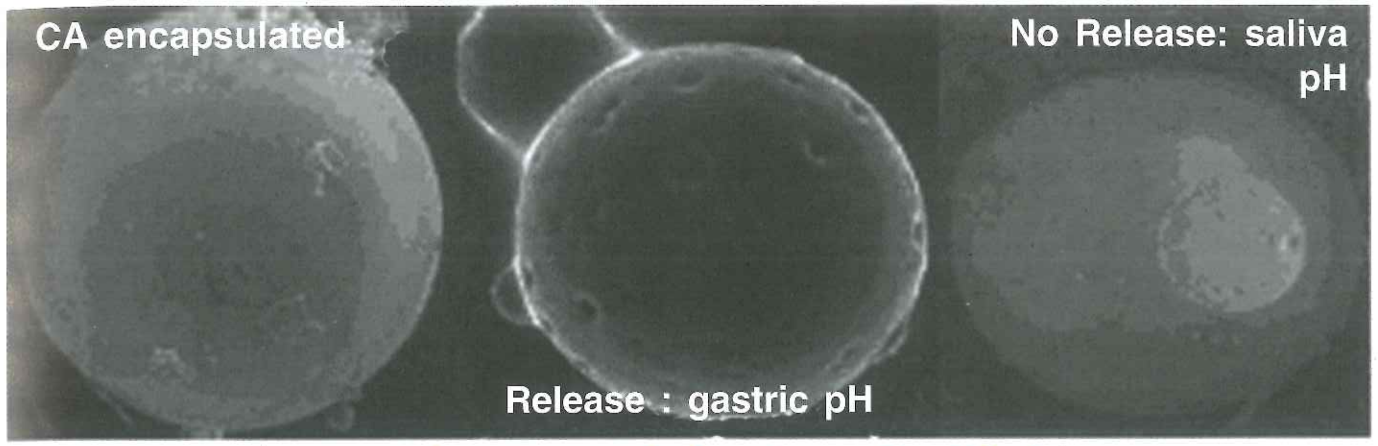
Drugs with limited absorption window, which in turn affects their absorption and consequently bioavailability, and those, which are inactivated due to the drug-polymer interaction, were identified. In particular, drugs such as cefuroxime axetil, ciprofloxacin hydrochloride and clarithromycin which are absorbed in upper gastric region and those required for local and immediate action were selected.

Development of a new reverse enteric polymer (NREP) which dissolves at gastric pH and can be used for the development of drug delivery systems for taste masking, immediate and sustained gastric release was undertaken. A detailed investigation of drug-polymer compatibility of the drug in active form was undertaken. The blends of NREP with other polymers to bring about sustained release of these drugs at gastric and intestinal pH were studied. The extent of interaction between polymer blends was quantified in terms of Schneider equation. The *in-vitro* drug release experiments were carried out to ensure the complete release of drugs.

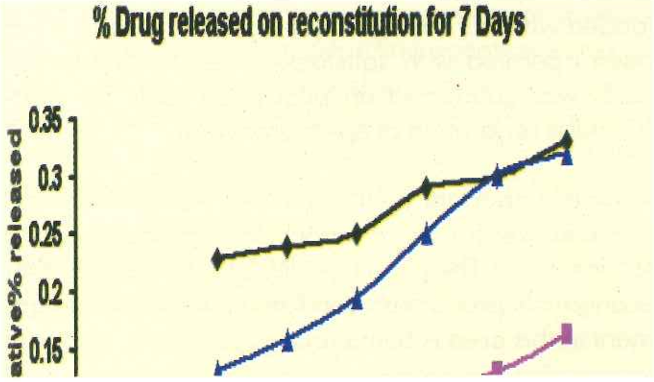
NREP was found to effectively taste mask the drugs with immediate release in gastric pH. Also sustained release formulation for gastric release of drugs can be formulated using NREP. This ensured the release of drugs better absorbed from gastric region at the right site and at the rate desired.



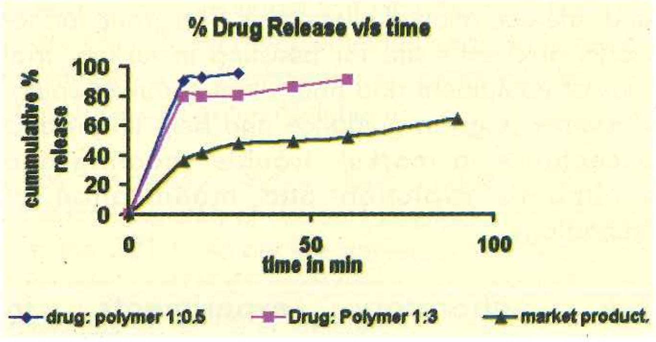
New reverse enteric polymer for drug delivery



Application of new reverse enteric polymer: taste masking of bitter drugs



Inhibition of drug release in reconstituted suspension enhancing palatability



Drug release from NREP in gastric pH

7. PROCESS DEVELOPMENT AND ENGINEERING

The group involved in process development and process design activity is responsible for translating laboratory innovations into commercial technologies. This activity is done with a multi-pronged approach like conducting laboratory experiments using special assemblies, experimental determination of physico-chemical data in order to develop a proper flow sheet, simulation of unit operations / processes using commercially available software, detailed process design calculations for establishing feasibility The complex work also involves design, construction and safe operation of pilot plants. The group further works at client's site for assisting in testing, trial runs of equipment and final plant commissioning. Customer is given guidance and help till product acceptance in market, trouble shooting and continuous evolution and modification of technology.

7.1 Laboratory experiments in specially designed assemblies.

Some of the common facilities for conducting laboratory experiments are small setups consisting of fractionation assemblies, rotary vacuum evaporators, packed bed-catalytic reactors with external re-circulation facility, high temperature furnaces and autoclaves. Data on reaction kinetics, thermal stability of products / reactants, screening of catalysts for activity / time-on-stream, separation of desired product by applying proper unit operations and alternative techniques of improving rates, yields and selectivity are collected by the experiments. The experiments establish the relative importance of various process parameters and enable one to do better scale-up.

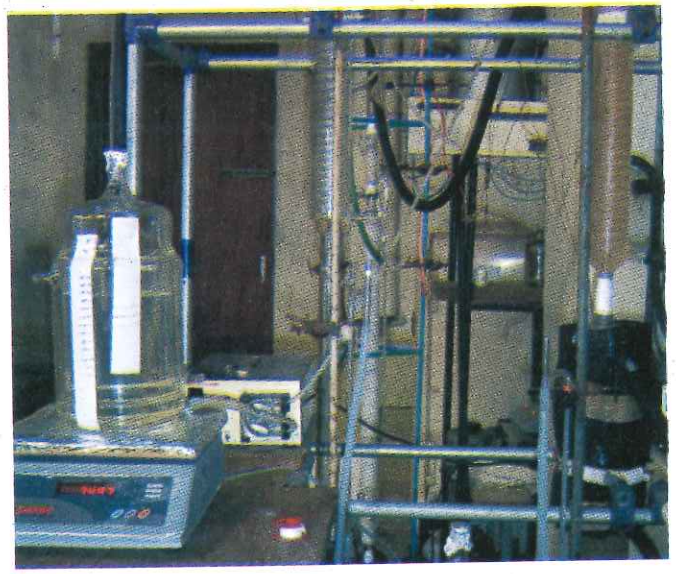
In the year of reporting, study was conducted, using novel laboratory equipment, for synthesis of extracting agents for highly critical applications. Application of short path distillation unit in separation and purification studies was established.

7.2 Construction and operation of pilot plants

Pilot plants are constructed after duly collecting / analyzing preliminary process data. In the event of uncertainty regarding some data affecting the process viability exists; and when some discrimination is required in choosing one or the other unit operation additional data on pilot plant scale is required. Due to the additional engineering data that is collected in such studies, one can enhance the confidence in design.

In the year of reporting, new pilot plants were constructed and operated; one of them deals with catalytic epoxidation; a novel tubular reactor unit loaded with extruded catalyst was erected and it has been operated with satisfactory results. Separation study was conducted on pilot plant scale for post-synthesis separation of epichlorohydrin.

Another important pilot plant that was erected and operated was for silicon tetrachloride production for a foreign client. The plant has yielded sufficient data for economical production and further work and assignment in this area is being taken up.



7.3 Experimental determination of physico-chemical data

Separation techniques require the knowledge of physico-chemical and thermo-chemical data. Although a large database is available in commercial simulation software, process development and design group feels the need of experimental data for multi-component systems in practice. Solubility, VLE, LLE, SLE and heats of reactions in multi-component mixtures are required for process design and scale-up. Heat of reaction data is not available in literature nor can it be computed based on information available for each step in critical reactions.

In the year of reporting, a large number of systems such as epichlorohydrin, extracting agents solvent etc. were studied for physico-chemical and thermo-chemical data with a view to assist process development and plant troubleshooting. Estimation of the heat of reaction data was done for several critical steps.

7.4 Simulation and preparation of design documents

The group is equipped with commercial software to do simulation studies of unit operations and obtain optimal design solutions to flow schemes and system synthesis. Preparation of engineering drawings and documents, including basic engineering packages was done with the software.

In the year of reporting, the group prepared several documents for clients. One of them deals with a promising catalytic process (epichlorohydrin using TS-1 catalyst). The other deals with conceptual design and validation of a complex distillation system (epichlorohydrin).

Group has potential for designing industrial reactors as per requirements. In one such assignment sulfur trioxide reactor unit for 25g/hr capacity was designed Basic engineering package for the same was also prepared NTPC will use these designs in their power production plants for injecting sulphur trioxide in flue gas systems for reducing fly ash emissions.

7.5 Ecology and environment

7.5.1 Technical and financial audit of CFC production sector in India

Chlorofluorocarbons (CFCs) have an adverse impact on the environment in the long run. They deplete ozone layer and allow harmful ultra violet radiations from the sun to reach the earth's atmosphere. Montreal Protocol is an international environment treaty concerned with protecting earth's ozone layer. This Protocol stipulates that CFCs and similar ozone depleting substances are to be completely phased out by 2010 in Article 5 countries. United Nations Environment Programme (UNEP) is the governing body monitoring the implementation of the Montreal Protocol. India is a signatory to the Protocol. The CFC phase out in India is implemented and monitored by the Ministry of Environment and Forests (MOEF) with the Ozone Cell as the nodal unit.

As per the protocol, Indian plants producing CFCs will have to completely phase out manufacturing CFCs by the year 2010. As per the agreement between CFC producers and MOEF, each enterprise is prescribed an annual quota for the CFC production by MOEF. MOEF (Ozone Cell) has mandated the National Chemical laboratory, Pune for monitoring the production phase out of CFCs by the Indian CFC producers as per the prescribed production quota. NCL is doing CFC Technical & Financial Audit of all four Indian production plants from 2000 till 2004. NCL is expecting to continue this assignment till 2010.

7.5.2 Technical appraisal of CTC consumption sector phase out proposals

As per Montreal Protocol commitments, India has to phase out production and consumption of carbon tetra chloride (CTC) for non-feed stock applications such as process agent and solvent use. The enterprises, which have to phase out CTC consumption as non-feed stock use, need to prepare a project document detailing CTC consumption, alternate technologies along with time plan and associated costs. NCL is doing the CTC consumption verification, technical feasibility of the alternate technology, changes required in the existing plant and equipment.

Work in above area was continued in this year under report and technology and financial implications audit was continued.

PUBLIC PRIVATE PARTNERSHIP PROGRAMMES

8. PUBLIC-PRIVATE PARTNERSHIP PROGRAMMES

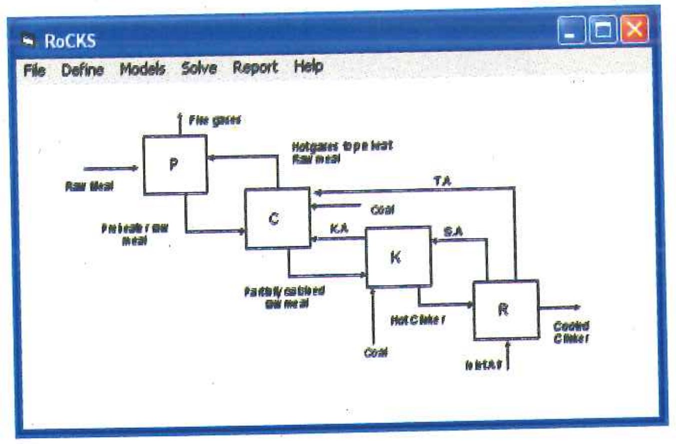
The New Millennium Indian Technology Leadership Initiative (NMITLI) envisages a symbiotic promotion and fostering of public-private partnership to enable Indian Industries to attain global leadership position in selected niche areas. The programme is backed by national determination to turn sound technological ideas into a reality through a systematic development of innovative projects. Over the last six years, CSIR has evolved 42 projects involving over 65 industry partners and 222 R&D Institutions of India. Following projects are undertaken at NCL:

8.1 Improved granular processing: towards energy efficiency and resource conservation in cement manufacture

(Grasim Industries Ltd., Mumbai, Indian Institute of Technology, Mumbai, Larson & Toubro Ltd., Mumbai, National Metallurgical Laboratory, Jamshedpur, The Associated Cement Companies Ltd., Thane and The India Cements Ltd., Chennai)

A comprehensive project was initiated under the NMITLI program in April 2002 to enhance performance of cement rotary kilns. Task of NCL was to develop computational models to enhance kiln performance. A comprehensive one-dimensional model for rotary cement kiln was developed. Furthermore a phenomenology based computational models for pre-heater, calciner and cooler were also developed. These models were coupled with the kiln model to develop a simulator for the entire cement plant. A menu driven, easy to use software called RoCKS (Rotary Cement Kiln Simulator) was developed to facilitate use of computational models to practising engineers.

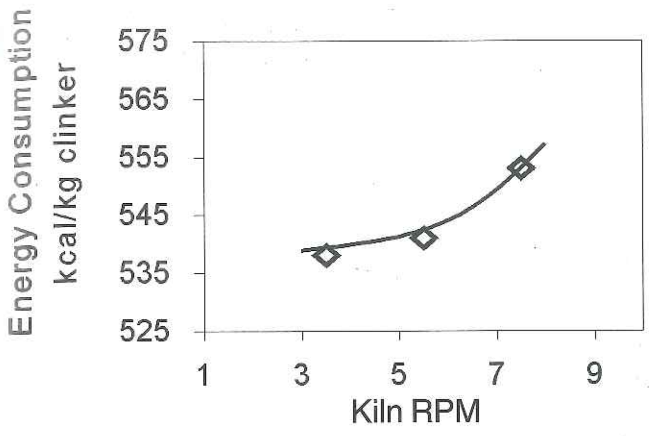
Separate models for pre-heater, calciner, kiln and cooler were developed initially. These individual models were coupled to each other to represent the clinker manufacturing process.



Screen shot of RoCKS

The model for calciner was formulated based on Eulerian-Lagrangian approach. The coal particles and raw meal particles were considered as discrete phases and gas phase was assumed to be completely back mixed. The model for cement kiln was developed by including coupling of the free board and the bed regions. Model for simulating variation of bed height was also included in the kiln model. The solid-solid reactions in the kiln bed were modelled assuming solids to be pseudo homogeneous. Combustion of coal in the freeboard region of calciner and kiln was modelled by accounting devolatilization, finite rate gas phase combustion and char reaction. The heat transfer between solids and air in individual models was predicted via empirical correlations. The coupled simulator was solved iteratively. The iterations were continued till the temperature of solids and gases at exit of individual modules are within one percent. Suitable under relaxation parameters were identified for faster convergence of the solution.

The integrated model was initially validated with available data from industry. On obtaining a reasonable agreement, various numerical experiments were carried out using the model to understand influence of key different design and operating parameters on performance of individual components. Thereafter several ways for reducing energy consumption were computationally investigated. As a sample of simulated results, the predicted influence of kiln rotational speed on overall energy consumption is shown in graph. These results showed that operating the kiln at lower RPM would be beneficial from energy conservation point. The models and the results show a promise in reducing energy consumption in cement industry.



Influence of RPM on energy consumption

8.2 Functionalization of alkanes: A catalytic process for the preparation of ethylene and acetic acid from ethane

(Indian Petrochemicals Corporation Limited, Vadodara)

The objective of the above project was to develop a catalyst formulation and a process for the economic production of acetic acid and ethylene (which are feed-stock for vinyl acetate monomer) from ethane by vapour-phase oxidation with oxygen. More than 200 catalyst compositions were prepared, characterized and screened using a state-of-the-art multiple high pressure reactors (with on-line analysis facility) for their catalytic activity for converting ethane to acetic acid and ethylene.

Among these at least three catalyst formulations were found which met the project targets, namely, 10 % conversion and a combined selectivity of more than 80 %. It was found that the selectivity of acetic acid and ethylene ratio could be controlled by small variations in the catalyst formulations. The catalysts were active and stable for several hours (more than 120 h) under the experimental conditions. The best catalyst formulation was scaled up to 650 g (final catalyst after calcination with 40 % binder) and three such batches were prepared. Finger prints for the final catalysts were developed based on IR, diffuse reflectance UV-Vis, powder XRD and XPS techniques.

Catalytic experiments were carried out with feed ethane/ molecular oxygen/steam where maximum acetic acid concentration in the liquid product was achieved more than 40 %. The data from the best result is: 10 % ethane conversion, 73 % selectivity to acetic acid. Reactor flow charts were made for ethane to acetic acid process as well as for the integrated process for making vinyl acetate monomer from ethane in two steps and preliminary economic analysis were carried out assuming 50,000 tpa capacity of acetic acid and vinyl acetate productions.

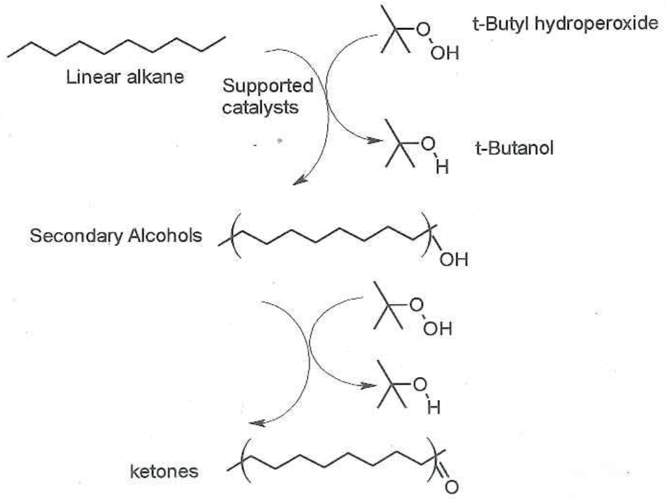
Impurity profile analyses for the liquid products as well as for the gaseous products were made at ppm levels. Economic analysis carried out by IPCL indicates that the project results are promising. The costing analysis suggested a need for few more optimizations and is being studied.

8.3 Detergent alcohols by oxidation of higher alkanes using alkyl hydroperoxide as oxygen carrier

(Indian Petrochemicals Corporation Limited, Vadodara)

The program was initiated with the following objectives: (i) Development of a process for the oxidation of $C_{11} - C_{13}$ alkanes to detergent alcohols using alkyl hydroperoxide as an oxygen carrier, (ii) Process for the preparation of t-amyl hydroperoxide using isopentane and oxygen/air, and (iii) Investigation on the role of catalysts in the cleavage of alkyl hydroperoxides as an alternate route to detergent alcohols.

A new iron based supported catalyst was developed which could oxygenate linear higher alkanes using tert-butyl hydroperoxide to ketones and alcohols primarily. With dodecane the catalyst gave about 20% conversion of the alkanes with ketone and alcohol selectivity in the range of 60 – 70%. The proposed reaction pathway was as follows:



The catalyst was also efficient for the oxidation of other linear alkanes in the range C_{10} to C_{16}, and even commercially available alkane mixtures were oxygenated to corresponding secondary alcohols and ketones. This catalyst was also prepared on granular supports so that a continuous operation could be feasible. A supported Pd catalyst has also been developed which is also active and selective in the oxidation of higher alkanes to alcohols and ketones.

The synthesis of tert-amyl hydroperoxide was also standardized and catalysts were developed for the oxidation of isopentane to TAHP in good yield. The schematic reaction is represented below:

The catalyst was also demonstrated to form the TAHP from a mixture of pentane and isopentane- a mixture that is available as a refinery stream.

8.4 Polymers from biomass: cellulose, hemicellulose and lignin

(*Godavari Sugar Mills Ltd, Mumbai*)

A variety of agricultural biomass is available in India for exploitation and development into value-added materials. A project was undertaken to fractionate waste agricultural biomass like sugarcane bagasse into cellulose, hemicellulose, and lignin. Extensive experimental work carried out at NCL was approved for taking forward to the next stage of setting up a semi-commercial facility, along with an industrial partner. Work on design of a suitable reactor for this purpose is underway. Further, work on conversion of hemicellulose to ethanol and other value-added derivatives such as xylose and xylitol is also being undertaken. Earlier, conversion of bagasse derived cellulose to cellulose triacetate, and lignin to lignosulfonate was also developed on a laboratory scale. Thus, a complete value chain has been developed for the polymers that can be derived from agricultural biomass. It is envisaged that in future, several petroleum based polymers can be replaced by polymers obtained from agricultural biomass.

8.5 Biotechnology of leather: Towards cleaner processing

(*SPIC Science Foundation, Chennai*)

Among several enzymes screened for application in leather manufacture, two proteases, a lipase and an amylase were found to be suitable. Optimization of protease production with respect to media composition, age of the stock, age and medium inoculum, pH and temperature were carried out in shake flasks. The production of both the proteases was scaled up in 5 L instrumented fermentor and yields were comparable to those obtained in shake flasks. protease 1 was also scaled up in 100 L fermentor. Maximum yields were obtained of Protease 1 and protease 3 in 60-72 h and 120 h, respectively. Complete dehairing of skins and hides was achieved with 0.5-2% Protease 1 and Protease 3 without lime and sulphide. Based on the evaluation trials conducted at CLRI, both the proteases viz. NCL protease 1 and NCL protease 3 were selected as lead products for enzymatic dehairing for commercialization in NMITLI phase II. Four industries interested in the products developed by the project were invited to participate in the phase II of the project aimed at commercialization of leads gained in phase I.

8.6 Stimuli sensitive polymeric nanoparticles for oral delivery of insulin

(*USV Ltd. Mumbai, National Institute of Pharmaceutical Education and Research, Chandigarh and Shree Chitra Institute of Medical Science and Technology, Trivandrum*)

Diabetes is a life style induced disease. In addition to the affluent countries of the west, diabetes has posed a serious threat to the population in the Indian subcontinent, in view of the genetic predisposition and changes in the life style influenced by globalization. Presently insulin is administered as an injection which is both painful and needs training to patients. Efforts are therefore in progress world wide to develop alternative delivery routes for insulin. Especially development of nasal insulin is fairly at an advanced stage but has not been fully commercialized.

A project on oral delivery of insulin was initiated at NCL three years ago. Based on the analysis of the fate of orally administered insulin, efforts were made to encapsulate insulin in carriers which will prevent degradation of insulin in the gastric region and enzymatic degradation in the intestinal route. Biodegradable polymers into which insulin can be encapsulated and released in the circulation system were identified and synthesized. Insulin has been encapsulated into the nanoparticles. The particle size ranges from 150 to 500 nm. The particles are expected to be transported across intestinal mucosa and release insulin in the biologically active form in circulation. Evaluation of these samples, to show that insulin is not degraded in the gastric as well as intestinal region as a result of encapsulation, is currently being undertaken at NIPER, Chandigarh.

8.7 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*)

India's annual soft woods and pulp imports are worth over Rs. 10,000 crores. The projected annual short fall of paper and paper products is expected to grow to approximately 4 million MT by the year 2010. Wood, agricultural residues and many other plant materials, which are used for pulp and paper production, consist largely of lignocellulose. The lignin is removed from the cellulose fibre using alkali. The pulp further requires bleaching treatment to remove lignin residues. The delignification process consumes large quantities of energy and chemicals, and also creates environmental concerns. Reducing the content or changing the quality of lignin in pulp wood species without compromising their mechanical strength is desirable.

Although a variety of plant species are of importance to the paper industry, *Leucaena sp.* is exclusively used in India. 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. This proposal will provide a strong technology base in India with the potential of providing leadership in raw materials for paper and pulp industries.

The mandate for NCL was to isolate the lignin biosynthesis pathway genes from *L. leucocephala*, and develop *in vitro* regeneration and transformation methodologies for *L. leucocephala*. So far isolated two genomic clones of the caffeoyl coenzymeA 3-O-methyl transferase (CCoAOMT), one genomic clone of the cinnamyl alcohol dehydrogenase (CAD), one cDNA clone each of CCoAOMT, CAD, coumarate-CoA-ligase (4-CL) and cinnamoyl CoA reductase (CCR) were isolated at NCL. The gene sequences have been deposited with the NCBI, USA. The accession numbers are as follows:

CCoAOMT : DQ174453, DQ174455, DQ313432, DQ219382, DQ313433,
CAD : DQ361031, DQ381538, DQ381539
4-CL : DQ267975
CCR : DQ313434, DQ287864

The cDNA gene clones have been individually cloned in pCAMBIA 1300 MCS binary vector in anti-sense orientation. The gene constructs have been placed under the control of cauliflower mosaic virus 355S promoter. The clones have been mobilized into *A. tumefaciens* strains LBA4404 and GV2260 which are used for transformation of *L. leucocephala*.

NCL has developed in vitro regeneration protocols for *L. leucocephala*. It was standardized using cotyledonary nodal explant in presence of TDZ.

The transformation protocol for *L. leucocephala* was standardized. Hygromycin was seen to be a better and reliable selectable marker as compared with kanamycin.

8.8 Development of novel fungicides

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

Development of 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 is necessary to ensure continuous production of wide variety of crops and sustainability of Indian agriculture.

In pursuit of this NCL has selected chitin synthase as initial target and has developed a small library of about sixty compounds. These have been obtained by adopting "diversity oriented synthesis" approach. Keeping in view of the functional aspects of the enzyme and the substrate basically ribose has been selected as a synthone and structural diversity has been introduced at various levels. These mainly include scaffolds such as steroids, heterocycles such as pyrimidines, purines, azoles, thio azoles, fused azoles and other other heterocycles. These have been tested and four molecules have shown promising fungicidal activity. Further work is in progress.

Furthermore, in addition to the synthesis of organic molecules, different microorganisms (mesophiles as well as extremophiles) have been isolated from a variety of soil samples which can be used as a potential source of enzyme inhibitors. So far forty-five bacterial strains have been identified for their potential antifungal activity using plate assay as well as hyphal tip bursting assay. The target plant pathogens used are *Sclerotium rolfsii* and *Fusarium* species. Three cultures, *Bacillus*, *Streptomyces* and *Psuedomonas* strains produce chitin synthase inhibitors. The purification of these inhibitors is in progress. A non-radioactive chitin synthase assay has been standardized in the laboratory for high throughput screening (HTS).

One of the novel *in vivo* target-based assays to screen fungicides is haplo-insufficiency measurement using nine mutants of *Saccharomyces cerevisiae* developed by IMTECH, Chandigarh. Initially five different organic molecules will be screened manually using this method. Further standardization using HTS will be carried for the screening of more number of samples.

8.9 Latent M. tuberculosis: New targets, drug delivery systems and bioenhancers and therapeutics:

(Bose Institute, Kolkata, Central Drug research Institute, Lucknow, Centre for DNA Fingerprinting and Diagnostics, Hyderabad, Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Science, Bangalore, Institute of Genomics and Integrative Biology, Delhi, Lupin Laboratories Ltd, Mumbai, Regional Research Laboratory, Jammu, Tuberculosis Research Centre, Chennai and University of Hyderabad)

The emergence of bacterial resistance to antibiotics has posed serious concern to medical professionals during the past decade. The focus is now on the multi-drug resistant gram positive organisms such as methicillin resistant *Staphylococci*, penicillin resistant *Pneumococci* and vancomycin resistant *Enterococci*. Therefore, the work was initiated to introduce and develop new antimicrobial agents.

Oxazolidinones belong to a new class of synthetic anti-microbial agents. They have a novel mechanism of action, selectivity and uniquely binding to the 50S ribosomal sub unit and inhibiting bacterial translation at the initial phase of protein synthesis. Structural variation in the oxazolidinone moiety led to the discovery of linezolid as a new anti-bacterial agent approved by US FDA in the year 2000. It is the first commercially available oxazolidinone antibiotic and is usually reserved for the treatment of serious bacterial infections where other antibiotics have failed due to bacterial resistance. It has been shown to be the valid alternative drug in the management of multi-drug resistant tuberculosis.

The excellent anti-bacterial activity of oxazolidinones has given a great impetus to synthesise and evaluate huge number of derivatives world over. NCL has synthesized 160 new chemical entities (NCEs) belonging to oxazolidinone class under this project on TB. The NCEs were synthesized by multi-step synthesis. The NCEs synthesized were racemic as well as chiral. They were submitted to CDRI, Lucknow and Lupin Laboratories Ltd., Pune for activity evaluation. Out of these NCEs synthesized, seven NCEs showed promising anti-bacterial activity.

8.10 Value added polymeric materials from renewable resources: lactic acid and lactic acid based polymers

(Central Food Technological Research Institute, Mysore, Central Salt & Marine Chemical Research Institute, Bhavnagar, Godavari Sugars Pvt. Ltd. (Somaiya Group of Industries), Mumbai, Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Technology, Bombay, Prathishta Biotech Industries Pvt. Ltd, Hyderabad and Reliance Industries Ltd, Mumbai)

A mutant of *Lactobacillus delbrueckii* capable of growing to high cell densities at 42°C and producing L-lactic acid as the main acid was isolated. Batch fermentation studies on 10 L and 100 L were performed using this mutant to optimize productivity of lactic acid at reduced cost. A volumetric productivity of 3.75 g/L/h and a final concentration of lactic acid, 110 g/ L could be achieved. The batch time could be reduced from five days, as is currently practiced in industry, to 30 hours.

Downstream processing of fermentation broth was examined by different routes such as extraction, distillation, electrodialysis, bipolar membranes, thermal cracking and adsorption. Experiments were conducted to determine the yields and efficiency of each of the above steps in downstream processing.

Based on experimental work conducted a laboratory scale process was developed to produce a lactic acid having a purity of 99.5% and lactic acid concentration of 88% w/v. A basic engineering package for a 1000 TPA plant has been prepared, with details on sizing of equipment, materials of construction, utility requirements and material balance at each stage of the process.

A detailed study on purity of commercial lactic acid of different sources and in-house lactic acid has been performed. This is in view of the stringent requirements for purity of polymer grade lactic acid. Methods for detecting Impurities at ppm level have been standardized. Lactic acid polymers were synthesized having molecular weight up to 1,00,000 Dalton.

8.11 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)

Since hydrogen provides an attractive method for generating clean energy a comprehensive programme on the generation, storage and conversion of hydrogen using fuel cells has been initiated building on the inherent strength of several CSIR laboratories in this area. The main goal is to create a focused group within CSIR for research and development into all aspects of hydrogen energy by creating a network of projects related to generation of hydrogen, storage with the help of several advanced materials followed by conversion using a variety of fuel cell technologies.

HYDROGEN GENERATION:

The focused activities of NCL, IIP, IICT and CMERI regarding hydrogen generation from various hydrocarbon and biomass feedstock have resulted in not only the development of new catalyst compositions for hydrogen generation from LPG/ methane, but a design of a batch bench scale pyrolysis unit (200-300 g) for hydrogen generation from biomass. For example, many rhodium based catalysts supported on mixed oxides were prepared and their performance towards methane reforming was evaluated using an indigenous catalyst evaluation facility for their use in autothermal reforming (ATR) based fuel processor. This is especially significant since a fuel processor working in steam reforming route is not ideal for quick start-up applications. Autothermal reforming of methane was carried out by placing a two layered steam reforming (SR) and partial oxidation (POX) wash coated monolith catalysts to test and evaluate. Its performance was close to that of Engelhard's patented catalyst. Experiments have been carried out to study the effect of oxygen/ nitrogen ratios, using mixtures of oxygen and air to explore the possibility of enhancing the H_2 concentration in the reformate. Two sets of (non-precious metal) copper based spinel catalyst systems Cu-Zn-Mn and Cu-Mn containing various atomic ratios of metals and Pt based catalysts were prepared and were evaluated for water gas shift reaction using synthetic gas mixtures that contain H_2, N_2, CO, CO_2 and water after characterization using XRD, TPR etc. Similarly a heat exchange integrated LPG ATR prototype (500W) was designed and fabricated and the reactor testing will start soon using ATR catalysts. A thermodynamic model to evaluate the performance of various catalysts for ATR of methane and LPG is in progress.

Experiments to investigate the process of syngas generation through thermo-chemical fluidized bed gasification of biomass followed by tar cracking have generated interesting results and various carbon based catalysts are being developed for obtaining COx- free hydrogen production by catalytic decomposition of methane. Similarly a batch bench scale pyrolysis unit (200 – 300 g biomass per batch) was designed, installed and operated using bagasse, *Calotropic procera* and *jatropha* oil cake as feed biomass. A fluidized-bed pyrolysis unit and a lab scale fluidized bed biomass gasifier for generation of hydrogen rich syngas have also been designed.

HYDROGEN STORAGE:

Several samples of multiwalled carbon nanotubes (CNT) were prepared by chemical vapor deposition (CVD) method by introducing the precursors like ferrocene-xylene and ferrocene-toluene mixture (0.75 at. wt. ratio) in a quartz tube in an electric furnace at 675 °C. The lumps of CNTs obtained on quartz substrates and along the side walls of the quartz tube were characterized using SEM, TEM and XRD, both before and after purification. Experiments on Pd functionalization by dispersing CNTs in acetone with the aid of ultrasonication (35 kHz) are in progress. A commercial CVD set up for the preparation of CNT has been installed (Fig. 2). The growth of carbon structures has been carried out on the catalyst provided by the same company, which was pre-patterned on silicon, alumina and mica.

HYDROGEN UTILIZATION: PEM FULE CELLS:

Concerted effort of CECRI, NCL and NPL has fructified the indigenous development of bipolar plates, porous carbon paper, and polybenzimidazole membranes, albeit in small scales. Preparation of new non-carcinogenic routes for monomers synthesis (3,3'-diaminobenzidine-DAB) followed by the casting of polybenzimidazole membranes(A4 size) has been achieved. Fabrication and testing of a 500 W (12-cell) PEFC stack assembly (electrode area 140 cm^2) with a peak power of 870 watt sustaining a power density of 520 mW/cm^2 using imported materials has been accomplished for PEFC and smaller modules of DMFC (power density of 50 mW/cm^2 at 45° C for an electrode area of 50 cm^2) and DBFC (A two-cell stack of 20 W DBFC with 100cm^2 area) have been fabricated with moderate current and power densities, which needs improvement.

Similarly a fuel cell test station (FCTS) has been installed and the operations of the different components (humidifier, mass flow controller etc.) in the FCTS were tested individually. Since FCTS is capable of analyzing the performance of the single cell as well as stack up to 32 cells, the long-term performance of the fuel can be monitored as a function of operating pressure, relative humidity and stoichiometry. Two Ballard fuel cells have been procured as bench marks and various test protocols are being developed for both the stack and the subsystem components.

HYDROGEN UTILIZATION - SOFC FULE CELLS:

Focused efforts of teams from CGCRI, NAL and NML have resulted in the fabrication of anode-supported SOFC single cells (50 mm x 50 mm x 1.5 mm planar configuration) and various compositions of ceramic materials to be used as cathodes, anodes and electrolyte components for both tubular and planar SOFCs. A planar 250W, 6 cell stack (100 mm x 100 mm x 1.5 mm size) with a power density of 0.5 W/cm^2 operating at 750°C is expected to be ready soon. Several other single phase compositions of ceramic materials $La_{1-x}Sr_xGa_{1-y}Mg_yO_{3-\delta}$ (x=0.0-0.2, y=0.0-0.2), new ways of coating process like electrophoretic deposition of La(Sr)GaO$_3$ on (NiO)YSZ substrates and gel-casted LSM tubes (250 mm length, 30 mm OD and 20 mm ID) have also been demonstrated.

RESOURCE CENTERS

Annual Report
2005-06

CATALYSTS PILOT PLANT

Catalyst pilot plant undertook the following activities :

- Development and supply of epichlorohydrin (ECH) and) morpholine
- Production and supply of TS-1 (25 Kg per month to Lyondell Corporation, USA)
- Fly ash based syntheses of high value zeolites like ZSM-12
- Demonstration of processes for the preparation of zeolite beta and KLTL to M/s Vamshi Exports, Mumbai
- Initiated activities for the catalyst identification, evaluation in batch as well as continuous for the bio-diesel and bio lubricants from vegetable oil. Catalyst identified and scaled-up to 500gm. Bio diesel process was scaled up to 7 kg product/batch, in batch process. Bio diesel product quality was confirmed by M/s HPCL, Mumbai, as far as fuel properties are concerned.

2. 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 include following major equipments that are 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.

2.1 Electron microscopy facilities

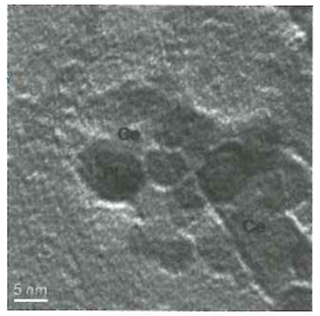
The electron microscope and image processing facility is a state-of-the-art facility dedicated to microscopy and microanalysis of materials to atomic levels. The Center has two transmission electron microscopes (TEM), two scanning electron microscopes (SEM) with extensive hardware/ software for image simulation, processing and analysis, and specimen preparation equipment.

2.1.1 Transmission electron microscope

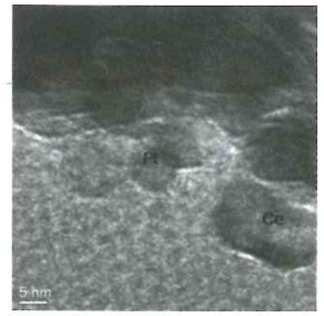
Conventional TEM studies are performed on a JEOL1200EX 120kV TEM equipped with a LaB_6 / tungsten filament, slow-scan and wide-angle TV-rate side mount CCD cameras and a variety of specimen holders, including a heating holder. This instrument has a point resolution of 1 nm and ± 15° tilt capability.

Another microscope, a FEI Tecnai G² F30 S-TWIN, offers accelerating voltages up to 300 kV allowing study of thicker and more challenging samples. It excels in versatility and flexibility by combining high performance in all TEM, STEM and EDX spectrum imaging modes. The "all-in-one" concept allows rapid switching between all data acquisition techniques with automatic recall of all operating settings required for ultimate performance. This microscope delivers atomic resolution in TEM, STEM and nano-analysis by high quality electron optics and high system. The facilities available are bright field/ dark field imaging, CBED, STEM with BF/DF and HAADF detector, diffraction studies, single tilt and double tilt holder and a low background double tilt beryllium holder.

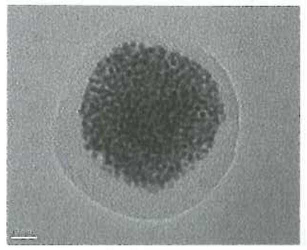
Tecnai G² F30 S-TWIN



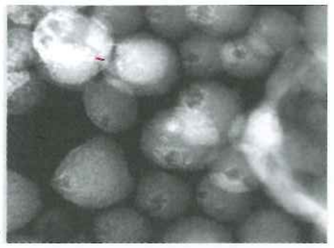
Pt loaded on CeZro fresh
Particle size of pt
nanoparticle 4 nm



Pt loaded on CeZro
Particle size of Pt
nanoparticle 8 nm



Porous Pt spheres,
particle size app 3nm



Stem of porous Pt balls with
spot EDAX

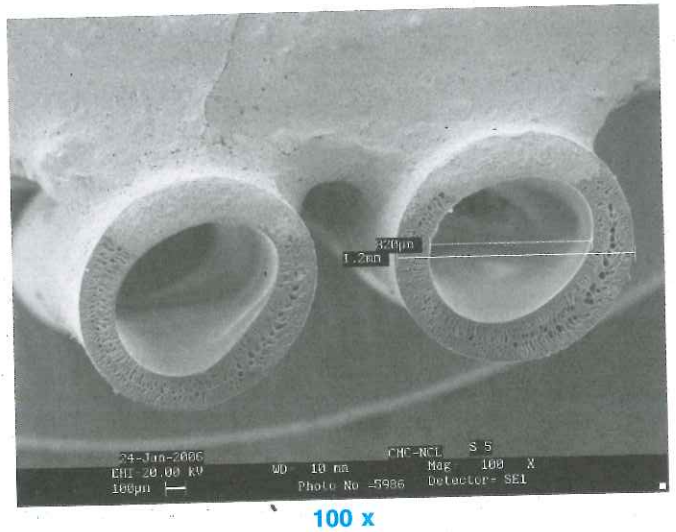
2.1.2 Scanning electron microscope

CMC is equipped with two scanning electron microscopes (SEM). Of these, Leica Stereoscan 440 with Phoenix EDAX/ EDXS performs day-to-day analysis of samples generated within the institute as well as of the samples submitted by the outside parties. SEM facility is extremely valuable in R&D areas that range from new polymeric materials to biological problems of interest. Some of the representative studies are given here.

- Drug release from porous material
- Poly(HIPE) materials for super absorption properties
- Poly(HIPE) synthesized materials for removing of toxic metal ion from drinking water
- Polymeric membranes for removal of pathogenic species from drinking water
- Sensilla on the antennae of male and female *Trichogramma chilonis*
- Sensilla on the maxillae of *Spodoptera litura*
- Interpenetrating hyperbranch Microstructures of Sb doped SnO_2 nanowires

The SEM images show cross section of porous, asymmetric tubular membrane. These images give information about pore size which is very small at skin layer and increases at the bottom and porosity of the membrane.

Another SEM – Quanta 3D - under installation is a DualBeam™ system with a tungsten electron column that uses environmental SEM (ESEM) technology to section, image and analyze a wide range of conducting and non-conducting samples. This system offers the capability for in-situ dynamic experiments, 3D imaging and analysis and TEM sample preparation for more in-depth analysis.



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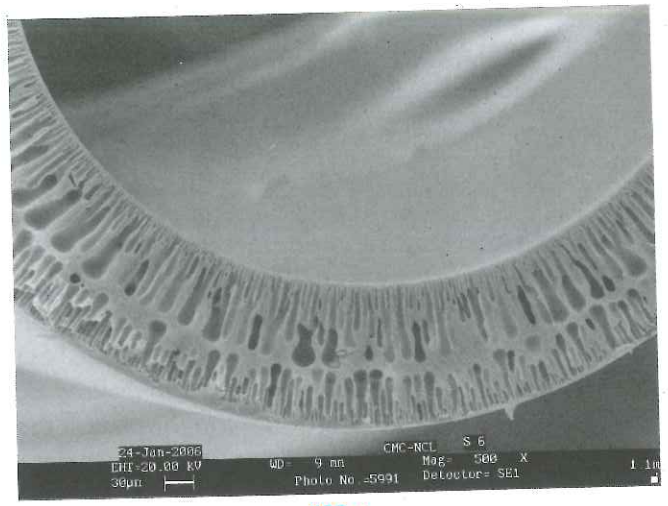

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2.2 Mass spectrometry facilities

2.2.1 MALDI-TOF-MS

This facility is mainly used for the study of

- Protein identification and characterization by peptide mass finger printing
- Polymer analysis and characterization
- Characterization of DNA, RNA, PNA interactions
- Protein-ligand interactions
- Intact cell MALDI for monitoring protein expression and microbial taxonomy
- Direct tissue profiling
- Drug discovery

Some of the major works carried out using MALDI-TOF are listed below:

- Intact cell matrix-assisted laser desorption ionization mass spectrometry as a tool to screen drugs in vivo for regulation of protein expression
- Taxonomical characterization of some Rhizobial species by intact cell MALDI mass spectrometry
- Direct tissue profiling for the identification of biomarker

2.2.2 LC-MS/MS-TOF

The instrument uses the following mass spectrometry techniques to analyze samples

- Two modes of single mass spectrometry (MS),
- Quadrupole-based single mass spectrometry (for calibration only),
- Time of flight-based single mass spectrometer,
- Two modes of tandem mass spectrometry (MS/MS),
- Product ion mass spectrometry, and
- Precursor ion mass spectrometry.

The major applications of LC-MS-MS-TOF are

- Identifying proteins in a database using intact protein masses, enzymitically generated peptide masses, or partial amino acid sequences (sequence tags)
- Accurate determination of molecular weights of proteins and peptides
- Generating lists of expected peptide fragments for comparison with MS/MS data
- Identifying and characterizing post-translational modifications
- Rapidly mapping identified sequences against the original data for results comparison
- Metabolite pathway identification
- Determining the unique elemental composition of all product ions in a spectrum for assigning definitive structures
- Quantification of proteins by ICAT or iTRAQ

2.2.3 High resolution mass spectrometry

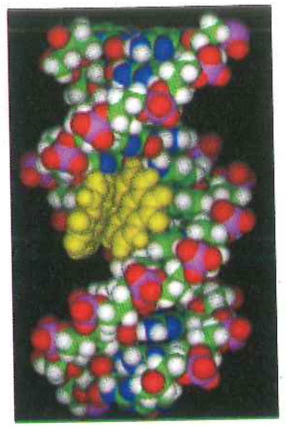
The high resolution mass spectrometer was installed and commissioned at CMC. Mass spectrometry can be used to find the relative molecular mass of a compound to a high degree of accuracy. Low-resolution mass spectrometry gives a value of m/e=101, high-resolution mass spectrometry can give a value of 101.0234. The high accuracy of the molecular weight calculation allows accurate determination of the molecular formula of a fragment.

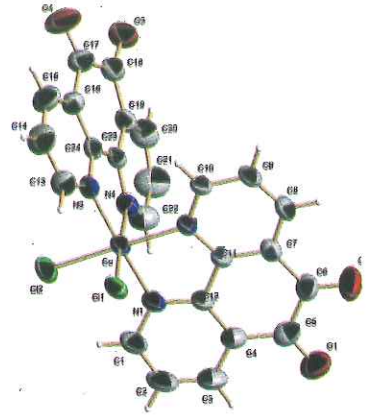
2.3 X-Ray diffraction facilities

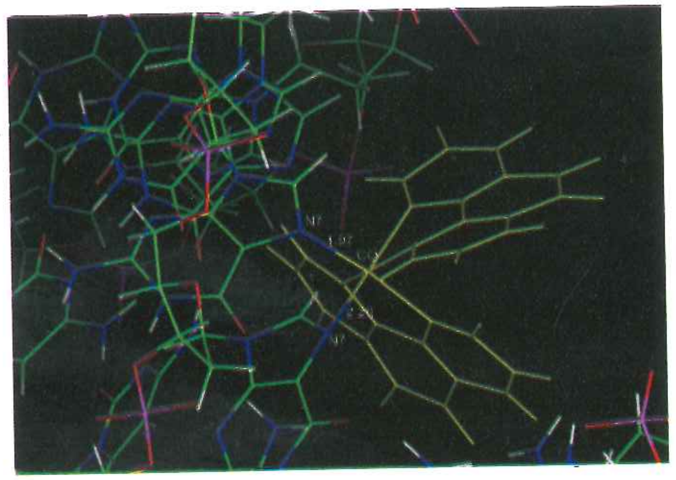
2.3.1 SMART APEX single crystals x-ray diffractometer

2.3.1.1 *cis*-Dichloro bis(diimine) Co(III) complexes show DNA-binding

A cobalt complex similar to cis platin, for anti cancer which can covalently bind to the major groove of DNA was obtained and further theoretical work was carried out.



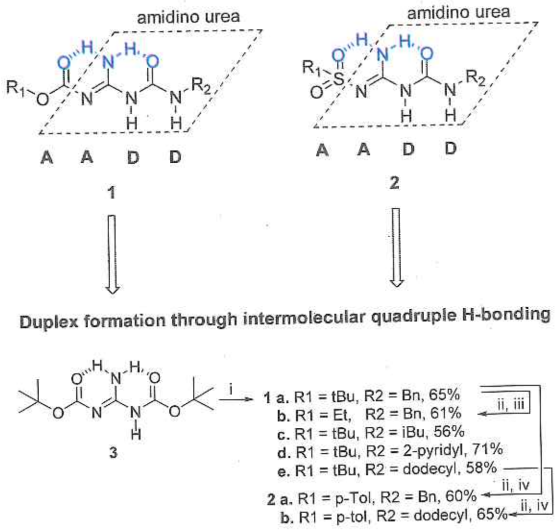




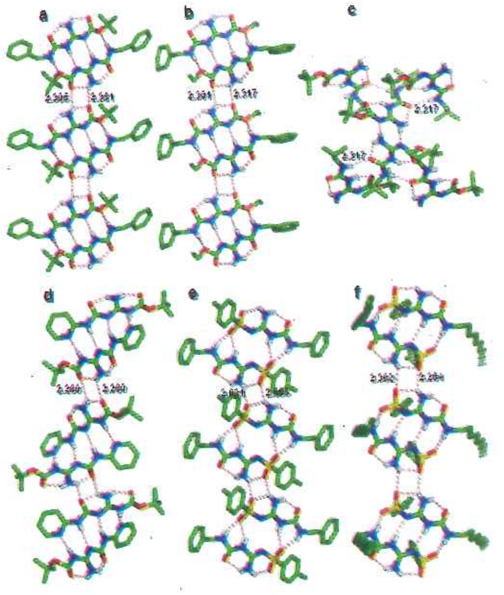
Experimental results indicated covalent binding of [Co(phendione)2Cl$_2$]$^+$ complex to the calf thymus DNA. The likely site of metalation has been shown to be the N7 of guanine, which is readily accessible in the major groove. *cis*-Platin has been shown to covalently bind to the N7 of guanine in the major groove. Because of this structural similarity the [Co(phendione)2Cl$_2$]$^+$ complex to *cis*-platin, our compound may covalently bind to the DNA in a similar fashion. Therefore, the initial structure of the ligand bound to DNA was constructed where the Co^{+3} forms a covalent bond to the two N7 atoms of adjacent guanines. Molecular modeling studies showed that the minimized structure of [Co(phendione)2Cl$_2$]$^+$, maintained the octahedral structure while binding to the N7 of guanines and the ligand fits into the major groove without disrupting the helical structure of the B-DNA. This work was done in collaboration with Department of Chemistry, University of Pune.

2.3.1.2 A novel approach to the formation of quadrapole H-bonded duplexes

In an effort to explore the potential of using intramolecular-hydrogen bonding as the sole driving force in pre-organizing linear hydrogen bonding arrays, a series of self-assembling modules whose linear quadruple hydrogen-bonding arrays embedded on an acyclic amidinourea framework were generated.

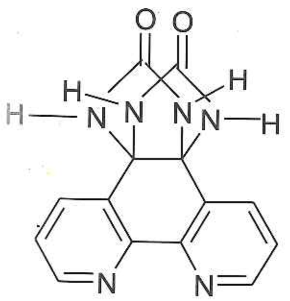


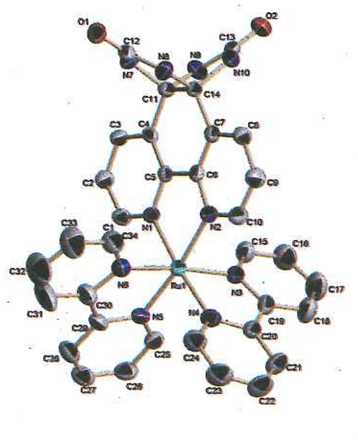
Single crystal X-ray structures of a (1.1a), b (1.1b), c (1.1c), d (1.1d), e (2.2a), and f (2.2b) were determined. All the quadruply hydrogen bonded dimers 1.1a,b,d and 2.2a,b undergo further self-assembly using the not-so-common 4-membered ring intermolecular hydrogen bonding interaction, forming extended sheet-like supramolecular networks. Many of these structures are disordered.



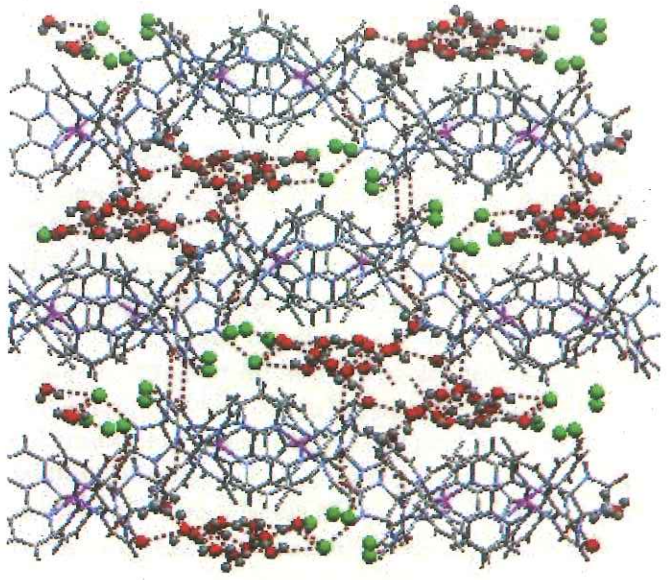
2.3.1.3 3D metal-organic framework encapsulate water molecules

Tecton (I) is a versatile ligand for the generation of supramolecular architectures and the judicious control of its stoichiometry and choice of ancillary ligands result in large number of diverse frameworks. Ruthenium complexes of the type [Ru(N-N)$_2$(tecton)]Cl$_2$, [Ru(N-N) (tecton)$_2$]Cl$_2$ and [Ru(tecton)$_3$]Cl$_2$ where N-N is 2,2′-bipyridine (bpy), 1,10-phenanthroline (phen), and tecton I is [4b,5,7,7a-tetrahydro-4b, 7a-epiminomethanoimino-6H-imidazo[4,5-f][1,10] phenanthroline-6,13-dione] have been synthesized and structurally characterized. The tecton (I) reacts with [Ru(bpy)$_2$Cl$_2$] in 1:1 molar ratio to form [Ru(bpy)$_2$(tecton)]Cl$_2$, (bpy=2,2′-bipyridine. $\{[C_{34}H_{26}N_{10}O_2Ru].[C_{35}H_{28}N_{10}O_2Ru]\}.Cl_4.5(CH_3OH).9.5H_2O$. Crystal structure revealed a 3-D metal-organic framework by a self-assembly process. The water cluster along with Chlorine anions makes a beautiful network of H-bonding in the channel parallel to "c" axis. The two symmetry related molecules are connected through N-H····O, N-H····Cl, C-H····O and C-H····Cl interactions arrange themselves forming 3-D arrays with the formation of channels. Water clusters buttressed by chlorine anions and fortified by N-H···O and C-H···O interactions are encapsulated within these channels. Heating the crystal at 250 °C eliminates water molecules from the channels, which reappear in the channels on exposure of the crystal to the moisture. The interchangeability of lattice water molecules and the corresponding effect on the overall structure was probed by IR and X-ray powder diffraction studies.

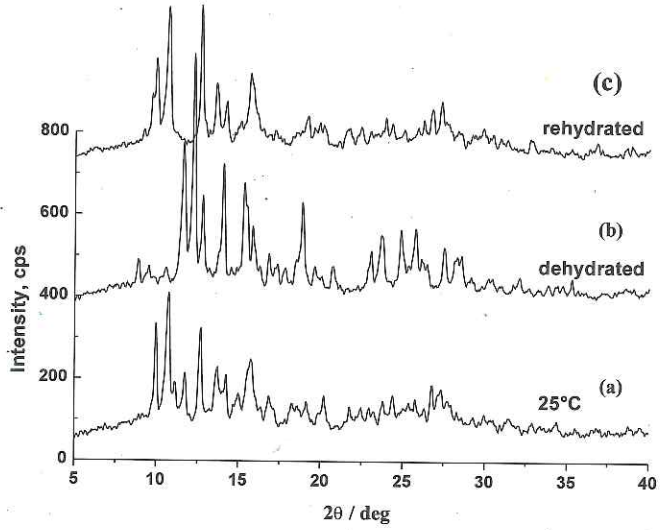


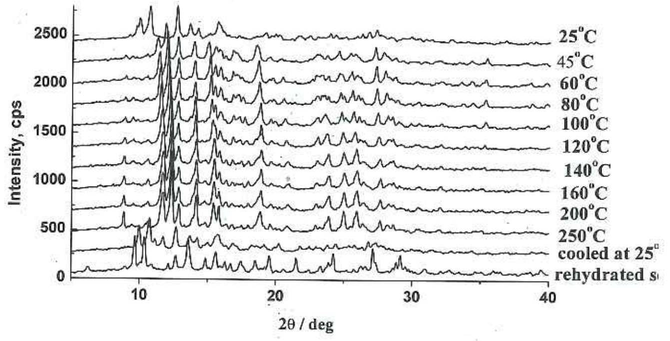


X-ray powder pattern



Packing of the molecules

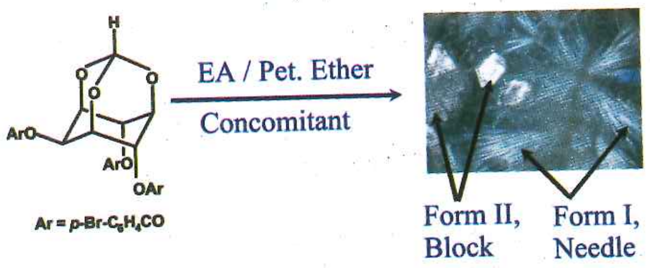


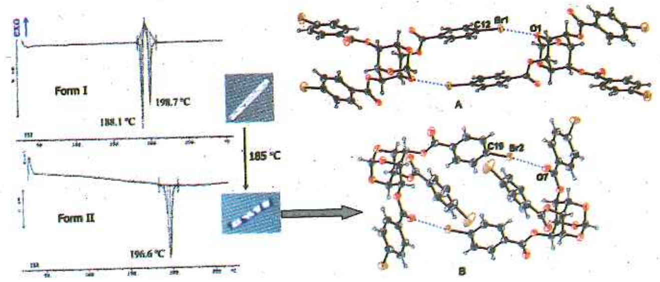


XRPD patterns at 25°C, 45°C, 60°C, 80°C, 100°C, 120°C, 140°C, 160°C, 200°C, 250°C, solid on cooling at 25C and rehydrated solid on standing overnight in the presence of atmospheric moisture.

2.3.1.4 First order crystal-to-crystal phase transition of kinetic form to the thermodynamic form

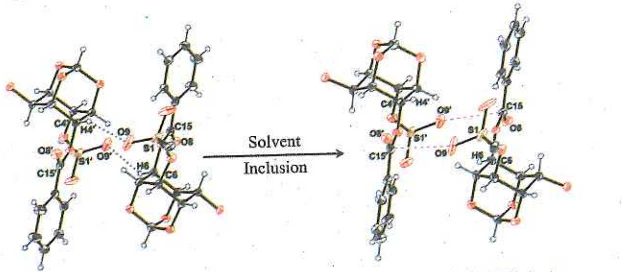
Polymorphism and crystal growth are among the most intensive areas of research because of interest in pharmaceutical solids. The polymorphic behavior exhibited by small organic molecules with no possibility of forming conventional H-bonding, offer an opportunity to study the interplay of weak interactions that take place in the nucleation event. We studied the structures of concomitant polymorphs of tri-O-[p-halobenzoyl]-*myo*-inositol 1,3,5-orthoformate. The form I crystals (needles) were kinetically produced within few hours and form II crystals (octahedral blocks) were obtained by slow evaporation (~ 2 days) in the same flask from 20% ethyl acetate-petroleum ether solution (v/v). Single crystal X-ray studies of the bromo-derivative revealed that both the forms utilized different 'halogen bonding' contacts; C-Br...O-C (ether oxygen) in Form I and C-Br...O=C (carbonyl oxygen) in Form II. DSC studies of the polymorphs suggested an irreversible phase transition of Form I to form II. Accordingly, heating a crystal of Form I to ~ 185-186 °C converted it to crystals of form II as revealed by X-ray crystallography.



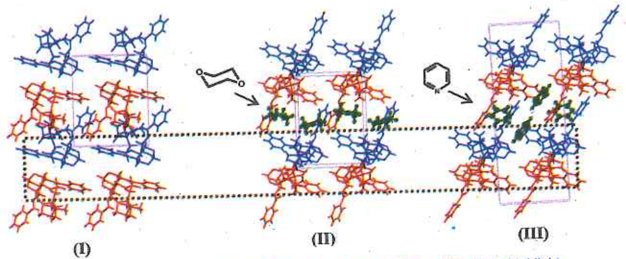


2.3.1.5 Subtle cross over from C-H···O to S=O···C=O short contacts upon formation of pseudopolymorphs

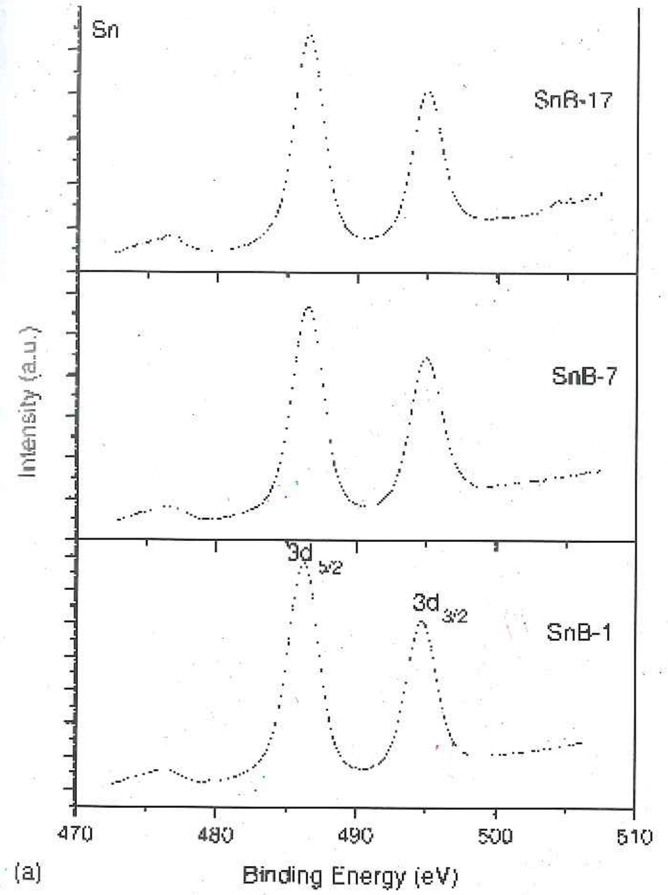
Diastereomers of 2,4(6)-di-O-benzoyl–6(4)-O-[(1S)-10-camphorsulfonyl]-*myo*-inositol 1,3,5-orthoformate associate via weak interactions to form 'head-to-head' dimers in their crystals. Molecular association through C-H···O short contacts do not leave any void for the guest inclusion, while association through S=O···C=O bridging produces pseudopolymorphs. Three crystalline modifications are observed for the title compound; Form I, monoclinic $P2_1$ without any guest solvent; solvated Forms II and III that belong to monoclinic space groups $P2_1$ and C2 respectively. A majority of solvates, that include pyridine, dichloromethane, benzene, tetrahydrofuran and cyclohexanone as guests belong to Form III. All these guests have two-fold symmetry axis (C2) with their electron count within 40-62 electrons; guest selectivity experiments indicated that planar aromatic guests (pyridine, benzene) bind better to the host molecules as compared to non-planar guests (dioxane, cyclohexanone). The molecular packing that creates through channels in the crystal (avoiding interpenetration of the layers) are of interest because of their potential application in molecular separation by forming selective inclusions. The diastereomeric association via S=O···C=O dipolar short contacts, a consistent feature observed in all the solvates, is thought to have relevance in binding of sulfonyl drugs to the C=O moieties of the receptor proteins.



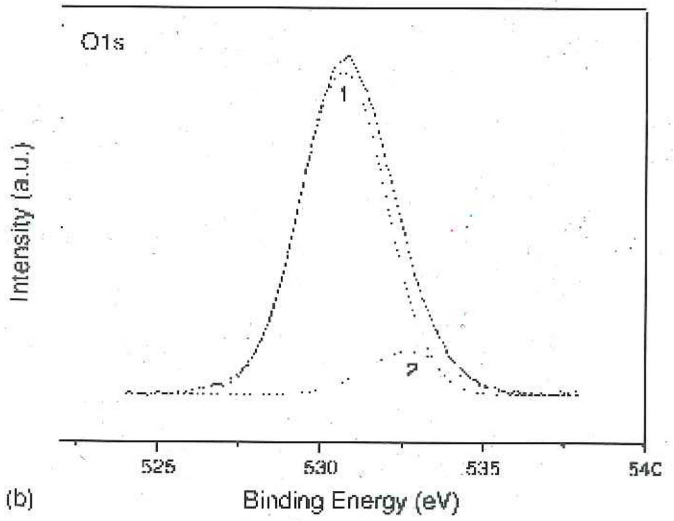
ORTEP view of the Form I with C-H···O bridging crossing over to S=O···C=O short contacts upon solvent inclusion



Molecular views down c -axis in Forms I, II and III. The dotted lines highlight unperturbed 1D- isostructurality of distereomeric association



(a)



(b)

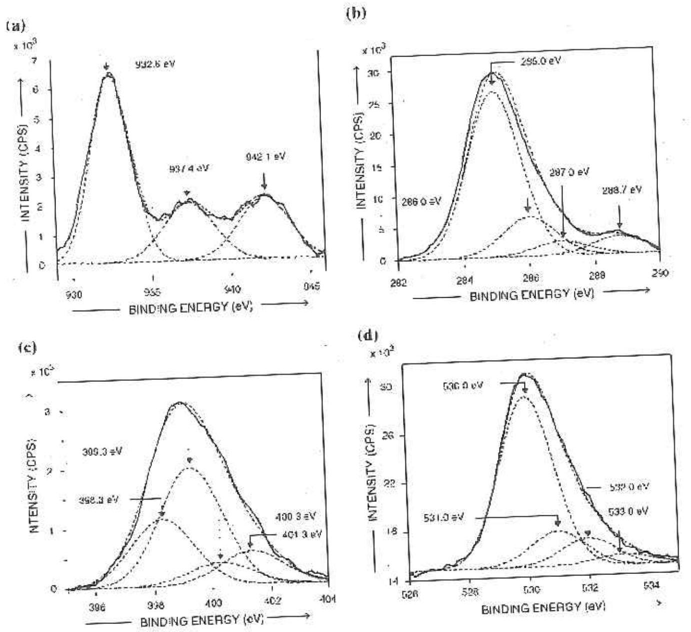
2.4 Electron spectrometer for chemical analysis

2.4.1 Effect of calcinations cycles on the preparation of tin oxide based traditional drug

The drugs known as *bhasmas* are used in the traditional Indian Ayurveda and these are mixed oxides of one or more metals. Traditional preparation of *bhasma* involves conversion of a pure metal into its oxide form. The effect of number of calcination cycles followed in the preparation of tin oxide, *vanga bhasma* was studied by a systematic characterization of the drug samples after various calcination stages. X-ray photoelectron spectroscopy (XPS) was used to test the chemical state for confirming the formation of metal oxide. It was found that tin was in the form of Sn^{4+} state and that the formation of SnO_2 proceeded step-wise through $Sn(OH)_4$.

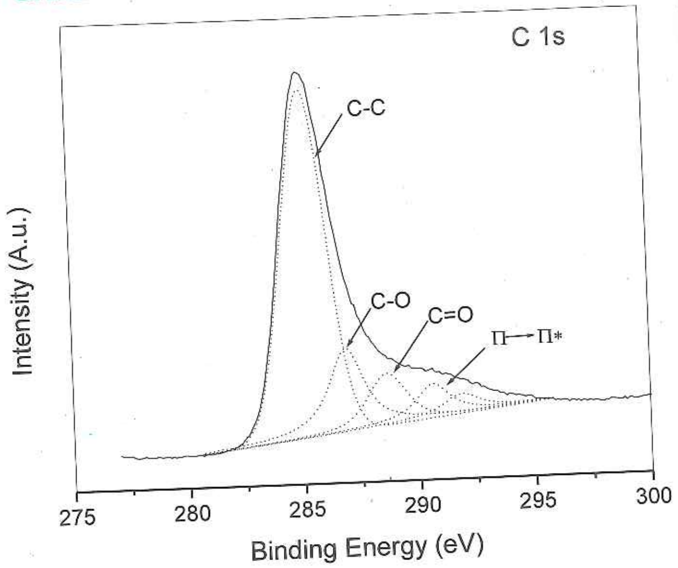
2.4.2 Formation of poly(o-anisidine) coatings on copper as anti-corrosion organic coatings

Due to the ability of the conducting polymer coatings to protect metal surfaces, there is a growing interest to synthesize these coatings on iron and aluminum and their alloys and to evaluate the corrosion protection. The electrochemical polymerization of o-anisidine from the aqueous salicylate solution results into the formation of uniform, compact and strongly adherent poly(o-anisidine) (POA) coating onto copper substrate. The preliminary study on the evaluation of the corrosion protection performance of these coatings revealed that POA can be considered as a potential coating material for protection of copper against corrosion in aqueous 3% NaCl. The surface modifications induced by polarizing the copper in the aqueous salicylate medium were characterized by XPS.



2.4.3 Mesoporous carbon material obtained by mesoporous silica template

Porous carbon with high surface areas, large pore volumes and chemical inertness are useful in many materials application areas, including water and air purification, adsorption, as a catalytic support and capacitors for energy storage. Ordered mesoporous carbon material was prepared by templating procedure using ordered mesoporous silica material as template. This mesoporous silica material was prepared using low cost templating agents such as hydroxy carboxylic acids and TEOS as silica source. Carbonization of sucrose inside the pores of silica material at 900° C followed by removal of silica framework using aqueous ethanoic solution of NaOH gives rise to carbon material with ordered mesoporosity. The resulting materials were characterized by XPS.



Analytical and testing facilities

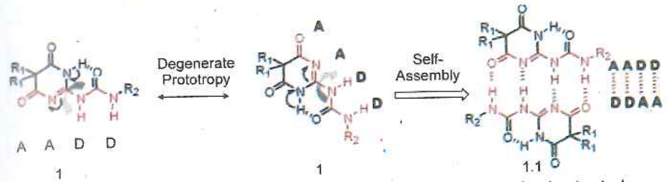
CMC also coordinated the analytical services from within CMC and other divisions. Elemental analysis, MS, surface area measurements (BATE), etc. were extended as research/ technical aid to various industries, research students and research institutes. The facilities like elemental analysis, XRD, NMR, 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 of these services is tabulated below:

Institute	Industry	Govt	Acad	Total
No	53	3	9	62
No. of Samples	377	19	26	422
Amount in Rs.	5,83,565.60	60,720.00	34,272.00	6,78,557.60

3 CENTRAL NMR FACILITY

3.1 Self-assembly with degenerate prototropy



Only one set of molecular duplex (no mixture of protamers)

This work describes a rational approach for addressing the prototropy-related problems in heterocycle-based self-assembling systems by the use of *degenerate prototropy*. As a proof of principle, the utility of *degenerate prototropy* is demonstrated herein by developing heterocycle-based AADD-type self-assembling modules that exist as "single set of protameric pair (duplex)" in both solution and solid states. These self-assembling modules are quickly accessible in good yield by reacting 2-amino-5,5-disubstituted-1*H*-pyrimidine-4,6-diones, available in one step by the condensation of R,R-dialkyl malonates and free guanidine, with isocyanates. Evidence from NMR spectroscopy, ESI mass spectrometry, and single-crystal X-ray diffraction studies confirmed the formation of molecular duplexes. The effect of electronic repulsion in duplex formation was also investigated. Their ready synthetic accessibility, remarkably high propensity to crystal formation, and the novel property of *degenerate prototropy* would make these novel self-assembling molecules promising candidates for many proposed applications.

3.2 Sensitivity enhancement of solid-state NMR experiments for half-integer spin quadrupolar nuclei

A significant number of the NMR active nuclei have spin>1/2. The Solid-State NMR spectra of these nuclei are broadened due to quadrupolar interaction. Obtaining high-resolution of these nuclei has been an important focus of solid-state NMR spectroscopy. The development of multiple-quantum magic angle spinning (MQMAS) was an important breakthrough in this area. Although this method has been very successful, it still has some problems with sensitivity and quantification. The problem of sensitivity is due to the fact that the multiple to single quantum transfer is very inefficient. There are many techniques that have been suggested to increase the MQ-SQ transfer. Currently we are exploring the use of various radio frequency modulation schemes to enhance the MQ-SQ transfer. We have demonstrated that we can increase MQ-SQ transfer using cosine amplitude modulated (RF) pulses. This project is in collaboration with TIFR, Mumbai and IIT Delhi.

3.3 Homonuclear correlation experiments for half-integer spin quadrupolar nuclei

The dipolar interaction is the crucial interaction that plays a major role in structural determination in NMR. This is the interaction that gives a direct distance measurement between nuclei. The dipolar interaction is averaged by magic angle sample spinning (MAS). One important area in solid-state NMR is the development of techniques to re-introduce the dipolar interaction averaged by MAS, so that distance measurement is possible. There are numerous techniques available in spin-1/2 systems using symmetry based pulse sequences. For quadrupolar nuclei, such schemes do not work due to the strength of the quadrupolar interaction. We are exploring the possibility of re-introducing the dipolar interaction in quadrupolar systems by spinning away from the magic angle. One of the methods that have been used for getting high resolution spectra of half-integer spin quadrupolar nuclei is double rotation in which the sample is spun *simultaneously* in two angles so that the quadrupolar interaction is averaged and we get high-resolution spectra in a one-dimensional experiment. This method is highly suitable for detecting the homonuclear correlation. This project is being carried out in collaboration with Radbound University Nijmegen, The Netherlands and NICPB, Talinn, Estonia.

3.4 Development of NMR methods for liquid crystals

The cross-polarization is one of the widely used methods in solid state NMR in which polarization transfer between two spins I and S in the rotating frame is used to enhance the signal intensity of a low gamma nucleus. Separated local field (SLF) spectroscopy based on transient oscillations observed during cross-polarization represents a class of two dimensional solid state NMR experiments in which the coherent transfer of energy between dipolar coupled spin systems provides a means of resolving heteronuclear dipolar couplings on the basis of chemical shifts and characterizing them. The basic experiment as well as the modifications to remove homonuclear dipolar couplings among protons have found extensive applications for the characterization of biological and liquid crystalline systems. One of the existing methods is the incorporation of an initial polarization inversion period to enhance the cross-peak intensities and to reduce the axial peak intensities. In a subsequent investigation, it was shown that the axial peaks arise from polarization build up in the double quantum sub-space of a two spin system. Polarization inversion ensures that the initial magnetization to be present essentially in the zero-quantum subspace thereby enhancing dipolar oscillations and the cross-peak intensities. We have suggested a modification to the standard cross-polarization experiment in which a 90 degree pulse on the X-nucleus is included and the pulse phases can be designed to promote the initial magnetization in the zero-quantum sub-space thereby significantly increasing the intensity of the cross-peaks in comparison to that of the axial peaks. The results are demonstrated for the case of nematic liquid crystal N-(4-methoxy-benzylidene)-4-n-butylaniline (MBBA) oriented in a magnetic field. This project is being carried out in collaboration with NMR Research Center, IISc Bangalore.

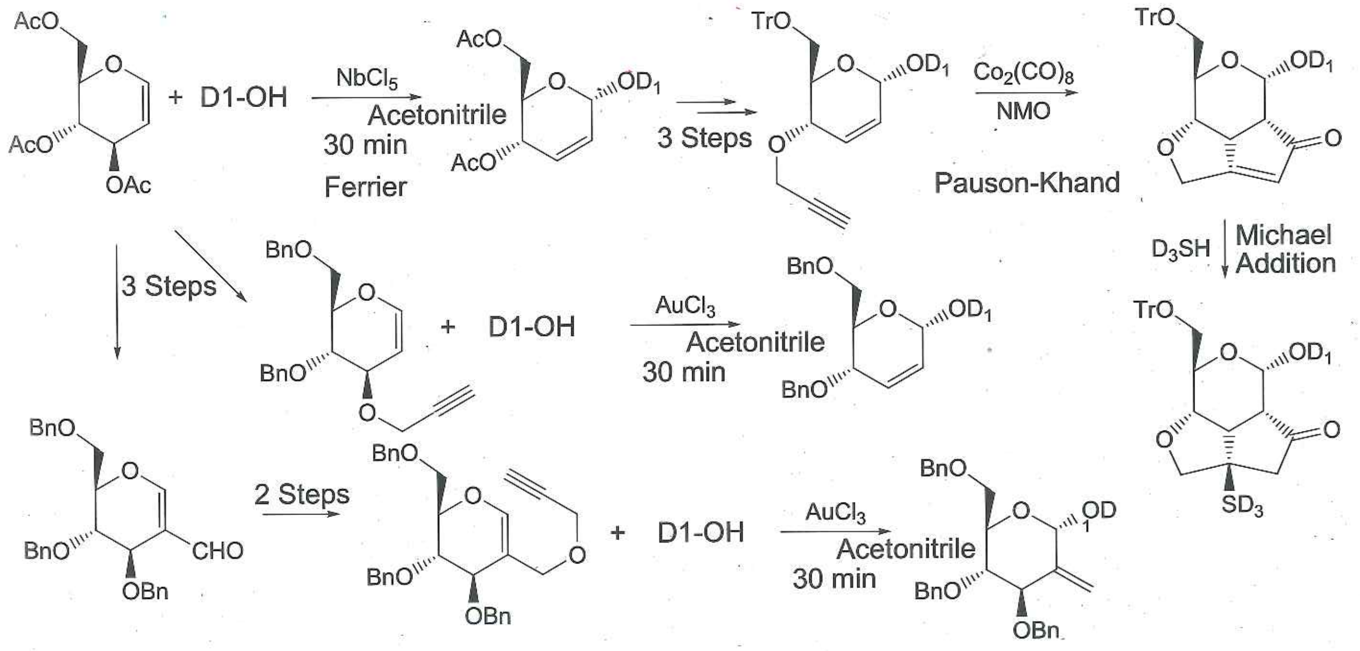
4 COMBI CHEM-BIO RESOURCE CENTER

Rapid identification of potent, selective and specific small molecules to macromolecular receptor(s) having defined biological function is a major challenge in the post-genomic era. For a long time, natural products are conceived to be of paramount importance in the identification of small molecule inhibitors. Later on, the focus shifted to the combinatorial chemistry; however, the anticipated result in the identification of the small molecule probes was not observed which was attributed partly to the clustering of small molecules in the three dimensional chemical space. In addition to this, a recent chemoinformatics data mining study revealed that on average, natural products have higher molecular weights; incorporate fewer nitrogen atoms but more oxygen atoms; and are sterically more complex with number of rings and chiral centers than the corresponding congeners from combinatorial libraries. Hence there exists a need to unravel the three dimensional chemical space by the use of less explored templates to generate novel complex, chiral and polycyclic compounds. Diversity oriented synthesis (DOS) of small molecules is a new algorithm that enables efficient synthesis of complex molecules. It can be hypothesized that the carbohydrate precursors enable us to develop diversity oriented pathways for the synthesis of novel chemical scaffolds decorated with chiral centers and a number of oxygen atoms embedded to fused rings.

4.1 Carbohydrate-based diversity oriented synthesis

A natural product-like small molecule library was achieved starting from glycals using a combination of Ferrier, Pauson-Khand and Michael addition reactions (Scheme 1). Later observations revealed an unprecedented behaviour of propargyl group to form 2,3-unsaturated α-glycosides when 3-O-propargyl bearing glucal was activated with $AuCl_3$ Spirocyclic skeletons are present in many biologically active natural products. Furthermore, molecules containing spirocycles have found many applications as the spiro system results in rigidity in the conformation of peptides, carbohydrates etc. As a result, the synthesis of spiro moieties has attracted a lot of attention in recent times.

Thus, in another effort, a DOS pathway was developed for spirocycles using Pauson-Khand reaction, Enyne metathesis and Intramolecular Diels Alder (IMDA) as complexity-generating reactions (Scheme 3). We are currently exploring second generation diversity exploiting acid sensitive isopropylidene groups in order to synthesize nucleosides and glycosides.



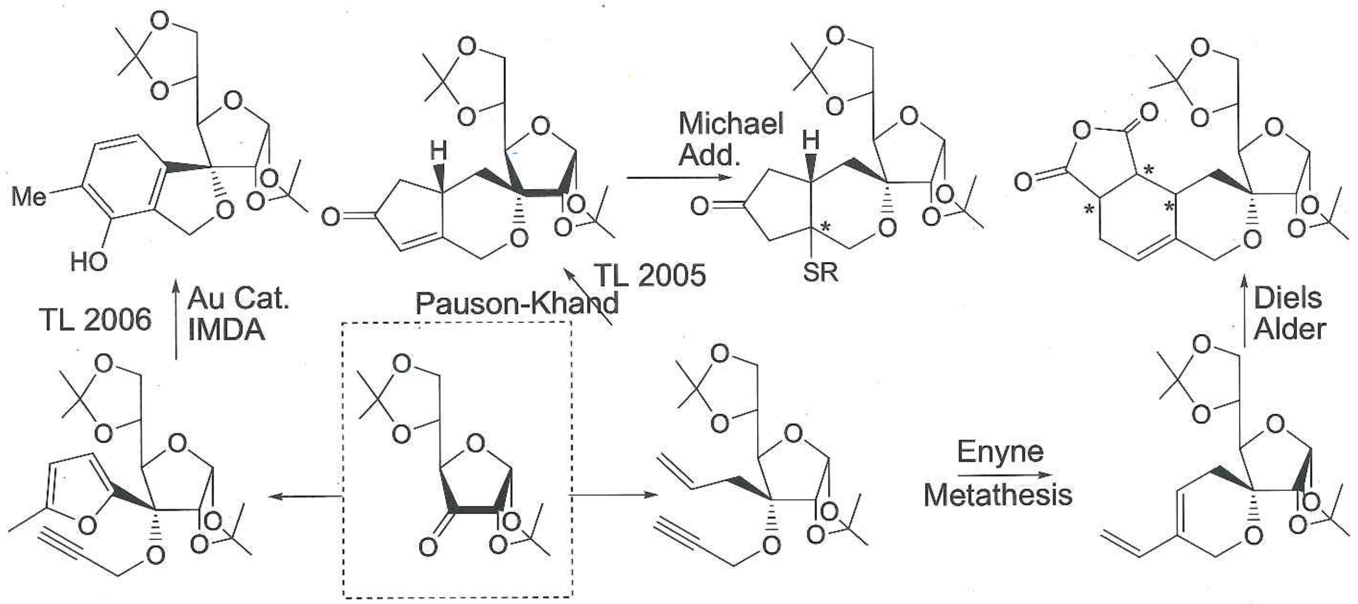
Scheme 1

COMBI CHEM-BIO RESOURCE CENTRE

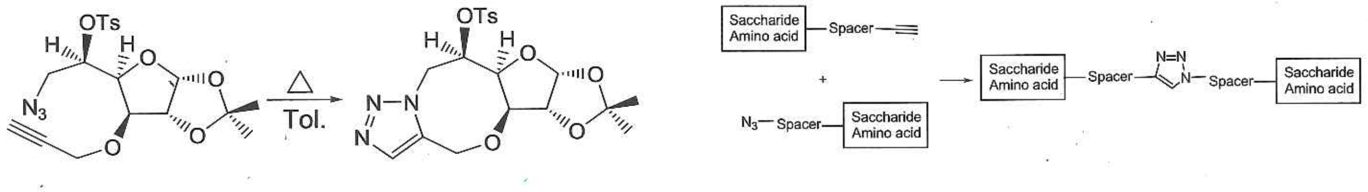
4.2 Application of "Click" chemistry to carbohydrate scaffolds

Several compounds of the 1,2,3-triazole class possess a broad spectrum of biological properties including anti-HIV, anti-allergic, anti-bacterial, herbicidal and fungicidal activity. 1,2,3-Triazoles are synthesized by 1,3-dipolar cycloaddition of the corresponding azide and alkyne, a procedure known as the Huisgen reaction. Furthermore, 1,2,3-triazole formation is a highly efficient reaction without any significant side products and is currently referred to as a "click" reaction. We have utilized 1,3-dipolar cycloaddition reaction (referred as 'Click' reaction) to carbohydrate moieties in order to achieve 1,2,3-triazole fused multi-cyclic frameworks (Scheme 2).

Oligosaccharides and glycopeptides play crucial roles in various cellular recognition events including signal transduction. Lack of sufficient quantities of oligosaccharides and peptides often limit the efficient conjugation of oligosaccharides to oligosaccharides/peptides. In continuation of our studies, "click" chemistry was employed for the synthesis of *pseudo*-oligosaccharides and amino acid glycoconjugates (Scheme 3). We are currently extending this concept for probing protein-protein interactions.



Scheme 2

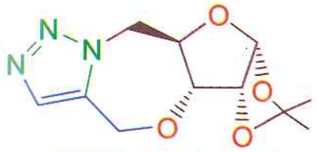


Scheme 3

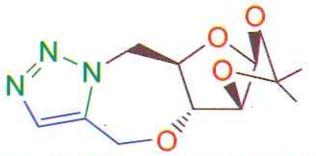
COMBI CHEM-BIO RESOURCE CENTRE

4.3 Novel fungicides

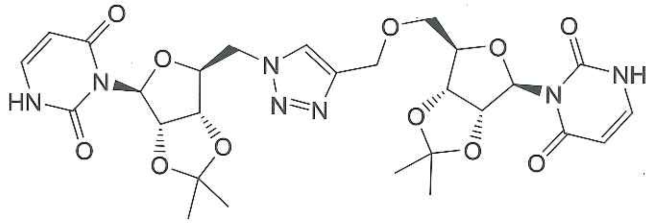
In continuation of our pursuit for the safer target based anti fungal agents a library of thirty compounds has been prepared based on the ribose based scaffold incorporating some heterocycles. These compounds have been synthesized employing diversity oriented approach and recently developed click chemistry approach. Some of them have shown encouraging activity against the *Candida albicans* and three other fungi. The library also showed the positive results in haplo insufficiency assay. Radioactive and fluorescent assays have been optimized for chitin synthase inhibition. Some of the representative members of the library are :

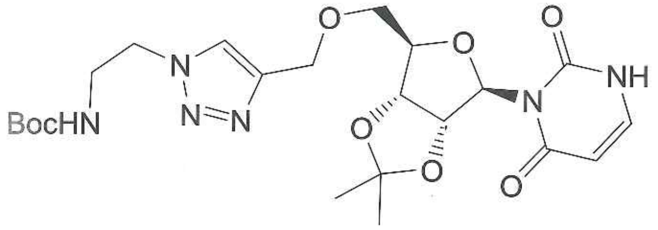


4bRibo-2 h,90%



4cArabino-3.5 h,92%





5 DIGITAL INFORMATION RESOURCE CENTER

5.1 Chemoinformatics

5.1.1 Design of a JavaRMI based architecture for distributed chemical informatics applications

An open client/server architecture based on JavaRMI has been established for distributed computing, distributed data mining from the Internet and focused *in-silico* library synthesis for virtual screening under additional restraints, such as drug-likeness. The major advantages of the distributed approach are that the implementation is both open source as well as very flexible and fine-tunable to a wide variety of distributed computing tasks. It is also the first scientific client/server approach that exploits the communication capabilities of JavaRMI for chemoinformatics research. This core architecture is compatible for information harvesting, chemical computing, virtual screening and chemical datamining.

5.1.2 Barcoding technology implementation for chemical structure based institutional inventory

In the present study a two-dimensional (PDF417) barcode representation of molecular structures in SMILES format is explored that enables the user to read and input molecular structures into computer systems in a fully automated fashion. The input via barcodes is fast, practically error free due to the 2D barcodes used which employ error correction and fully automatic. A Web application interface is developed which interprets these barcodes and export them as optimized 3D chemical structures. Applications of this representation range from keeping automated storage systems to Web-based tracking systems of molecular samples. NCL employs 2D barcode encoded structures for in-house repository management, where barcodes can also be used for querying the database for similar or substructures of the query structure.

5.1.3 General melting point prediction using artificial neural networks

The melting point is a fundamental physicochemical property of a molecule that is controlled by both single-molecule properties and intermolecular interactions due to packing in the solid state. Thus, it is difficult to predict, and previously only melting point models for clearly defined and smaller compound sets have been developed. Here we derive the first general model that covers a comparatively large and relevant part of organic chemical space. We reported the development of a robust and general model for the prediction of melting points. It is based on a diverse data set of 4173 compounds and employs a large number of 2D and 3D descriptors to capture molecular physicochemical and other graph-based properties. Dimensionality reduction is performed by principal component analysis, while a fully connected feed-forward back-propagation artificial neural network is employed for model generation.

5.1.4 Dspace@NCL

An open archive Initiatives was established to archive digital version of a range of institutional scientific documents including PhD theses, publications accepted in the peer reviewed journals, selected research reports, etc. The additional bibliographic information such as list of authors, title and abstracts can be searched by the users. Currently, the Dspace@NCL holds 349 scientific documents including 200 PhD Theses, 42 research reports and 107 patents from NCL and is being updated regularly.

5.2 Biodiversity informatics

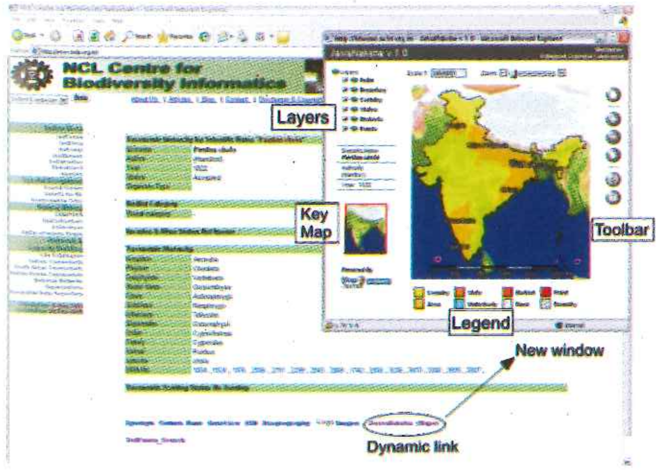
Biodiversity informatics encompasses collection, collation, analysis, prediction, and dissemination of knowledge about biotic resources. The efforts are aimed at developing tools, standards, and protocols that would help improve infrastructure and capacity building leading to acceleration of national and regional progress in this emerging new discipline.

5.2.1 IndOBIS – Indian Ocean node of ocean biogeographic information system

IndOBIS is one the seven southern regional nodes of the ocean biogeographic information system (OBIS). During the year IndOBIS launched its web portal http://www.indobis.org/. Currently, IndOBIS catalogue of life (IndOBIS CoL). disseminates baseline information on over 20,000 faunal species known from Indian Ocean. Other than accepted scientific names, it collates information on synonyms, common names, and occurrences.

5.2.2 SaGrIS -Sacred groves information system

Sacred groves (SGs) are patches of forests that are dedicated to gods and goddesses; hence remain undisturbed and well conserved. There are believed to be nearly 100,000 such sacred patches of pristine forests spread all over India. Web based information infrastructure for collating data related to these sacred groves was developed. Information about sacred groves of the northeastern state of Arunachal Pradesh has been collated using SaGrIS. NCL and North Eastern Regional Institute of Science & Technology (NERIST), Nirjuli, Itanagar. NERIST has collated data on nearly 70 SGs using SaGrIS under the pilot project from DSIR.



JaivaNaksha maps the occurrences of Indian faunal species

5.2.3 IndFauna – Electronic catalogue of known indian fauna

During the year, over 20,000 records for three orders *Coleoptera*, *Hymenoptera* and *Lepidoptera* was scrutinized. DiGIR server was established to facilitate caching of data by the Global Biodiversity Information Facility, who has awarded a contract to conduct taxonomic scrutiny of these three orders mentioned earlier. ***JaivaNaksha***, web-mapping tool was developed to map the occurrences of Indian Fauna as reported in variety of publications spanning over 250 years. A unique feature of JaivaNaksha is its ability to map areas, water bodies, geo-coordinate ranges together with point localities in the same map.

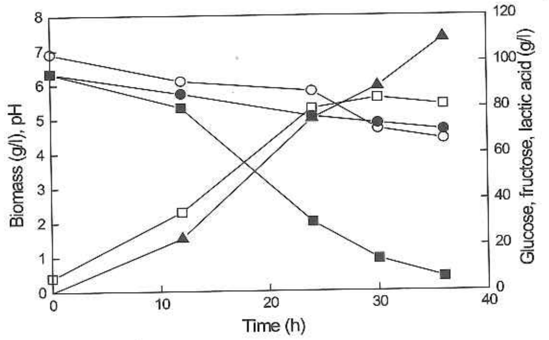
5.2.4 IndCollections

Biological collections are essential to biodiversity research as they are the fundamental underpinning of all the biological information. Digitization of these collections is essential as the data associated with specimens contributes to the overall understanding of evolution of species, ecological process, and relations of a species with other living forms and abiotic factors. In order to overcome the challenge of making this information accessible, web based infrastructure called ***"IndCollections"*** was developed. Currently, three museums namely, Regional Centre, National Institute of Oceanography, Kochi; Gujarat Ecological Society, Vadodara; and Department of Zoology, Modern College, Pune are using IndCollections to digitize their collections.

6 NATIONAL COLLECTION OF INDUSTRIAL MICROORGANISMS

6.1 Strain improvement for production of lactic acid

Lactic acid is an important bulk chemical produced by fermentation. The present technology for fermentation employs highly selected strains for rapid fermentation, high lactate tolerance and ability to ferment at high temperature. The activity of the strains, however, decreases with lowering of pH due to accumulation of lactic acid in the medium. Lactobacillus strain, which produced 90g/l of lactic acid with productivity of 1.2g/l/h was subjected to UV-mutagenesis to isolate mutants. One of the mutants yielded lactic acid (105g/l) with increased productivity (4.7g/l/h). This could be a suitable candidate for lactic acid production at commercial level. The property of the mutant to utilize preferentially glucose from hydrolysed sucrose was exploited to produce lactic acid and high fructose syrup (HFC). The lactic acid yield was more than 90%, which can be separated as calcium lactate. The syrups obtained after separation of lactic acid contained more than 90% fructose when media with 100-200 g/l of hydrolyzed cane sugar were used for fermentation. Even at 250 g/l of hydrolyzed cane sugar concentration, the produced syrup contained 75% fructose which is richer in fructose content than the ordinary cane sugar and 55% HFCs. Unwanted by-product like acetic acid was not detected in the fermented broth. These finding will be useful in the production of lactic acid and high fructose syrups using media with high concentrations of sucrose based raw materials. This approach can lead to modification of the traditional fermentation processes to obtain value added by-products, attaining better process economics.



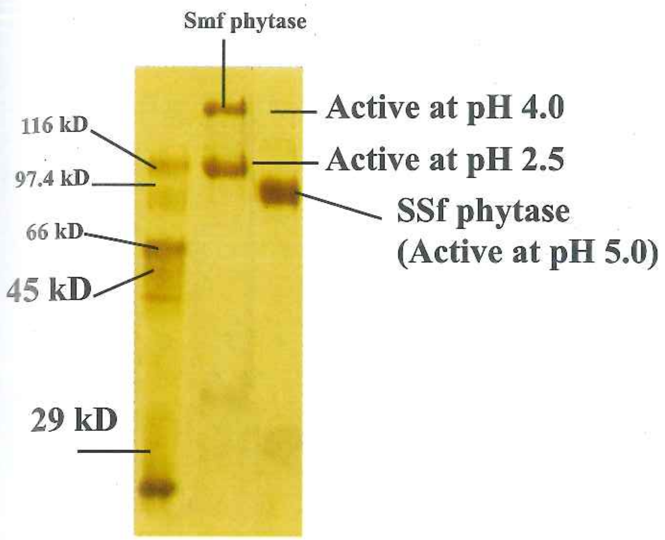
Kinetics of growth of Lactobacillus delbrueckii mutant Uc-3 and lactic acid production and fructose accumulation in synthetic medium containing 190 g l-1 of hydrolyzed cane sugar: (□) biomass, (■) glucose, (○) pH, (●) fructose, (▲) lactic acid

6.2 Highly Acidic Lipase from *Aspergillus niger*

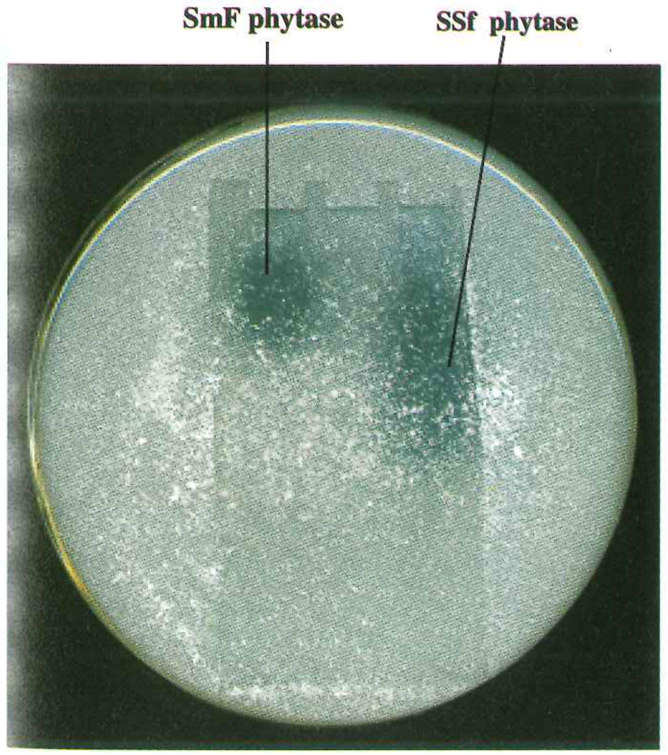
Aspergillus niger produces high levels of lipase which is stable and active at extremely acidic pH. The mycelium lipase has been used for conversion of isoamyl alcohol to isoamyl acetate (80g/l) with 90% conversion efficiency. Mutants are also isolated capable of producing enhanced levels of extra-cellular acidic lipase. The extracellular preparation of lipase is being investigated for fusel oil conversion to isoamyl acetate. The initial experimentation demonstrated the possibility of using fusel oil for bioconversion to isoamyl acetate.

6.3 Novel Phytase production from *Aspergillus niger* NCM 563

Phytase is one of the most industrially important enzymes used in animal feed industry especially poultry feed industry. Phytases hydrolyze phytic acid, myo-inositol-hexakisphosphate, to less phosphorylated myo-inositols and inorganic phosphate. Screening of more than 200 strains of A. niger from our culture collection (NCIM) resulted in identification of A. niger 563 as novel phytase enzyme producer. It produced phytase under both submerged and solid-state fermentation. Maximum phytase activity (108 IU/g dry mouldy bran) was produced with cowpea meal as substrate within 7 days with pH optimum 5.0. Recently, it was found that phytase secreted under submerged fermentation condition has two pH optima viz. 2.5 and 4.0 i.e. it belongs to phytase A (phy A) but novelty of the phytase is its activity at pH 2.5 is five times higher than at pH 4.0, which is very unusual, as phytase B (phyB) reported in the literature show two pH optima i.e. 2.2 to 2.5 and 4.0 to 5.0 with higher activity at pH 4.0 to 5.0. Our preliminary work indicates that phytase produced under SSF and SmF is different.



Compartive zymogram of phytase by Smf and SSf



6.4 Alpha-galactosidase from thermophilic fungus Humicola and thermophilic strain of *Bacillus stearothermophilus*

α-Galactosidase is industrially important enzyme used in food and feed industry. It is used to remove galactooligosaccharides viz. raffinose and stachyose which are present in soya milk which otherwise cause intestinal discomfort and flatulence. This is the first report of extracellular α-galactosidase (44.6 U/g of original substrate) from thermophilic fungi using solid-state fermentation technology. This enzyme, active at pH 5.0 and temperature 60°C, removes raffinose and stachyose from soyamilk within 2h at 50°C. *B. stearothermophilus* produces highest levels of á-galactosidase (101 IU/l) which is active at 65°C and at pH 6.5. This enzyme removes galactooligosaccharides from soyamilk within 2 h at 65°C thus useful in pasteurization of milk. This could be useful in removal of galactooligosaccharides from animal feed ingredients like guar powder, sunflower cake and cotton seed cake, the property, which is helpful to increase the digestibility of animal feed.

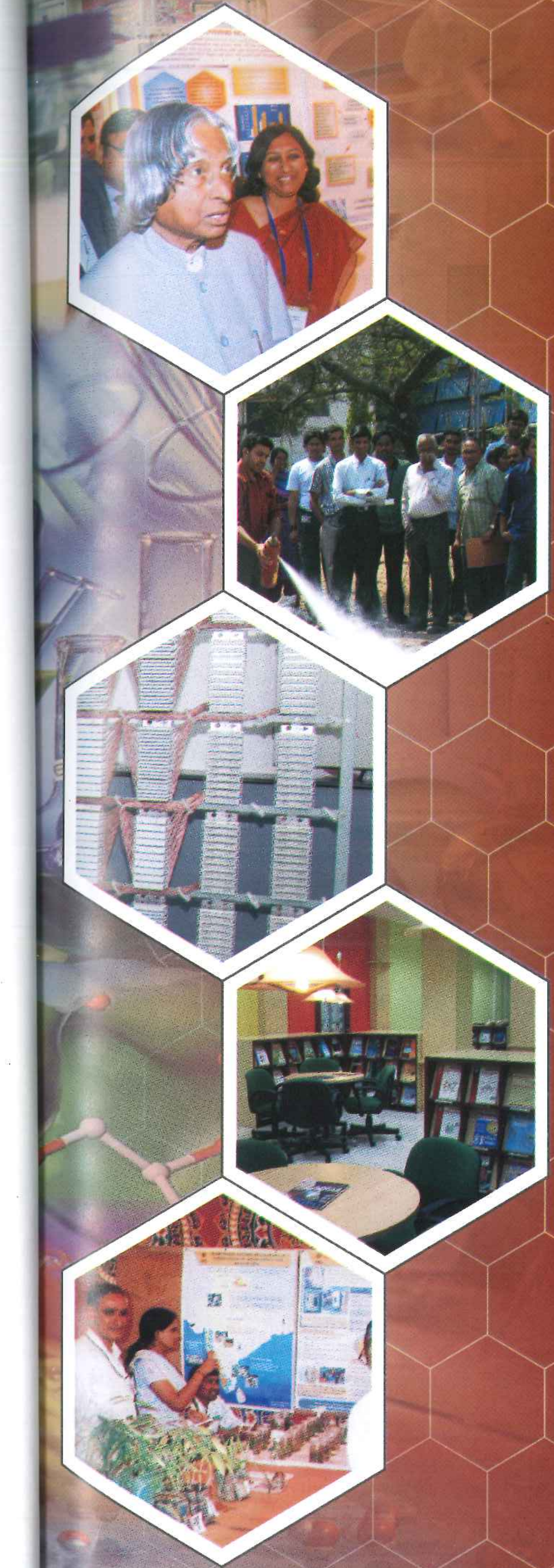
6.5 Strain Improvement for cellulase production

A mutant, EMS-UV-8, of *Penicillium janthinellum* capable showing enhanced zone of Walseth cellulose hydrolysis was isolated using EMS treatment followed by UV irradiation of the spores. The treatment of spores with only UV irradiation did not result in getting improved strain. The further mutation and selection resulted in isolation of 2 promising mutants, one selected on the basis of Avicel hydrolysis (EU1) and other on the basis of hydrolysis of Walseth cellulose in presence of 2-deoxy-D-glucose (EU2D-21). All these mutants produced two times Fpase and CMCase activities than the parent strain. Enzyme preparation derived from EU1 mutant hydrolyzed Avicel to greater extent. The enhanced hydrolysis yields could be correlated to the selection of EU1 mutant on the basis of Avicel hydrolysis, which is more crystalline substrate. The enzyme preparation from one of the mutants (EMS-UV-8) for hydrolysis of delignified

NATIONAL COLLECTION OF INDUSTRIAL MICROORGANISMS

bagasse sample generated was evaluated to produce fermentable sugars, which could be converted to either ethanol or lactic acid. This study shows the high potential of agricultural waste biomass as important sources of sugars for fermentation to commodity chemicals like ethanol or lactic acid.

Zone of hydrolysis of Phosphoric acid swollen cellulose exhibited by parent and mutants



S&T SUPPORT SERVICES

**Annual Report
2005-06**

BUSINESS DEVELOPMENT

NCL has a separate Business Development Division (BDD) to take 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 laboratory The division is staffed with engineers and management graduates who work as technology facilitators interfacing with scientists, industries, government, financial institutions and other statutory agencies.

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.

Public relations & events management

The public relations and events management group provided management services in planning, coordination, and organization of events and public relation activities, particularly in industrial liaison, exhibitions, seminars, conferences, business meetings, HRD programmes, etc.

- Exhibitions:

NCL participated in the exhibitions like CSIR Foundation Day Exhibition at New Delhi (25-26 September 2005), R & D Meet 2005 at Technology Bhavan, New Delhi (5-9 November 2005), CSIR Exhibition at Bio-Asia 2006 at Hyderabad (9-11 February 2006), Science Day Exhibition at TIFR, Khodad (28 February - 1 March 2006), etc.

- National Science Day Exhibition at GMRT:

NCL participated in National Science Day Exhibition (28 February - 1 March 2006) at Giant Metrewave Radio Telescope, Khodad near Pune which is the sub center of Tata Institute of Fundamental Research. Scientists from Tissue Culture Pilot Plant presented the salient achievements in the area of plant biotechnology with special reference to micropropagation of economically important tree species, plantation and horticulture crops, medicinal plants and its demonstration at grass root level. The work done in the area of plant molecular biology such as, early sex determination in papaya plants, and studies on insect resistance in plants were also highlighted. Around 7000 visitors including graduates, school students, farmers, and people from various strata of the society visited the stall and showed keen interest in the advancements exhibited at the stall.

- Science Expo-2005:

NCL participated in the Science Expo-2005 from 23rd to 27th November, 2005 organised by Nehru Science Centre, Mumbai. The function was inaugurated by Dr. K.A. Dinshaw, Director, Tata Memorial Centre, Mumbai. Dr. A.A. Natu and Dr. B.L.V. Prasad delivered special science lectures on "Newer developments in drug discovery" and "Current trends in nanoscience & technology", respectively.

Visit of Dr. K.A. Dinshaw and Shri G.S. Rautela, Director, Nehru Science Centre to NCL Stall

India R&D 2005: The event 'India R&D 2005 - The World's Knowledge Hub of the Future' was held on November 7-8, 2005 at Vigyan Bhavan, New Delhi. This event was organized by FICCI in partnership with Department of Science and Technology (DST), Department of Industrial Policy and Promotion (DIPP) and CSIR. Along with the conference an exhibition showcasing specific research and development activities in various fields was also organized. NCL was showcased as a global R&D based platform in the area of chemical and allied sciences.

Honorable President of India Dr. A.P.J. Abdul Kalam visits NCL stall

- Symposia/ Seminars:

During the year, NCL organized twelve national / international conferences symposia/ workshops / seminars /meetings including Visit of Parliamentary Standing Committee on S & T, Environment and Forest, Interactive Meet with Seed Industry, and Joint International Conference on Building Bridges, Forging Bonds for 21st Century Organic Chemistry and Chemical Biology (ACS-CSIR OCCB 2006).

- Annual Events and Lectures:

NCL organized various Memorial lectures, Endowment lectures, Special lectures, besides CSIR Foundation Day, NCL Foundation Day, National Science Day, National Technology Day, National Safety Day, Hindi week, and Vigilance awareness week events.

- Training and HRD Programmes:

CSIR Programme on Youth for Leadership in Science (CPYLS) for X std. meritorious students was organized. Interactive Programme on Finance & Accounts for Controllers of Finance & Accounts & Finance & Accounts Officers (19-20 September 2005) and a symposium on science education "Emerging trends in Teaching and Learning" were organized (7-8 May 2005).

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. Twenty-eight foreign and forty-six Indian patent applications were processed in addition to the ongoing work of the patent applications from the previous years.

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.

Customer satisfaction index

CSIR, the parent body of NCL, has launched an independent unit called the "Customer Satisfaction and Evaluation Unit" (CSEU) that monitors the levels of satisfaction of our clients with R & D services that the CSIR laboratories offer.

Customers were asked to grade the laboratory on the following parameters with respect to the project that they had undertaken with NCL on a defined scale.

- **Objective:** To check if the broad direction of the achievements intended at the start were accomplished or not
- **Schedule:** To ascertain if work is accomplished, as per the time schedule committed at the start
- **Output:** To ascertain how much of the minimum tangible which is of value to the customer, has been as committed at the start
- **Usability:** To ensure that the customer is able to readily use the output without further processing and with prolonged impact

The latest CSI score available is for the year 2004-05. NCL is one of the seven laboratories that are categorized in chemical sciences group amongst CSIR labs. NCL's CSI for the last three years is as follows:

Year	CSI
2002-2003	3.175 (out of 4)
2003-2004	3.447 (out of 4)
2004-2005	4.24 (out of 5)

NCL's customers

Global customers

Alcoa
BASF
Biotechnology Consulting & Research Inc.
D&O Pharmachem Inc.
DuPont
Galelio Pharma
General Electric
Honeywell International Inc.
Invista
Lanxess
Lyondell
Millenium Research Laboratories, Inc
Nikem Research
Proctor & Gamble
SC Johnson
Scios Corporation
Thai Organic Chemicals Company Ltd.

Indian customers

Ajeet Seeds
Alkyl Amines
Altana Pharma
Ankur Seeds
Asian Paints
Atul
Chembiotek
CIPLA
Dabur
Dr. Reddy's Laboratory
Dura-Line India
Emcure
Emmeellen Biotech Pharmaceuticals Ltd.
FDC
Garware Polyesters
Glenmark
GSFC
Hindustan Lever
Hindustan Polyamides and Fibres
Innovasynth Technologies

Indian customers cont'd

Kanoria Chemicals
Kirloskar Oil Engines Limited
Lupin
NTPC
ONGC
Ranbaxy
Reliance Industries
S.C. Johnson
Shasun Chemicals
Shriram Vinyl & Chemical Industries
Shymal Organics
Tata Chemicals
Tata Steel
Transmetal
United Phosphorus Limited
USV
Vamshi Exports
Schenectady Herdillia

Unencumbered Patents

Unencumbered Foreign Patents: Biochemistry

Patent No.	Title
5,455,163	Process for producing alcohol.
5,534,429	Strain of cephalosporium having ATCC accession no. 74297, A process of isolating said strain of cephalosporium and a process for preparing extracellular endoxylanase
5,750,401	Cultural medium for bamboo shoot sprouting and multiplication and a method for sprouting and multiplication of bamboo plantlets.
6,015,699	Process for the production of alcohol.
6,037,128	Process for the preparation of semisynthetic amplicon useful for sex determination of the papaya plant.
6,121,024	Halophilic pseudomonas strain having accession no. NCIM 5109 (ATCC 55940) and a process for preparing D(-)N-carbamoylphenyl glycine using said strain.
6,180,345	Process for simultaneous preparation of sex specific and gender-neutral semisynthetic amplicons useful for sex determination.
6,365,407	Culture medium composition useful for induction and proliferation of *Taxus calli*.
6,379,937	Process for the preparation a mixture of 19hydroxyeicosatetraenoic acid and 20 hydroxyeicosatetraenoic acid (19 HETE and 20 HETE).
6,448,051	Process for the preparation of 4(R) hydroxy cyclopent-2-en-1(S) acetate.
6,448,060	Alkalothermophilic bacillus that produces a protease inhibitor
6,514,748	Strain of streptomyces for the preparation of an alkaline protease inhibitor
6,534,303	Process for the preparation of acidic lipase
6,692,945	A process for the production of polyhydroxyoctanoate by streptomyces
6,756,222	Novel *Escherichia coli* having Accession No. PTA 1579 and its use to produce polyhydroxybutyrate
6,777,219	Process for the preparation of alkaline protease
6,846,664	Process for the preparation of protease inhibitor using novel alkalothermophilic *Bacillus* sp.

BUSINESS DEVELOPMENT

Unencumbered Indian Patents: Biochemistry

Patent No.	Title
185720	An improved process for producing ethanol using alumino silicate zeolite
179018	A novel process for the production of d(-) Carbamoyl phenyl glycine from 5- phenyl hydantoin.
187087	An improved process for the preparation of Ethanol
183287	Treatment of stable intergeneric hybrid Zm/c 041 with synthetic zeolites to enhance the extracellular activities of the industrially important enzymes like xylanase
183286	Treatment of stable intergeneric hybrid Zm/c 041 with synthetic zeolite to enhance the extracellular activities of amylase
186995	A process for the preparation of novel protease stable at high pH
182520	A process for the production of extracellular endoxylanase active at high alkaline pH from alkalotolerant fungal strain cephalosporium
189297	A process for the preparation of alkaline protease from an alkalophilic streptomycete in semi solid fermentation
183925	An improved process for the production of penicillin V acylase using *Bacillus sphaericus*
186723	An improved process for thermostabilizing of alpha-L-arabinofuranosidase enzyme
186894	A composition useful for the propagation of phragmites species
189032	A process for the preparation of an improved composition useful for promoting development of shoots from the excised embryo-axis of cotton
193289	An improved process for simultaneous preparation of sex specific and gender neutral semi synthetic amplicons useful for sex determination
191262	A process for the preparation of protease inhibitor using novel alkalothermophilic *Bacillus* sp.
192501	A process for the preparation of cellulase free alkali tolerant xylanase
191097	A process for the preparation of a proteinaceous alkaline proteinase inhibitor having antifungal properties
191418	A process for the preparation of 4(R)-hydroxy cyclopent-2-en-1 (S) acetate
193300	A process for the preparation of mycolytic enzymes containing mainly chitosanase
192348	An improved process for the preparation of acidic lipase

Unencumbered Foreign Patents: Catalysis

Patent No.	Title
0442173	Process for the preparation of alkyl methyl carbamates.
0867424	A process for the preparation of alpha and beta naphthol by hydroxylation of naphthalene using an organotransition metal complex.
1229064	Process for the preparation of a polyester.
1229065	Process for the preparation of a polyesteramide.
1277650	Lanthanum silicate catalyst composite, its preparation and its use for conversion of alkanols to light olefins.
2025449	Catalyst composite material for hydrocarbon reactions.
22474	A process for reforming of pyrolysis naphtha.
246301	An improved process for the conversion of natural gas into middle distillates.
352378	Nickel containing catalyst.
382960	An improved reforming process for the catalytic conversion of petroleum fractions to a mixture of hydrocarbons rich in aromatics.
4,902,659	An improved catalyst useful for thepreparation of carboxylic acids and improved process for the preparation of carboxylic acids.
4,950,385	aromatics An improved reforming process for the catalytic conversion of petroleum fractions to a mixture of hydrocarbons
474928	Catalyst composite material for hydrocarbon reactions
5,141,908	Catalyst composite material for hydrocarbon reactions.
5,219,813	A process for the preparation of novel crystalline molecular sieves.
25,262,045	A process for reforming of pyrolysis.
5,453,553	Process for the production of linear alkylbenzenes.
5,493,061	Process for the conversion of phenol to hydroquinone and catechol.
5,498,801	Process for the catalytic hydroformylation of alkenes.
5,502,241	An improved process for the preparation of alkyl carbamates.
5,650,546	Process for the catalytic hydrogenation of organic compounds.
5,693,869	Process for the single step oxidation of 3-phenoxytoluene to 3-phenoxybenzaldehyde.
5,723,679	Process for the preparation of methyl ethyl ketone from secondary butyl alcohol using an improved copper silica catalyst.
5,767,320	Process for the oxidation of cyclohexane to a mixture of cyclohexanone and cyclohexanol.
5,792,875	Catalytic production of butyrolactone or tetrahydrofuran.
5,795,555	Micro-meso porous amorphous titanium silicates and a process for preparing the same.
5,811,599	Process for the selective oxidation of hydrocarbons and their derivatives.

BUSINESS DEVELOPMENT

5,856,575	Process for the preparation of N-acetyl aminophenols.
5,885,546	Process for the preparation of titanium silicates.
5,892,138	Process for the preparation of halocumenes
5,932,752	Process for the C-C bond forming reaction using solid acid catalysts.
5,932,773	Process for the preparation of alpha and beta naphthol by hydroxylation of naphthalene using organotransition metal complex.
551688	A process for the preparation of crystalline molecular sieves.
564724	A process for the production of linear alkylbenzenes.
577793	Iron sodium silicate catalyst.
6,028,227	Single step process for the preparation of p-aminophenol.
6,166,269	Process for the preparation of 2-phenyl ethanol.
6,294,687	Process for the preparation of saturated carboxylic acids and their esters.
6,331,502	Catalyst system containing a semilabile anionic ligand and a use of such catalyst system to produce alpha, beta-unsaturated carboxylic acids and their esters.
6,335,415	Process for the preparation of a polyester.
6,376,701	Process for the transesterification of keto esters using solid acids as catalysts.
6,380,426	Process for the preparation of a carboxylic acid.
6,392,093	Process for the oxidation of cyclohexane to adipic acid.
6,403,833	Single step hydrogenation of nitrobenzene to p-aminophenol.
6,410,681	Process for the preparation of a polyesteramide.
6,420,615	Process for the conversion of 1,4-butynediol to 1,4-butenediol.
6,444,844	Process for the preparation of a carboxylic acid.
6,469,169	Water soluble palladium complexes and process for the preparation thereof
6,469,221	Process for the conversion of 1,4-butynediol to 1,4-butanediol or a mixture of 1,4-butenediol and 1,4 butanediol.
6,479,693	Process for the preparation of a saturated carboxylic acid.
6,492,566	Process for the preparation of dihydroxydiphenylmethanes.
6,521,784	Process for the preparation of acetic acid or methyl acetate.
6,521,789	Process for the preparation of adipic acid.

BUSINESS DEVELOPMENT

6,528,689	Noble metal containing hydrogenation catalyst for selective hydrogenation of 1,4-butynediol to 1,4 butenediol, and a process for the preparation thereof.
6,537,344	Process for the preparation of a nanosized colloidal metal particle.
6,559,322	Process for preparation of a lactone from a cyclic ketone.
6,593,499	A process for the preparation of phenyl ketones.
6,649,791	Process for the preparation of an aromatic carboxylic acid.
6,660,675	Noble metal containing hydrogenation catalyst for the selective hydrogenation of 1,4 butynediol to 1,4-butenediol and a process for the preparation thereof.
6,660,883	Process for the preparation of 2-aryl propionic acids.
6,791,000	Process for vapour phase nitration of benzene using nitric acid over molybdenum silica catalyst.
6,800,221	Conductive polymer blend and a process for the preparation thereof.
6,825,388	Process for the preparation of 4-nitro-o-xylene.
6,858,753	Process for the preparation of carboxylic acids from aliphatic alcohols.
6,894,191	Process for the preparation of arylamines.
6,921,843	Process for the preparation of dimethyl cumenes.
6,924,379	Process for preparation of cyclic carbonate.
6,979,753	Process for the preparation of 2-phenyl ethanol.
621640	An improved process for the conversion of natural gas into middle distillates.
625926	Catalyst composite material for hydrocarbon reactions.
784045	A process for the preparation of adipic acid.
8803781.9	An improved catalyst useful for the preparation of carboxylic acids and improved process for the preparation of carboxylic acids.
GB2389324	A novel catalytic formulation and its preparation.
PI8803781.9	An improved catalyst useful for the preparation of carboxylic acids and improved process for the preparation of carboxylic acids.
1325814	Process for the conversion of natural gas into middle distillates.
1325901	Process for the preparation of adipic acid.
135159	A commercial process for the preparation of p-diethyl benzene from dilute ethyl alcohol and ethyl benzene.
135162	A commercial process for the preparation of p-diethyl benzene from dilute ethyl alcohol and ethyl benzene.
1974954	An improved catalyst useful for the preparation of carboxylic acids and improved process for the preparation of carboxylic acids.

1974954	An improved catalyst useful for thepreparation of carboxylic acids and improved process for the preparation of carboxylic acids.

Unencumbered Indian Patents: Catalysis

Patent No.	Title
185935	An improved process for the preparation of iron-molybdate catalyst
185627	An improved process for the preparation of formaldehyde using improved Iron molybdate catalyst
185720	An improved process for producing ethanol using alumino silicate zeolite
179276	A process for the production of ortho chlorotoluene
187354	An improved naphtha reforming process for the preparation of a mixture of hydrocarbon rich in aromatics
187087	An improved process for the preparation of ethanol
182357	An improved process for the preparation of 4-chloro-o-xylene
186074	An improved process for the preparation of epoxides of olefinic organic compounds
193288	A process for the preparation of stabilised zirconia
183287	Treatment of stable intergeneric hybrid Zm/c 041 with synthetic zeolites to enhance the extracellular activities of the industrially important enzymes like xylanase
183286	Treatment of stable intergeneric hybrid Zm/c 041 with synthetic zeolite to enhance the extracellular activities of amylase
189140	An improved process for the preparation of N-acetyl amino phenol
188690	An improved process for the preparation of monochlorophthalic anhydride free from dichloro component.
189161	An improved process for the preparation of aromatic aldehydes
189203)	A process for the preparation of 1-chloro naphthalene.
188874	A process for the preparation of high silica sodium aluminosilicate
190725	A process for the production of benzophenones
189381	An improved process for the preparation of Titanium silicates
189405	An improved process for the conversion of phenol into amixture of hydroquinone and catechol.
192816	An improved process for the preparation of para-di-alkyl benzene.
189460	An improved process for the preparation of Tin containing crystalline molecular sieves of MEL type
189306	An improved process for the preparation of a novel porous crystalline tin containing crystalline molecular sieves
190356	An improved process for the selective oxidation of hydrocarbons and their derivatives
189703	A process for the preparation of micro-meso porous amorphous titanium silicates
189479	An improved process for the preparation of copper-silica catalyst supported on a metal oxide
190552	An improved process for the preparation of aniline by hydrogenation of nitrobenzene using an improved copper silica catalyst
190733	An improved process for the preparation of composite catalytic material
190273	An improved process for the preparation of a crystalline titanosilicate molecular sieve
187347	A process for the preparation of molybdenum-silicate molecular sieves
190557	A process for the preparation of arsenic modified porous crystalline silicas
184802	A process for the preparation of L-dopa from L-tyrosine
193302	An improved process for the preparation of sulphated mixed metal oxides
192732	An improved process for the oxidation of cyclohexane and cyclohexanol.
193308	An improved process for the manufacture of hydroquinone and catechol
185325	An improved process for the preparation of alpha and beta naphtha by hydroxylation of naphthalene
192383	An improved process for the preparation of cumene hydroperoxide
184428	An improved process for the hydroxylation of ethyl benzene
192547	An improved process for the preparation of mixture of guaiacol and p-methoxy phenol
193301	An improved process for the oxidation of benzene
192396	A process for the preparation of cresols
185074	An improved process for the preparation of m-dichlorobenzene
190813	An improved process for the preparation of 2,4-dichlorotoluene
186078	An improved process for the oxidative halogenation ofaromatic compounds
185806	An improved process for the preparation of substituted acetophenones
188375	An improved process for the preparation of halocumenes
184740	An improved process for the preparation of cyclopropylamine
190793	An improved process for the production of epichlorohydrin
189048	An improved process for the preparation of unsaturated hydroxy lactones
190582	An improved process for the preparation of 4-hydroxy-cyclic and acyclic-2-enones
190825	An improved process for the production of aminocarboxylic acid salts
193312	An improved process for the preparation of meta-chlorotoluene

178254	An improved process for the preparation of chlorobenzenes
191516	A process for the preparation of hydroxy benzyl alcohols
193309	An improved process for the preparation of keto-isophorone
191624	Process for the manufacture of epoxides of olefinic compounds
191839	An improved process for preparation of ibuprofen
192841	An improved process for the preparation of 2-aryl propionic acids
191096	An improved process for the preparation of 2-aryl propionic acids
191704	An improved process for the preparation of 2-aryl propionic acids
191417	An improved process for the preparation of 2-aryl propionic acids
191702	An improved process for the preparation of 2-aryl propionic acids
191703	An improved process for the preparation of 2-aryl propionic acids
191360	An improved process for the preparation of 2-aryl propionic acids
191488	An improved process for the preparation of 2-aryl propionic acids
191234	An improved process for the preparation of 2-aryl propionic acids
191705	An improved process for the preparation of 2-aryl propionic acids
191706	An improved process for the preparation of 2-aryl propionic acids
191235	An improved process for the preparation of 2-aryl propionic acids
193298	An improved process for the single step hydrogenation of nitrobenzene to p-aminophenol
192391	An improved process for preparation of N- substituted carabamates

Unencumbered Foreign Patents: Chemical engineering and process development

Patent No.	Title
5,080,121	A process for the preparation of a new polymer useful for drag reduction in hydrocarbon fluids in exceptionally dilute polymer solutions.
5,118,654	A process for the preparation of an improved Li-promoted magnesium oxide catalyst useful for oxidative coupling of methane to ethane and ethylene.
5,306,854	A two step process for production of liquid hydrocarbons from natural gas.
5,336,825	An improved integrated two step process for conversion of methane to liquid hydrocarbons of gasoline range.
5,336,825	An improved integrated two step process for conversion of methane to liquid hydrocarbons of gasoline range

5,338,488	An improved process for the production of synthesis gas by oxidative conversion of methane using composite catalyst containing transitional and alkaline earth metal oxides.
5,368,835	Process for production of synthesis gas by oxidative conversion of methane methane (or natural gas) using composite catalyst.
5,411,927	Process of preparing composite catalysts for production of synthesis gas by oxidative conversion of methane or natural gas.
5,594,137	An improved process for the preparation of caprolactum from cyclohexanone oxime using micella solutions, macroemulsion and microemulsion systems.
5,712,217	A process for the preparation of improved supported catalyst use-ful for the oxidative coupling of methane to higher hydrocarbons, oxidative conversion of natural gas to thylene and lower olefins.
5,744,419	Process for the preparation of an improved supported catalyst.
5,756,421	Composite catalysts containing transitional and alkaline earth metal oxides useful for oxidative conversion of methane (or natural gas) to carbon monoxide and hydrogen (or synthesis gas).
5,763,725	Process for the production of ethylene by non-catalytic oxidative cracking of ethane or ethane rich C.sub-2-C-sub-4 paraffins.
5,786,519	Process for the preparation of a mixture of guaiacol and p-methoxy phenol.
5,936,135	Process for the preparation of hydrocarbons.
582004	Novel composite catalysts and their use in process for the oxidative conversion of methane or natural gas to synthesis gas.
6,020,534	Process for production of propylene and ethylene by non catalytic oxycracking of propane or propane-rich C2-C4 paraffins.
6,087,545	Process for oxidative conversion
6,093,830	Enantioselective resolution process for arylpropionic acid drugs from the racemic mixture.
6,180,557	Supported catalyst useful for Friedel-Crafts reactions and process for the preparation of aralkylated aromatic compounds using the catalyst.
6,197,719	Process for the activation of perovskite type oxide.
6,208,951	Method and an apparatus for the identification and/or separation of complex composite signals into its deterministic and noisy components.
6,215,035	Process for the preparation of aralkylated aromatic compounds using heterogeneous catalyst.
6,293,979	Process for the catalytic conversion of methane or natural gas to syngas or a mixture of carbon monoxide and hydrogen.
6,346,228	Hydrophobic multicomponent catalyst useful for direct oxidation of hydrogen to hydrogen peroxide
6,420,596	Process for the selective esterification of tertiary alcohol by an acid anhydride using a reusable solid catalyst.

BUSINESS DEVELOPMENT

6,432,376	Membrane process for the production of hydrogen peroxide by non-hazardous direct oxidation of hydrogen by using a novel hydrophobic composite Pd-membrane catalyst.
6,437,191	Process for the acylation of aromatic compounds using a reusable solid catalyst comprising indium halide.
6,448,199	Hydrophobic composite Pd-membrane catalyst useful for non-hazardous direct oxidation of hydrogen by oxygen to hydrogen peroxide and method of its preparation.
6,459,000	Process for the liquid phase acylation of aromatic compounds.
6,504,050	Process for the preparation of 2-acrylamido-2-methyl-1-propanesulfonic acid.
6,509,000	Low temperature process for the production of hydrogen.
6,525,226	Process for preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst.
6,534,440	Process for the activation of a metallic palladium based catalyst useful for the direct oxidation of hydrogen to hydrogen peroxide.
6,548,722	A process for the preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst.
6,589,427	Process for treatment of mixture of spent wash from distillery and black liquor from pulp and paper industry.
6,657,082	An improved process for the preparation of thiourea.
6,660,882	Process for the preparation of 2-methyl-2-propene-1-sulfonic acid, sodium salt.
6,825,383	A new catalytic process for regiospecific chlorination of alkanes, alkenes and arenes
6,826,513	Method and apparatus for online identification of safe operation and advance detection of unsafe operation of a system or process.
6,828,463	Processes for the preparation of carboxyl compounds with carboxyl group attached to the aromatic ring.
6,835,854	Process for the production of 3,3',4,4'-Tetraaminobiphenyl.
6,858,141	Process for the preparation of ultrafiltration membranes of polyacrylonitrile, using malic acid as an additive.
6,872,857	Process for the conversion of phenol to hydroquinone and quinones.
6,894,183	Method for the improvement of gas-solid contacting in a bubbling fluidized bed reactor.
6,900,286	Process for preparation of conducting polyaniline.
6,929,942	A process for the treatment of industrial effluents using marine algae to produce potable water.
6,933,397	Process for the epoxidation of liquid olefinic organic compound using a supported nano-gold catalyst.
6,979,749	Catalytic process for the production of 3,3',4,4'-Tetraaminobiphenyl.
7,022,307	Method for the improvement of Gas-Solid contacting in a bubbling fluidized bed reactor.

BUSINESS DEVELOPMENT

Unencumbered Indian Patents: Chemical engineering and process development

Patent No.	Title
185714	An improved process for the preparation of hydrogenated esters of dicarboxylic acid
185715	A process for the preparation of supported bimetallic catalyst useful for the hydrogenation of esters of dicarboxylic acid
179018	A novel process for the production of d(-) carbamoyl phenyl glycine from 5-Phenyl hydantoin.
184871	A process for the preparation of macroporous glycidyl co-polymers
187915	A process for the preparation of ankle block component useful for artificial foot
187419	A process for preparation of a novel macroporous glycidyl copolymers beads useful as matrix for anchoring hydrophobic biomolecules
189045	An improved process for the preparation of caprolactam
182590	A process for the preparation of hydrolytically stable macroporous beads
189145	An improved process for the preparation of an improved supported catalyst useful for oxidative conversion of methane, natural gas and biogas to synthetic gas
188329	A process for the preparation of syngas
183663	A process for the preparation of pendent chain linked amino acids containing biodegradable polymers.
188871	An improved process for the preparation of ethylene and higher olefins, using the improved supported catalyst
188332	An improved process for the catalytic hydroformylation of alkanes
183195	An improved process for the catalytic hydrogenation of organic compounds
188334	An improved process for the production of ethylene by non-catalytic oxidative cracking of ethane or ethane rich C2-C4 paraffins
188538	A process for the preparation of improved supported catalyst useful for the oxidative coupling of methane to higher hydrocarbons, oxidative conversion of natural gas to ethylene and lower olefins
188872	An improved process for the preparation of ethylene, ethane and higher hydrocarbon
190179	An improved process for the preparation of aryl substituted acids and their alkaline salts
183618	A process for the separation of racemic mixture of chiral drugs to optically active enantiomers
193284	An improved process for the treatment of distillery effluent
191260	An improved process for the preparation of naringinase enzyme using penicillium citrinum
188412	An improved process for the preparation of alpha-cyclodextrin glycosyltransferase enzyme
190793	An improved process for the production of epichlorohydrin

189741	A new enantioselective resolution process for arylpropionic acid drugs from the racemic mixture
192166	An improved process for the preparation of immobilized penicillin acylase
192158	A process for the preparation of carotenoids mainly B- carotene and other
184642	An improved process for the separation of Gibberellic acid from the fermented broth containing other gibberellins
185325	An improved process for the preparation of alpha and beta naphtha by hydroxylation of naphthalene
192547	An improved process for the preparation of mixture of guaiacol and p-methoxy phenol
184739	An improved process for the recovery of thiocarbamide
190987	An improved process for recovery of glycerin from fermented molasses

Unencumbered Foreign Patents: Organic chemistry

Patent No.	Title
0564723	An improved process for the synthesis of D(+) biotin.
1219625	Novel substituted 2-(6-benzyl-5-oxo-3-phenyl-(S3,7S,7AR)-perhydroimidazol (1,5-C)(1,3) thiazol-7YL) compounds.
1238965	A process for the preparation of 1-[2-dimethylamino-(4-methoxyphenyl)-ethyl] cyclohexanol.
1238965	One pot process for the preparation of 1-[2-dimethylamino-(4-methoxyphenyl)-ethyl] cyclohexanol.
1238967	A process for the preparation of 1-[cyano(aryl)methyl] cyclohexanol.
2565977	A process for the preparation of alpha-aryl propionic acids.
4,906,343	A process for the photochemical production of alpha-aryl propionic acids.
5,066,819	An improved process for the preparation of aryl-N-alkyl carbamates.
5,274,107	An improved process for the synthesis of D(+) biotin.
5,395,951	Triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity and a process for extracting such compounds from the neem plant.
5,510,490	A process for the preparation of B-chloro-3-vinyl pyridine.
5,510,490	Process for preparation of epibatadine.
5,602,261	A process for the preparation of an active composition containing triterpenes including azadirachtin and its derivatives possessing antifeedant and growth inhibitory activity from parts of neem plant.
5,654,439	N-1-1 alkyl-2,5 di(trilakyl silyl) pyrolidines.
5,750,757	Pesticidal ester preparation.
5,756,773	Triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity.

5,869,697	Process for preparing diltiazem.
5,900,493	Triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitoryactivity.
6,008380	(2R, 3S, 24S)-2,3-diacetoxy-22,23-epoxy24-ethyl-.beta.-homo-7-oxa-5-.alpha.cholestan-6-one and a process for preparing the same.
6,087,136	Microbial process for the production of D(-)-N-carbamoylphenylglycine.
6,090,952	(2R,3S,22R,23R)-2,3,22,23-tetrahydroxy-24-ethyl-beta-homo-7-oxa-5-alpha-cholestan-6-one and a process for preparing the same.
6,180,785	Process for preparing diltiazem.
6,191,279	Dipyrano-quinolinones useful as anti viral agents and a process for preparing the same
6,350,881	Process for the preparation of 5-methoxy-4-(methylthioalkyl)-1,3-bis(phenylmethyl)-2-imidazolidone.
6,350,912	One pot process for the preparation of 1-[2-dimethylamino-(4-methoxyphenyl)-ethyl] cyclohexanol.
6,376,683	Process for the preparation of (4R,6S)-4-hydroxy-6-hydroxymethyl-tetrahydropyran-2-one.
6,388,097	Process for the preparation of beta hydroxy-delta lactone using novel intermediates.
6,417,374	Process for the preparation of beta-hydroxy-delta-lactone using novel intermediates.
6,486,328	Substituted 2-[-6-benzyl-5-oxo-3-phenyl-(3S, 7S, 7AR)-perhydroimidazol [1,5-C] [1,3] thiazol-7yl] compounds.
6,504,044	Process for the preparation of 1-[cyano (aryl) methyl] cyclohexanol.
6,512,130	Mifepristone analogue, process for the preparation thereof and use thereof.
6,562,983	Process for the preparation of alkyl 4[2-(phthalimido)ethoxy]-acetoacetate.
6,608,206	Process for making S(-) amlodipine salts.
6,645,917	Composition for hybrid seed production, process for the preparation of such composition and use thereof.
6,713,639	A process for preparing enantiomerically pure (S)-3-hydroxy-gamma-butyrolactone.
6,780,635	Process for the preparation of optically active azabicycloheptanone derivatives.
6,818,786	Process for the preparation of ethyl3-ethoxy-4-ethoxycarbonyl-phenylacetate.
6,825,378	A process for the synthesis of enantiomerically pure cyclohexylphenyl glycolic acid.
6,838,581	An improved process for the preparation of enantiomerically pure 3-phenyl-3-hydroxypropylamine.
6,846,932	An improved process for the preparation of chiral amlodipine salts.
6,852,864	Process for the synthesis of dipyrromethanes.
6,919,471	Process for preparing alkyl/aryl chloroformates.
63554E	Process for the preparation of codeine from morphine.

BUSINESS DEVELOPMENT

Unencumbered Indian Patents: Organic chemistry

Patent No.	Title
185630	An improved process for the preparation of 2-alkoxyphenols
182439	An improved process for the preparation of -halo ketones
182446	An improved process for the preparation of 5S(p-alkoxyphenyl)-4R-(carboalkoxy)-1,3,2, dioxthiolane-2-oxide
182445	An improved process for the preparation of 2-R-hydroxy-3S-[(2-aminoarylthio)]-3-(p-alkoxyaryl) propionic acid alkyl ester
180508	A process for the preparation of 2,5-di(trialkyl silyl pyrrolidine-t-butyl carbonate.
182838	An improved process for the preparation of organic halides.
184108	An improved process for the preparation of dialkyl 2,2,2-trichloroethylidene propanedioate
183298	A process for the preparation of alpha-chloro-beta-(4-methoxy phenyl) propionitrile
184694	A process for the preparation of cheatomellic acid A anhydride
184878	A process for the preparation of 3-Tetradecyl 2-oxo-3H-imidazo[1,2-a] pyridinium bromide (IV)
183338	A process for the preparation of N-(2-pyridyl)-alpha bromo palmitamide
18480	A new process for the preparation of (2R,3S,24S)-2,3-diacetoxy-22-bromo-24-ethyl-B-homo-7-oxa-23-hydroxy-5a-cholestan-6-one
184686	A new process for the preparation of (2R,3S,24S)-2,3-diacetoxy-22,23epoxy-24-ethyl-B-homo-7-oxa-5a-cholestan-6-one
185115	A new process for the preparation of (2R,3S,22R,23R)-2,3,22,23-tertahydroxy-24-ethyl-B-homo7-oxa-5a-cholestan-6-one
184684	A new process for the preparation of (2R,3S,22E,24S)-24-ethyl-2,3-dihydroxy-5a-choplestan-22-ene-6-one
185277	An enzymatic process for the preparation of optically pure isomers of ethyl 2,3-dihydroxy-3-(4 methoxyphenyl) propanoate
185785	A process for the preparation ofalkyl 2-(substituted amino)-1-carbalkoxy acrylates
186134	A process for the preparation of estra-5 alpha-hydroxy-9-en-11 beta-[4-(2-methyl-1,3-dioxolyl)phenyl]-17 beta-hydroxy-17 alpha-(3-methyl-1-butynyl)-cyclic-3-(1,2-ethandiyl)acetal
191577	A process for the preparation of 3ß-hydroxy-(20R)-20-hydroxydithianepregna-5-one
190796	A process for the preparation of 2,4(6)-di-O-alkyl-myo-inositol-1,3,5-orthoformate sulphonic acid esters
191924	A process for the preparation of 2,4(6)-di-O-deacytyl -6(4)-0-tosyl-myo-inositol-1,3.5-orthoformate
163810	A process for the separation of stigmasterol derived products

BUSINESS DEVELOPMENT

192836	A new process for the preparation of (2R,3S, 22S, 23S)-2, 3, 22, 23-tetraacetoxy-B-homo-7-oxastigmastan-6-one
192156	An improved process for the preparation of (2R, 3S, 22S, 23S)-2, 3, 22, 23-tetraacetoxy-B-homo- 7-oxastigmastln-6-one
179018	A novel process for the production of D(-)carbamoyl phenyl glycine from 5-phenylhydantoin.
179530	An improved process for the preparation of sodium p-hydroxy mandelate
182837	An improved process for the preparation of D(-)-phenylglycine from D(-) carbamoyl phenylglycine
182528	A process for the preparation of DL-5-phenylhydantoin
185701	An improved process for the preparation of sulfoxides
184645	An improved process for the preparation of chlorinated arenes
190435	An improved process for the preparation of alpha-bromo phenyl acetic acid
184650	An improved process for the preparation of ciprofloxacin
185783	An improved process for the preparation of 3-(N-substituted amino)-3-oxo-propionic acid esters
185379	An improved process for the preparation of hydroxy compoundsof steroids
184735	An improved process for the preparation of misopristol
185389	A process for the preparation of E(-) silane, {[1-(2-iodoethenyl)-1-methylhexyl]oxy} trimethyl
185790	A process for the preparation of 5,6-didehydro 15-methyl PGF-alpha 2 derivative
188978	An improved process for the preparation of (1R,cis)-(-)-caronaldehydic acid hemiacetal
186339	A process for the preparation of optically active carboprost methyl ester
184740	An improved process for the preparation of cyclopropylamine
185768	An improved process for the preparation of optically active carboprost methyl ester
192297	A process for the preparation of dimer of 4-methodxy-5(mercaptomethyl)-1,3-bis(phenylmethyl)-2-imidazolidinone, D(+)-biotin intermediate
190795	A process for the preparation of substituted 2-heptyne, 1(arylmethoxy)
189048	An improved process for the preparation of unsaturated hydroxy lactones
190582	An improved process for the preparation of 4-hydroxy-cyclic and acyclic-2-enones
191418	A process for the preparation of 4(R)-hydroxy cyclopent-2-en-1 (S) acetate
193287	A process for the preparation ofsubstituted 2-heptyne, 4-ol-1-(arylmethoxy)
192844	An improved process for the preparation of cycloalkylphenols
192827	A process for the preparation of 3-sulfanyl cyclic ketones

192052	An improved process for preparation of aziridines
192849	A process for the preparation of a novel cis, cis-3-hydroxy-5-methylcarbonyloxy-cyclohexylacetate useful as an intermediate for 6-hydroxymethyl-4-(tert-butyldimethylsilyloxy)-(4R, 6S)-tetrahydro-2H-2-pyranone
192170	A process for the preparation of a novel 3-tetrahydro-2H-2-pyranyloxy-5-(tert-butyldimethylsilyloxy)-(1S,3R,5R)-cyclohexan-1-one useful as an intermediate for 6-hydroxymethyl-4-(tert-butyldimethylsilyloxy)-(4R,6S)-tetrahydro-2H-2-pyranone

Unencumbered Foreign Patents: Material Chemistry

Patent No.	Title
5,461,013	Process for the preparation of lithium stanates doped with transition metal cations.
5,549,931	Process for the preparation of uniform ultra thin films of metal oxide, metal chalco-genides and metal halides.
5,643,508	Process for the preparation of nanodimensional particles of oxides and sulphides of metals.
6,783,963	Process for the preparation of metal sulfide nanoparticles.TZ/P/05/00082 A new process for the synthesis of mono and bimetallic nano particles.

Unencumbered Indian Patents: Material chemistry

Patent No.	Title
189191	A process for the preparation of ultra-thin films of inorganic compounds by liquid interface reaction technique
191575	A process for the preparation of boron phosphate useful for humidity sensing and a humidity sensor made threrefrom

Unencumbered Foreign Patents: Polymer science and engineering

Patent No.	Title
0477444	Carbanionic polymerisation initiators.
0878484	A process for the preparation of a magnesium halide supported metallocene catalyst.
0982334	A process for producing polycondensable macromonomer
2023298	Process for the preparation of a new polymer useful for drag reduction in hydrocarbon fluids in exceptionally dilute polymer solutions.
471116	A polymer useful for drag reduction in hydrocarbon fluids and its preparations.
5,194,537	An improved process for the preparation of nitrile group containing polymers.
5,266,659	Solid state process for the preparation of high molecular weight poly(arylcarbonate)s.
5,266,702	A process for the preparation of new reactive anionic initiators useful for polymerisation of vinyl monomers.

5,288,838	Preparation of polycarbonates with bioxyanion catalyst.
5,451,611	Process for the conversion of poly(ethylene terephthalate) waste to poly(alkylene terephthalate).
5,952,411	Compound bearing an urethane linkage which is an adduct of ricinoleic esters and an isocynate, useful as a plasticizer for polyvinylchloride (PVC) and a process for preparing such compound.
5,955,554	Process for polymerization and copolymerization of olefins.
5,962,003	Process for the preparation of polyurethane microcapsules containing monocrotophos.
5,962,360	Process for the preparation of a magnesium halide supported metallocene catalyst.
5,965,477	Process for the preparation of supported metallocene catalyst.
5,973,086	Process for the living anionic polymerization of alkyl (methacrylic) monomers using a novel initiator system.
5,994,533	Process for the recovery of tartaric acid and other products from tamarind pulp.
5,647,27	Process for the preparation of arylpolycarbonates in the presence of bioxyanion catalysts.
6,002,060	Process for oligomerisation of alpha-olefins.
6,015,768	Process for preparation of a heterogeneous catalyst useful for preparation of super high molecular weight polymers of alpha-olefin.
6,022,930	Process for pro macromonomer ducing polycondensable
6,118,012	Compound bearing a urethane linkage, which is an addict of ricinoleic esters and an isocynate, useful as a plasticizer for polyvinyl chloride (PVC) and a process for preparing such compound.
6,123,988	Process for the preparation of polyurethane spherical particle.
6,187,882	Process for polymerization of olefins.
6,239,213	Process for the preparation of stable aqueous urethane dispersions.
6,239,252	Single step process for the preparation of poly(oxyalkylene)-alpha, omega-dicarboxylic acid.
6,284,895	Bromo-functionalized benzotriazole UV absorbers.
6,307,055	Diol-functionalized UV absorber.
6,316,585	Process for the preparation of enzymatically degradable polymers.
6,316,615	Process for the recovery of potassium bitartrate and other products from tamarind pulp.
6,320,056	Process for the preparation of bromo-functionalized benzotriazole UV absorbers.
6,320,056	Process for the preparation of bromo-functionalized benzotriazole UV absorbers.
6,346,643	Process for the preparation of diesters of poly(oxyalkylene glycol) and amino acids.
6,369,249	Process for the preparation of N-substituted acrylamides.

6,369,249	Process for the preparation of N-substituted acrylamides
6,379,599	Process for the preparation of molecularly imprinted polymers useful for separation of enzymes.
6,420,487	Process for the preparation of thermoprecipitating affinity polymers
6,420,511	Process for the preparation of aromatic polyesters.
6,437,032	Compound bearing an urethane linkage, which is an addict of ricinoleic esters and an isocynate, useful as a plasticizer for polyvinyl chloride (PVC) and a process forpreparing such compound
6,489,482	Process for the preparation of novel vinylic hindered amine light stabilizers.
6,492,518	Tinuvin P-hindered amine light stabilizer and derivatives thereof.
6,500,913	Polyimides, process for the preparation thereof, and use thereof as alignment films for liquid crystal devices
6,559,311	Process for the synthesis of a photo-stabilizer
6,605,714	Thermoprecipitating polymer containing enzyme specific ligands, process for the preparation thereof, and process for the separation of enzymes using such polymers.
6,610,856	Tinuvin P-hindred amine light stabilizer and derivatives thereof.
6,689,836	Process for the preparation of thermoprecipitating affinity polymers.
6,737,528	Vinylic hindered amine light stabilizers.
6,756,499	Process for the preparation of noveldiol functionalised UV absorbers
6,770,785	Antioxonant cum antioxidant, process for preparation.
6,790,993	1,1-BIS(4-aminophenyl)-3-alkylcyclohexanes and method for their preparation.
6,794,467	Process for the preparation of polymeric absorbents.
6,822,064	Polymerizable macromer and preparation thereof.
6,825,308	Copolymers and preparation thereof.
6,867,268	Thermoprecipitating polymer containing enzyme specific ligands,process for the preparation thereof, and use thereof for the separation of enzymes.
6,916,960	Diol functionalised antioxidant and process for their preparation.
6,936,717	Tinuvin P-hindered amine light stabilizer and derivatives thereof.
6,977,285	Oligomers and preparation thereof.
908483	A process for the preparation of poly (ester-carbonates).
982331	Process for the preparation of aqueous urethane dispersions.

Unencumbered Indian Patents: Polymer science and engineering

Patent No.	Title
188894	An improved process for the preparation of polymer containing metal composite materials
189146	An improved process for the preparation of polymer containing ceramic composites materials
191257	A process for the preparation of conducting polymer composite useful for positive temperature coefficient resistance devices
183923	A process for the preparation of trifunctional amino acid derivatives of dicarboxylic acid chlorides
187374	An improved process for the preparation of photocrosslinkable polymers
189324	A process for hydrophilic stable macroporous beads.
183922	A process for the preparation of chemically linked biodegradable polymers
183657	A process for the preparation of Trifunctional amino acids based IMIDO acids for the synthesis of pendent chain linked biodegradable polymers.
183899	A process for the preparation of molded polymer for controlled release of physiologically active agent
190556	An improved process for the deposition on insulating substrates of conducting polymer films having enhanced stability
192400	A process for the preparation of a new polymeric composition for the controlled release of active ingredient in response to pH.
192558	An improved process for the conversion of esters and amides to corresponding alcohols and amines
189033	A process for the preparation of an improved polymeric device
192831	A composition of polymeric blends and devices made thereof
185076	A new process for the recovery of tartaric acid and other products from tamarind pulp
187315	An improved process for the preparation of novel crosslinked macroporous glycidyl methacrylate-pentaerythritol triacrylate copolymers (Jointly with HAL, Pune)
186455	An improved process for the production of immobilized D-amino acid oxidase (Jointly with HAL, Pune)
186430	An improved process for the preparation of novel crosslinked macroporous crosslinked glycidyl methacrylate-pentaerythritol triacrylate copolymers (Jointly with HAL, Pune)
187316	An improved process for the production of immobilized milk clotting protease (Jointly with HAL, Pune)
186454	An improved process for the continuous production of cheese free from aspartic protease (Jointly with HAL, Pune)
191019	A new process for the recovery of potassium bitartarate and other products such as Pectin, Sugars, Fruit acids as by-products from tamarind pulp
190971	A process for preparation of diesters of poly(oxyalkylene glycol) and amino acids

BUSINESS DEVELOPMENT

192067	An improved process for the separation of lysozyme
192969	A process for the extraction of penicillin G acylase from enzyme extract of *Escherichia coli*.
192740	A process for the purified penicillinase
178867	An improved process for the preparation of Poly(alkylenecarbonate)s
186303	A process for the preparation of a soluble homogeneous catalyst useful for the preparation of high molecular weight, narrow molecular weight distribution of non crystalline polymers of alpha olefins containing at least four carbon atoms
185719	An improved process for the preparation of high molecular weight narrow molecular weight distribution non crystalline hydrocarbon soluble poly (alphaol efins)
184951	An improved process for the preparation of polyolefins bearing pendant reactive vinyl unsaturation.
186839	An improved process for the preparation of thin semipermeable membrane
187889	A process for the preparation of polyalkylene terephthalate containing at least 3 carbon atoms from polyethylene terephthalate (PET) waste useful as an engineering thermoplastic
188825	A process for the preparation of a compound containing urethane linkage useful as plasticizer for polyvinylchloride (PVC)
188046	A process for the preparation of improved compounded poly(vinylchloride) (PVC)
190733	An improved process for the preparation of composite catalytic material
192765	An improved process for the anionic polymerization of alkyl(methacrylic) monomers using a novel initiator system
184975	An improved process for the preparation of microcapsular formulations of agrochemicals
187237	An improved process for the production of THPE [1,1',1"-tris (4'-hydroxyphenyl) ethane]
190819	A process for the preparation of polyurethane micorspheres

INFORMATION DIVISION

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 intellectual 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. Besides, the division conducts research on Chemical Informatics and Biodiversity Informatics.

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:

- Centralized e-mail with web mail facility
- Centralized antivirus for SMTP, Desktop, Gateway and servers
- Upgraded divisional uplinks to gigabit speed
- Deployment of Intrusion Prevention System
- Upgradation of 64 KBPS VSNL radio link to 256 KBPS
- Local hosting of all NCL web sites
- Development and deployment of an online recruitment system – the system has been successfully used in the recent recruitments of group IV staff at NCL
- Development and deployment of an online ARP system
- Development and deployment of an online conference management system

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 ARP
- Finance and Accounts
- Staff welfare club
- Resources for employees
- Students and career
- NCL alumni association
- Medical services

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. The user community consists of NCL scientists, research scholars as well as industrial and academic sector situated in and around Pune. Broadly, the activity includes procurement of printed, online version of documents, document delivery services, maintenance of stacks and users facilities. This is a continuous activity which supports research and hence requires continuous efforts. Library has taken steps towards developing a hybrid library. It has rich collection of current and old printed journals and books. Library is subscribing to many electronic resources. NISCAIR, on behalf of CSIR, has concluded agreements with 11 international publishers to have access to over 3300 journals across all the labs. Besides, library is subscribing major publisher's back files, Scopus and J Gate portal. Links for all these resources are provided on Library homepage, which is available on ncl@home, a local intranet. Library provides Document Delivery Services to in- house and industrial clientele. About 300 members which include post-graduate students, faculty members from various colleges, institutions and industries personnel use the NCL Library facility.

INFORMATION DIVISION

During 2005-06, Library procured 537 books and subscribed to 250 journals. The total library collection is 1,33,960 which includes books and bound volumes of journals. Exhibition of latest scientific and technical books was organized in Aug 2005. This provided an opportunity to scientists and students to browse the new books and recommend for purchase. Library catalogue, WebOPAC is now available on NCL's academic site http://www.ncl.res.in/ which helps to check availability of documents at NCL library from any corner of the world. "Reading Lounge", a new reading room for current periodicals, was inaugurated at the hands of Prof. M. M. Sharma, Chairman, Research Council of NCL in Mar 06.

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 send 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 and 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 makes 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 overall 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 monitors the expenditure twice 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

Training

Training on micropropagation :

An advanced training programme on micropropagation was organized by NCL during May 2-13, 2005. The aim of this programme was to encourage educated unemployed people to take up tissue culture as a viable venture and to train them for tissue culture industries. Teachers who are entrusted with designing and commissioning tissue culture laboratories at their respective colleges / institutes also participated in the programme. Total 8 persons participated in the Training Programme including students and teachers from various universities of Maharashtra. The training programme included training of basic laboratory techniques like glassware preparation, media preparation, and advanced training on micropropagation of horticulture and tree crops. The training programme also included the component on quality testing of plants using molecular markers and demonstrations on mycorrhizal association with tissue culture propagules.

Training on plant tissue culture:

An advanced training programme on 'Plant tissue culture' was organized by NCL from December 12-16, 2005 for a group of fifteen officials from Department of Horticulture, Jammu and Kashmir. The programme included lectures, practicals on different aspects of plant tissue culture such as general laboratory techniques, media formulations, and detailed training on micropropagation consisting of all stages such as selection of explant, surface sterilization, initiation of cultures, establishment of cultures, multiplication / proliferation of cultures, rooting in vitro / ex vitro, transfer to soil and hardening.

Training programme for researchers at GE's JW Technology Centre :

NCL organized a specialized training programme for researchers at GE's Jack F. Welch Technology Centre at Bangalore between 19 and 23 Dec 2005 at the company's site in Bangalore. The training programme aimed to provide a comprehensive and coherent introduction to polymer science and engineering. The course also leveraged the extensive consulting and research experience to provide specific and detailed insights on relevance and application of these concepts to plastic materials manufactured by GE Plastics. The course was attended by 34 researchers with diverse backgrounds — spread across chemistry, physics & materials science, and engineering. The course was designed and delivered with extensive use of electronic media, and was fashioned to be comparable in standards to global continuing education programmes. The course was well received and appreciated by the participants and GE-JFWTC management who rated the course at 6 on a scale of 0-7 in the course evaluation.

Workshop on design and scale-up of catalytic multiphase reactors:

NCL organized a two-day workshop on design and scale-up of catalytic multiphase reactors in January 2006. The workshop was aimed at providing up-to-date and comprehensive information on catalytic multiphase reactors to the participants. It was mainly meant for i) industry managers to enable more enlightened decision-making, ii) research engineers working in industries to enhance productivity, and iii) staff and Ph.D. students from Academia.

The workshop also offered an opportunity for discussing the progress of research in the design and scale-up of multiphase reactors with colleagues from industries and academia. About 20 participants both from industry and academia attended the workshop. The faculty members Prof. P.A. Ramchandran, Dr. R.V. Chaudhari and Dr. V.V. Ranade who conducted the workshop had an extensive experience in research and development. They shared their experience of implementing designs about multiphase reactors in practice. The workshop started with brief introduction on Emerging Multiphase Catalytic Processes. This was followed by detail lectures on "Theoretical concepts about Design and Scale-up of Multiphase Reactors". Case studies on industrial problems were also discussed. Finally, there was one to one interaction between the participants and faculty.

Student academic activities

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.

Ph.D. Degrees (2005)

Author	Title	University	Guide
Banerjee, P.	Intra molecular (3+2) Cycloaddition of Non stabilized Azomethine Ylide: Synthesis of Monotanine type Amaryllidaceae Alkaloids	Pune	Pandey, G.
Bera, S.	Synthetic Studies towards Slagenins B and C, Some Rigid Bicyclo Heterocyclic Scaffolds and Histrionicotoxin 235A	Pune	Gurjar, M.K.
Bhowmick, K.C.	Synthesis and Applications of a New C2 Symmetric Chiral 1, 3 Diol	Pune	Joshi, N.N.
Chaki, N.K.	Synthesis, Characterization and Electrochemical Studies of Metal Nanoclusters and their Possible Applications	Pune	Vijayamohanan, K.
Chatterjee, A.	Chral Ti(III) complexes for Catalytic Pinacol Coupling and Related Reactions	Pune	Joshi, N.N.
Chaube, V.D.	Synthesis, Characterization of Zeolites and Metal Complex Immobilized Mesoporous Alumina for Acylation, Alkylation and Oxidation Reactions	Pune	Singh, A.P.
Chaudhuri, S.R.	Synthetic Studies toward Nagahamide A, Sanglifehrin A, L-ido-Carba-Sugars and Hydroxyglimepiride	Pune	Gurjar, M.K.
Cherukupally, P.	Synthetic Studies towards Lipoic Acid, other Biologically Active Compounds and development of some useful Synthetic Methodogies	Pune	Chavan, S.P.
Chidambaram, M.	Organo Functionalized Zr- TMS Catalysts: Synthesis, Characterization and their Applications in Environmentally Benign Organic Transformations	Pune	Singh, A.P.
Dandekar, D.H.	Studies on DNA- Protein Interactions: HIV- 1 Tat as a Novel DNA Binding Transcriptional Activator	Pune	Ganesh, K.N. & Mitra, D.
Devassy, B.M.	Acid Catalysis using Zirconia- Supported Keggin Heteropoly Acids	Pune	Halligudi, S.B.
Dhage, S.R.	Studies on Non- Linear Current- Voltage (I-V) Characteristics in Doped SnO2 and Related Systems: Synthesis and Characterization	Pune	Ravi, V.
Gholap, S.G.	Hydrogel Membranes for Bio- Separations	Pune	Badiger, M.V.
Govande, V.V.	Studies in Synthesis and Transformations of Substituted Azetidin- 2- Ones	Pune	Deshmukh, A.R.A.S.
Govindaraju, T.	Conformationally Preorganized Carbocyclic and Backbone Extended Pyrrolidine Peptide Nucleic Acids: Chemical Synthesis and Biophysical Studies	Pune	Ganesh, K.N.
Gowd, E.B.	Effect of Additives and Co-monomers on Crystallization and Solid State Polymerization of Polyesters	Pune	Ramesh, C.
Gunjal, P.R.	Flow Modeling and Mixing in Packed Bed Reactor	IIT Bombay	Chaudhari, R.V.
Jayanthi, A.	Studies in Polycyclic Beta Lactam Synthesis	Pune	Deshmukh, A.R.A.S.

HUMAN RESOURCE MANAGEMENT

Author	Title	University	Guide
Jha, R.	Organic Reactions using Novel Reusable Solid Catalysts for the Synthesis of Fine/ Specialty Chemicals	Pune	Choudhary, V.R.
Jha, R.K.	Synthesis and Characterization of Mesoporous Materials and their Applications in Fine Chemical Synthesis	Pune	Singh, A.P.
Kandula, S.V.	Asymmetric Transformations Employing II face Stereoselection and Enantioselective Synthesis of Bioliogically Active Natural Products	Pune	Pradeepkumar
Kar, A.	Studies on Total Synthesis of Bioctive Natural Products Chaetomellic Acid A, 1, 7(Z)- Nonadecadiene -2, 3- Dicarboxylic Acid, 2-(beta carboxyethyl)- 3- Octylmaleic Anhydride, 2- Carboxymethyl- 3- 3- Hexylmaleic Anhydride, Nostoclide I, Sarkomycin, Homosarkomycin, Secocrispiolide, Mitomycin K and Mitomycin C	Pune	Argade, N.P.
Kar, S. B.	Studies on electromechanical sensors and actuators based on conducting polymers.	Pune	Kulkarni, B.D. & Radhakrishnan, S.
Khopkar, A.R.	Gas- Liquid Flows in Stirred Reactor	Mumbai	Pandit, A.B. & Ranade, V.V.
Kulkarni, N.G.	Studies in Polyester Forming Reactions	Pune	Sivaram, S.
Kuriakose, J.	Modeling, Characterization and Analysis of Systems Exhibiting Complex Spatiotemporal Dynamics and Patterns	Pune	Kulkarni, B.D.
Mahajan, V.A.	Design and Synthesis of Beta- Substituted- Gamma- Methylenefuranones, Related Lignan Analogues and Synthetic Studies Towards Saintopin	Pune	Wakharkar, R.D.
Manish Chandra, P.	Studies on the Catalysis and Post Translational Processing of Penicillin V Acylase	Pune	Suresh, C.G.
Pai, S.M.	Alkylation and Disproportionation of Aromatic Compounds over Molecular Sieve Catalysts	Pune	Satyanarayana, C.V.V.
Paraskar, A.S.	Enantioselective Synthesis of Bioactive Molecules via Metal- Catalyzed Asymmetric Reductions, Oxidations of Alkenes and Addition by Nucleophiles onto Imines	Pune	Sudalai, A.

HUMAN RESOURCE MANAGEMENT

Author	Title	University	Guide
Patel, R.	Compatibilisation by chain Coupling Agents: Engineering Polymers/ Thermotropic Liquid Crystalline Polymer Blends	Pune	Ponrathnam, S.
Priya, L.	Polyvinylidene Fluoride/ Clay Nanocomposites: Preparation and Characterization	Pune	Jog, J.P.(Ms)
Rahman, I.	Application of Artificial Intelligence Techniques to Chemical Engineering Problems	Nagpur	Kulkarni, B.D.
Ramakrishna, G.	Synthetic Studies Towards D(+)- Biotin and Development of other Useful Synthetic Methodologies	Pune	Chavan, S.P.
Ramalingam, S.	Synthetic Studies Towards Bioactive Molecules using Asymmetric Dihydroxylation and Organic Transformation using Yttria- Zirconia and other Heterogeneous Catalyst	Pune	Pradeep Kumar
Rohini Devi, D.	Biosynthesis of Polyhydroxyalkanoates by Bacillus Sp.	Pune	Rawal, S.K.
Sajeev, Y.	Electronic Resonances by the Method of Complex Scaling and Complex Absorbing Potentials within the Framework of Coupled Cluster Theory	Pune	Pal, Sourav.
Salokhe, S.G.	Studies on the Effect of a New Insect Growth Regulators on the Biology and Biochemical Parameters of Tribolium castaneum	Pune	Mukherjee, S.N. & Pal, J.K.
Sarkar, A.	Synthesis and Characterization of Polyamides, Polyimides and Polyesters containing Flexibilizing Groups	Pune	Wadgaonkar, P.P.
Sarmah, M.P.	Chemistry of Inositols: Investigation on the Solid State Acyl transfer Reactions of Inositol Derivatives and the Use of Sulfonate Protecting Groups for the Synthesis of Cyclitol Derivatives	Pune	Shashidhar, M.S.
Sattar, A.K.	Catalytic Transfer Hydrogenation of Organic Functional Groups using Ni, Ru Complexes and Asymmetric Induction using Racemic Chiral and Achiral Ligands and Synthetic Applications	Pune	Iyer, S.
Selvakannan, P. R.	New Methods for the Synthesis of Metal Nanoparticles	Pune	Sastry, M.

Author	Title	University	Guide
Senapati, S.	Biosynthesis and Immobilization of Nanoparticles and their Applications	Pune	Kumar, R.
Sharma, N.K.	Pyrrolidine and Pyrrolidinone Peptide Nucleic Acids: Synthesis and Comparative Studies of the DNA Binding Activities	Pune	Ganesh, K.N.
Shetty, S.G.	Study of Structural and Bonding Properties of Some Mixed Metal Clusters and Beta Zeolite using Density Functional Theory	Pune	Pal, Sourav
Shirude, P.S.	Synthesis and Biophysical Evaluation of Modified and Fluorescent PNAs: Applications in Antisense Therapeutics and Diagnostics	Pune	Ganesh, K.N.
Shiv Shankar, S.	New Methods for Synthesis of Inorganic Nanoparticles in Lipid Thin Films and in Solution	Pune	Sastry, M.
Srivastava, R.	Activation of Small Molecules for Cycloaddition and Coupling Reactions Over Transition Metal Catalysis	Pune	Srinivas, D.
Subramaniyam, S.	Structure and Properties of Nano-particulate Mica-Thermoplastic Composites	Pune	Radhakrishnan, S.
Wagholikar, S.G.	Studies on C-C Bond Formation Reactions of Organic Molecules Over Zeolites and other Molecular Sieve Catalysts	Pune	Sivasanker, S.

NCL Scientists recognized by different universities as research guides

Name	University
Dr. Adikane, H.V.	Pune
Dr. Agrawal, D.C.	Pune
Dr. Anil Kumar	Pune
Dr. Argade, N.P.	Pune, Mumbai
Dr. Asthana, (Mrs.) Saroja	Pune
Dr. Avadhani, Ver Chilukuri	Pune
Dr. Badiger, M.V.	Pune
Dr. Bakre, P.P.	Pune
Dr. Bastawde, K.B.	Pune, Shivaji University, Kolhapur
Dr. Bhadbhade, M.M.	Pune, Bhavnagar

Name	University
Dr. Bhattacharya, A.K.	Pune
Dr. Borate, H.B.	Pune
Dr. Chanda, (Mrs) Bhanu	Pune
Dr. Chandwadkar, (Ms) A.J.	Pune
Dr. Chaudhari, R.V.	Pune, Mumbai, Shivaji University, Kolhapur
Dr. Chavan, S.P.	Pune
Dr. Chumbhale, V.R.	Pune, Shivaji University, Kolhapur, Swami Ramanand Tirth University, Nanded
Dr. Deshmukh, A.R.A.S.	Pune
Dr. Deshmukh, M.N.	Osmania
Dr. Deshpande, M.V.	Pune, Shivaji University, Kolhapur, North Maharashtra University, Jalgaon
Dr. Deshpande, R.M.	Pune
Dr. Dongare, M.K.	Pune, Mumbai
Dr. Gadre, R.V.	Pune
Dr. Gaikwad, (Mrs.) Sushama Mugutarao	Pune
Dr. Gaikwad, A.G.	Pune
Dr. Ganapathy, S.	Pune
Dr. Ganesh, K.N.	Pune
Dr. Garnaik, (Ms.) B.	Pune
Dr. Gokhale, D.V.	Pune, Shivaji University, Kolhapur
Dr. Gopinath, C.S.	Pune
Dr. Gupta, (Mrs) Vidya	Pune
Dr. Gupte, S.P.	Pune
Dr. Gurjar, M.K.	Pune, Mumbai, Osmania University, Hyderabad
Dr. Guruswamy, K	Pune, IIT-Mumbai
Dr. Halligudi, S.B.	Pune, Bhavnagar
Dr. Hazra, (Mrs) Sulekha	Pune
Dr. Hazra, B.G.	Pune
Dr. Hegde, S.G.	Shri Ramanand Tirth University, Nanded
Dr. Hotha, Srinivas	Pune.
Dr. Idage, B.B.	Pune
Dr. Iyer, Suresh	Pune

HUMAN RESOURCE MANAGEMENT

Name	University
Dr. Jaganathan, R.	Pune
Dr. Jayaraman, V.K.	Pune
Dr. Jog, (Mrs) J.P.	Pune, Shivaji University, Kolhapur
Dr. Joshi, (Mrs) S.P.	Pune
Dr. Joshi, N.N.	Pune
Dr. Joshi, P.N.	Swami Ramanand Tirth University, Nanded
Dr. Joy, P.A.	Pune
Dr. Kalkote, U.R.	Pune
Dr. Kelkar, A.A.	Pune
Dr. Khan, B.M.	Pune
Dr. Khan, M.I.	Pune, North Maharashtra University, Jalgaon
Dr. Kharul, U.K.	Pune
Dr. Khire, J.M.	Pune
Dr. Kolar, (Mrs) Lalitha Sunilkumar	Pune
Dr. Krishnan, S.	Pune
Dr. Kshirsagar Suresh Tukaram	Pune
Dr. Kulkarni, B.D.	Pune, Mumbai, Nagpur, Shivaji University, Kolhapur
Dr. Kulkarni, M.G.	Pune, Mumbai
Dr. Kulkarni, R.A.	Pune
Dr. Kumar, (Mrs) V.A.	Pune
Dr. Lachke, Anil	Pune
Dr. Lele, A.K.	Pune, Mumbai
Dr. Manikandan, P.	Pune
Dr. Mayadevi, (Mrs) S.	Pune, Mumbai and Shivaji University, Kolhapur
Dr. Mohapatra, D.K.	Pune
Dr. Deshmukh, (Ms) Sumedha Sharad	Pune
Dr. Mukherjee, S.N.	Pune
Dr. Mulla, I.S.	Pune
Dr. Nadgauda, (Mrs) Rajani	Pune
Dr. Natarajan, Upendra	IIT-Mumbai
Dr. Natu, A.A.	Pune, Shivaji University, Kolhapur
Dr. Pal, Sourav	Pune

HUMAN RESOURCE MANAGEMENT

Name	University
Dr. Pandey, Ganesh	Pune, Osmania University, Hyderabad, Shivaji University, Kolhapur
Dr. Pedireddi, V.R.	Pune
Dr. Ponrathnam, S.	Pune
Dr. Pore, (Mrs) V.S.	Pune
Dr. Prabhune, (Mrs) Asmita	Pune
Dr. Prasad, B.L.V.	Pune
Dr. Prasad, S.D.	Pune
Dr. Pundle, (Ms) Archana	Pune
Dr. Puranik, (Mrs) V.G.	Pune
Dr. Radhakrishnan, S.	Bharati Vidyapith, Pune, Pune
Dr. Rajamohanan, P.R.	Pune
Dr. Rajiv Kumar	Pune
Dr. Ramana, C.V.	Pune
Dr. Ramaswamy, (Mrs) Veda	Pune
Dr. Ramesh, C.	Pune
Dr. Ranade, V.V.	Pune, Mumbai
Dr. Rao, (Mrs) Mala	Pune, Shivaji University, Kolhapur
Dr. Ravi Kumar, V.	Pune
Dr. Ravi, Venkatanarayanan	Pune
Dr. Rawal, S.K.	Pune
Dr. Rele, (Mrs.) M.V.	Pune
Dr. Rode, C.V.	Pune, Swami Ramanand Tirth University, Nanded
Dr. Rojatkar, S.R.	Pune
Dr. Sainkar, S.R.	Pune
Dr. Sanjayan, G.J.	Pune
Dr. Sarkar, Dhiman	Pune
Dr. Sastry, Murali	Pune
Dr. Satyanarayana, C.V.V.	Pune
Dr. Seetalaxman, (Mrs) R.	Pune
Dr. Shashidhar, M.S.	Pune
Dr. Singh, A.P.	Pune
Dr. Singh, R.P.	Pune

HUMAN RESOURCE MANAGEMENT

Name	University
Dr. Sivaram, S.	Pune, Mumbai, IIT-Mumbai
Dr. Srinivas, D.	Pune, Bhavnagar
Dr. Srinivasan, K.V.	Pune
Dr. Sudalai, A.	Pune
Dr. Suresh, C.G.	Pune
Dr. Suryavanshi Gurunath	Pune
Dr. Tambe, Sanjeev	Pune
Dr. Tare, (Mrs) V.S.	Shivaji University Kolhapur, North Maharashtra University, JalgaonYashwantrao Chavan Maharashtra Open University, Nashik
Dr. Tewari, R.	Pune
Dr. Thengane, (Mrs.) S.R.	Pune
Dr. Thomas Daniel	Pune
Dr. Tripathi, P.K.	Pune
Dr. Umbarkar, (Ms) Shubhangi Balchandra	Pune
Dr. Varma, A.J.	Pune
Dr. Vijayamohanan, K.	Pune
Dr. Wadgaonkar, P.P.	Pune, Shivaji University, Kolhapur
Dr. Waghmare, Kashinath	Pune
Dr. Wakharkar, (Mrs) R.D.	Pune

PUBLICATION AND SCIENCE COMMUNICATION

The Publication and Science Communication

The Publication and Science Communication (PSC) unit manages i) addition / modifications of applications and content for NCL website (both English and Hindi versions) ii) addition / modifications of applications and content for NCL local intranet, iii) Press releases, iv) Digitization of archives, v) Publications, vi) Still and video photography, CSIR and NCL films, and vii) Liaison with CSIR. The effective use of information technology is being made to collect, retrieve and disseminate the data.

Website:

The unit manages the content on the NCL website (http://www.ncl-india.org). It also makes applications, modifies the existing applications as per the requirement and updates the website continuously so as to provide latest information to the user may it be research publications, patents, press releases, organisation of conferences, symposia or communicating the exiting research happening at NCL through R&D feature. Hindi version of the NCL website is also developed. The static pages of the Hindi version were also updated periodically. Webpage on right to information (RTI) act was added to the NCL website this year. NCIM database was revamped completely to enable the NCIM staff to add / delete the entries of microbial species in the database.

Conference management system:

The unit assists the organisers of the conferences to manage various aspects of conference management through launching the website for the particular conference. The website for managing conference is mainly divided in two parts – one static pages and other dynamic pages. Static pages are mainly informative whereas dynamic pages are interactive wherein the user can register, upload / withdraw abstract, pay registration fee, book hotel accommodation, etc. Besides, the conference organisers were given continuous support on various aspects of printing the conference material both in hard copy soft copy – CD format. The area in and around auditorium was made wi-fi enabled and internet surfing facility was made available to the participants. Workshop on new solid state NMR methods and materials characterisation, International symposium on ionic polymerization, and Joint International Conference on Building Bridges, Forging Bonds for 21st Century Organic Chemistry and Chemical Biology (ACS-CSIR OCCB 2006) were organised using the conference management system.

Intranet / ncl@home:

New modules like photo gallery and CSEU reports were added to ncl@home. Revision of booking lecture hall page was coordinated. The modules such as safety page, students academic committee page, job vacancy page, NCL in news page, archive page, publication page, DG's page, General interest/ CSIR news/ articles, major events page, science day posters, medical center page with the information on authorized doctors, hospitals and health related articles were updated continuously. NCL/ CSIR office forms and announcements page was modified and Administrative Section on was encouraged to use revised page which has reduced the load on mail server and at the same time user can browse the list of such uploaded forms and circulars. A database for mailing list was prepared. The database has the various categories like 'Central /State Agency' , 'CSIR HQ / CSIR Lab', 'Current NCL HoD', 'Foreign Company', 'Former HoDs / Directors', 'Hindi advisory committee for ministry of S&T', 'IIT', 'Indian Company', 'NCL alumni', 'Press / Media', 'Pune – local', 'Research Council Member', 'RF Donor' and 'University'. The database has the facility to categorize one address under four categories.

Press releases:

The unit releases press notes on all important occasions and events. It communicates important R&D reports for publication in CSIR News and CSIR Samachar. The unit also attends to press enquiries from local media, magazines dedicated to chemical industries, etc.

PUBLICATION AND SCIENCE COMMUNICATION

Digitisation of archives:

The unit digitised and archived several NCL project reports and CSIR and NCL review reports. The posters displayed by the students on the occasion of National Science Day were also archived. The unit also digitised summary/ synopsis pages of around 1000 theses from NCL library.

Publications:

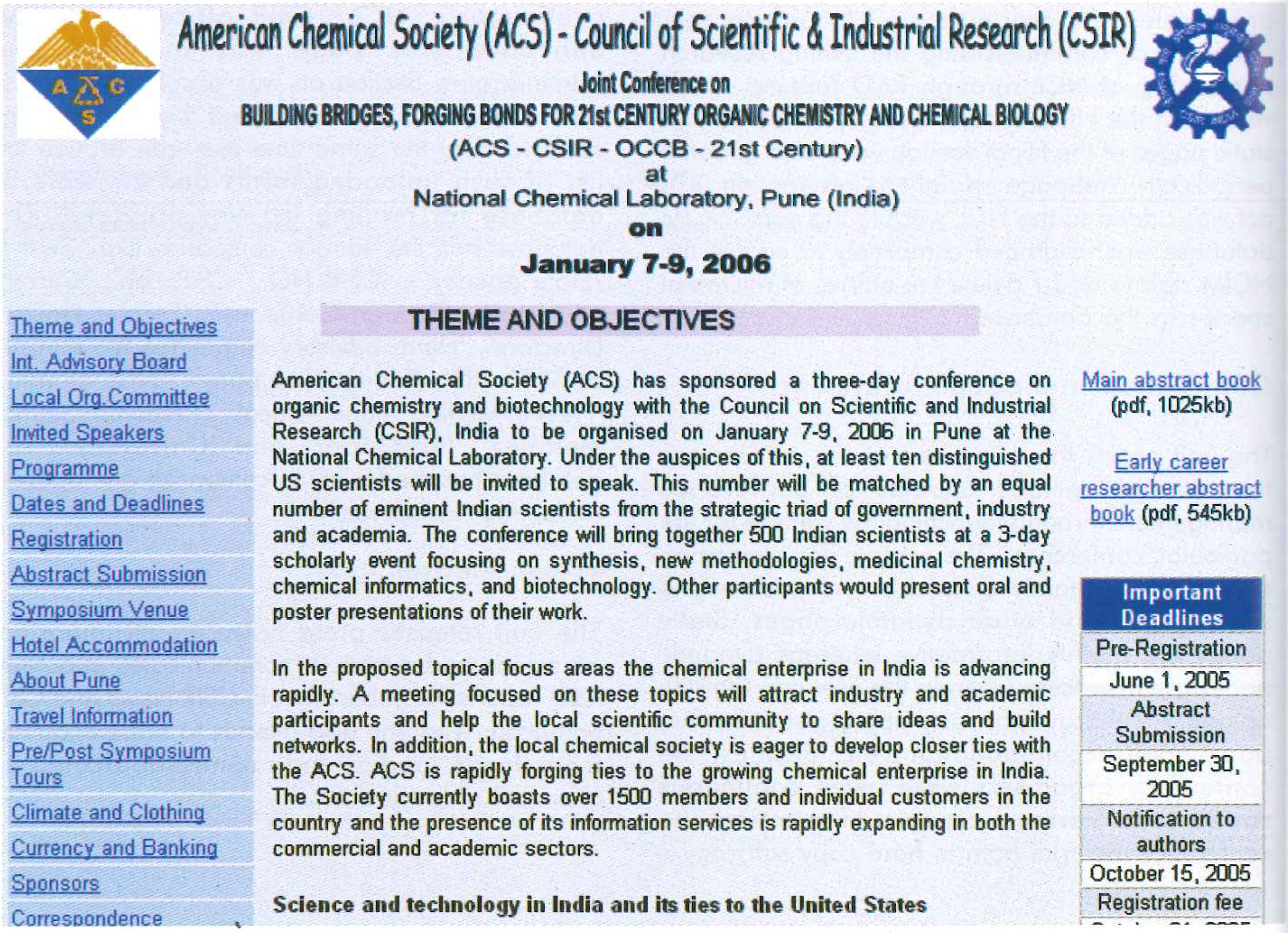
The unit brings out NCL annual report, besides providing customised NCL reports for various publications brought out by CSIR and other publishing agencies including CSIR annual report.

Audio, Video, Still photography and NCL film:

The Unit coordinated the still and video shooting of the events organized at NCL. Some of these photographs were also uploaded in photo gallery page at ncl@home, the local Intranet. The Unit organized video shooting of CSIR films on 'chemical technology' and 'herbal therapeutics' and the TV serial on Nanoscience and NCL part of Pest Control Association of India film. Video shooting organized by electronic media was also coordinated. The NCL input for CSIR film on 'drugs for poor' was provided to the film coordinator (CDRI, Lucknow). The walkthrough film on NCL was also produced.

Liaison with CSIR:

The unit attended to various queries of CSIR Hq. related to information dissemination. The unit also provided NCL information for CSIR website.



American Chemical Society (ACS) - Council of Scientific & Industrial Research (CSIR)

Joint Conference on
BUILDING BRIDGES, FORGING BONDS FOR 21st CENTURY ORGANIC CHEMISTRY AND CHEMICAL BIOLOGY
(ACS - CSIR - OCCB - 21st Century)
at
National Chemical Laboratory, Pune (India)
on
January 7-9, 2006

- Theme and Objectives
- Int. Advisory Board
- Local Org.Committee
- Invited Speakers
- Programme
- Dates and Deadlines
- Registration
- Abstract Submission
- Symposium Venue
- Hotel Accommodation
- About Pune
- Travel Information
- Pre/Post Symposium Tours
- Climate and Clothing
- Currency and Banking
- Sponsors
- Correspondence

THEME AND OBJECTIVES

American Chemical Society (ACS) has sponsored a three-day conference on organic chemistry and biotechnology with the Council on Scientific and Industrial Research (CSIR), India to be organised on January 7-9, 2006 in Pune at the National Chemical Laboratory. Under the auspices of this, at least ten distinguished US scientists will be invited to speak. This number will be matched by an equal number of eminent Indian scientists from the strategic triad of government, industry and academia. The conference will bring together 500 Indian scientists at a 3-day scholarly event focusing on synthesis, new methodologies, medicinal chemistry, chemical informatics, and biotechnology. Other participants would present oral and poster presentations of their work.

In the proposed topical focus areas the chemical enterprise in India is advancing rapidly. A meeting focused on these topics will attract industry and academic participants and help the local scientific community to share ideas and build networks. In addition, the local chemical society is eager to develop closer ties with the ACS. ACS is rapidly forging ties to the growing chemical enterprise in India. The Society currently boasts over 1500 members and individual customers in the country and the presence of its information services is rapidly expanding in both the commercial and academic sectors.

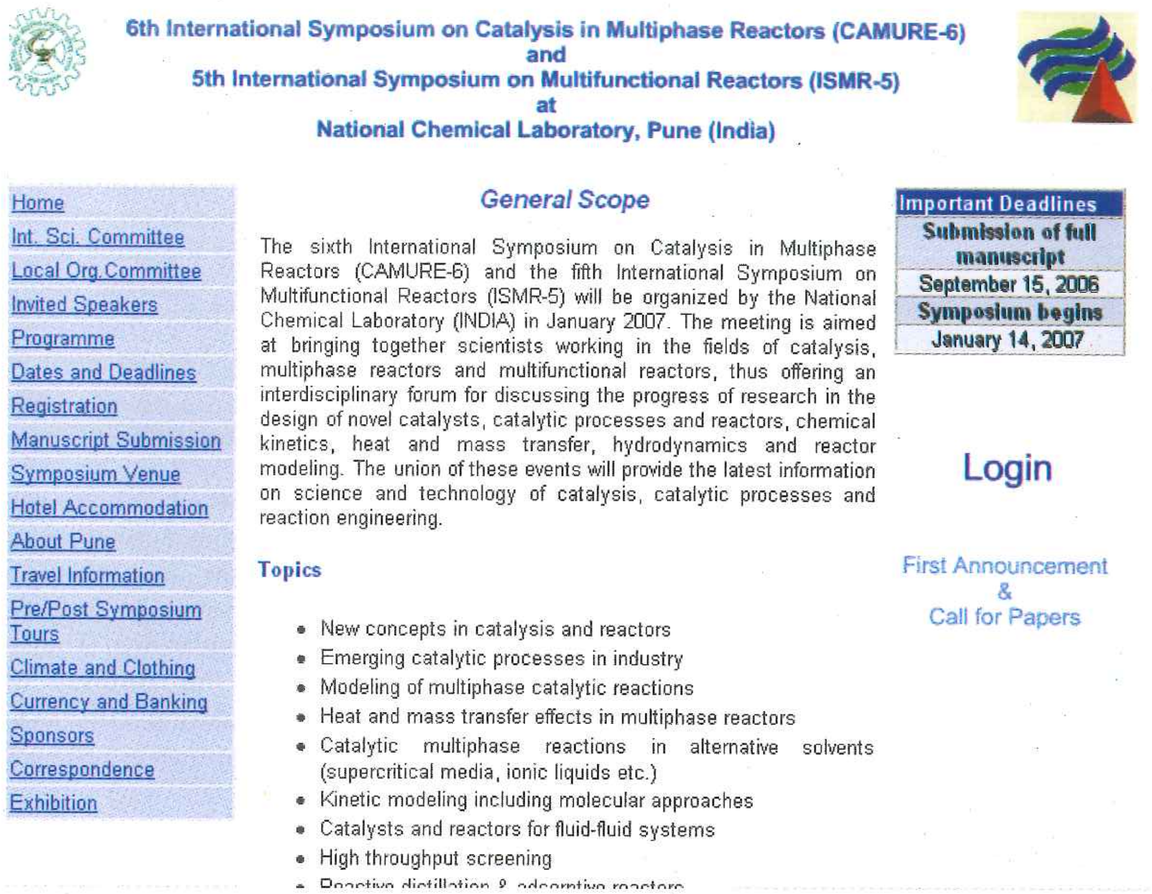
Science and technology in India and its ties to the United States

Main abstract book (pdf, 1025kb)

Early career researcher abstract book (pdf, 545kb)

Important Deadlines
Pre-Registration
June 1, 2005
Abstract Submission
September 30, 2005
Notification to authors
October 15, 2005
Registration fee

PUBLICATION AND SCIENCE COMMUNICATION



6th International Symposium on Catalysis in Multiphase Reactors (CAMURE-6)
and
5th International Symposium on Multifunctional Reactors (ISMR-5)
at
National Chemical Laboratory, Pune (India)

- Home
- Int. Sci. Committee
- Local Org.Committee
- Invited Speakers
- Programme
- Dates and Deadlines
- Registration
- Manuscript Submission
- Symposium Venue
- Hotel Accommodation
- About Pune
- Travel Information
- Pre/Post Symposium Tours
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- Currency and Banking
- Sponsors
- Correspondence
- Exhibition

General Scope

The sixth International Symposium on Catalysis in Multiphase Reactors (CAMURE-6) and the fifth International Symposium on Multifunctional Reactors (ISMR-5) will be organized by the National Chemical Laboratory (INDIA) in January 2007. The meeting is aimed at bringing together scientists working in the fields of catalysis, multiphase reactors and multifunctional reactors, thus offering an interdisciplinary forum for discussing the progress of research in the design of novel catalysts, catalytic processes and reactors, chemical kinetics, heat and mass transfer, hydrodynamics and reactor modeling. The union of these events will provide the latest information on science and technology of catalysis, catalytic processes and reaction engineering.

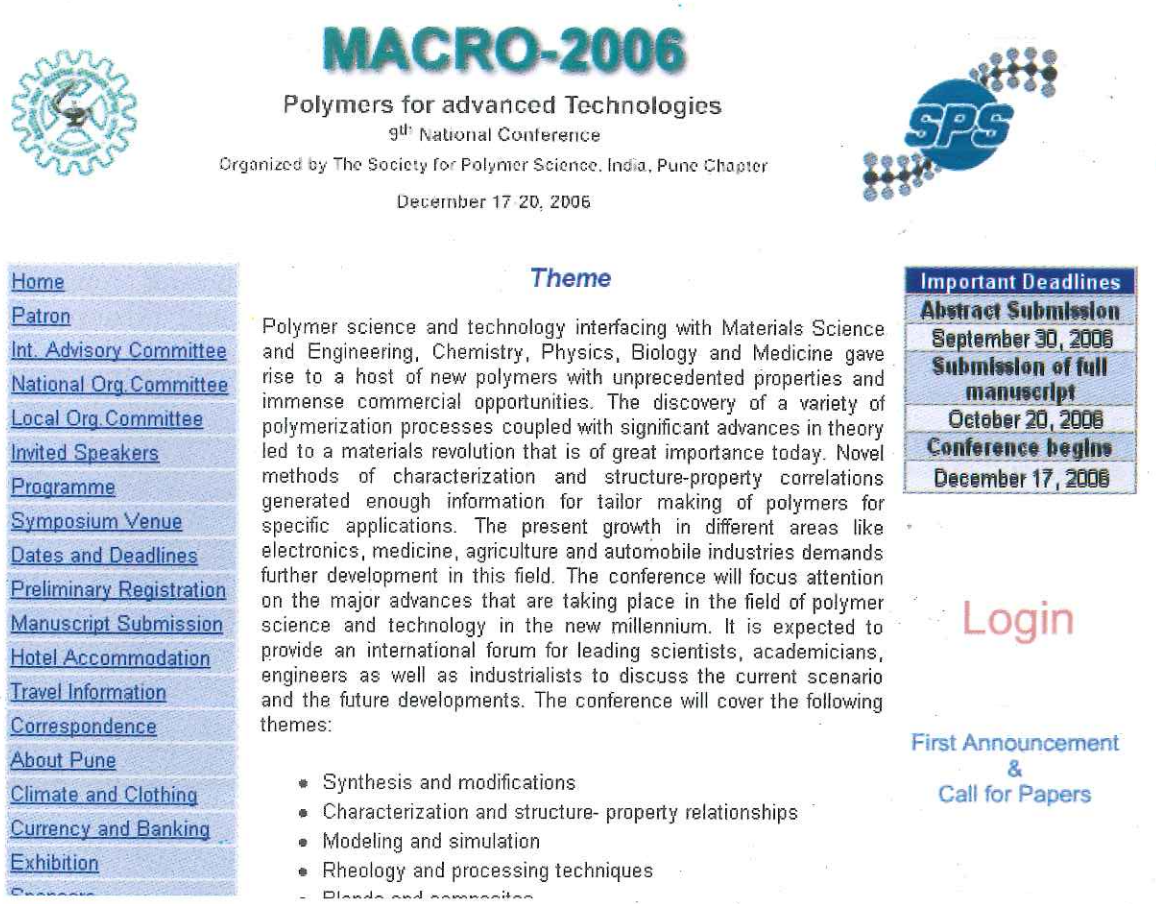
Topics

- New concepts in catalysis and reactors
- Emerging catalytic processes in industry
- Modeling of multiphase catalytic reactions
- Heat and mass transfer effects in multiphase reactors
- Catalytic multiphase reactions in alternative solvents (supercritical media, ionic liquids etc.)
- Kinetic modeling including molecular approaches
- Catalysts and reactors for fluid-fluid systems
- High throughput screening
- Reactive distillation & adsorptive reactors

Important Deadlines
Submission of full manuscript
September 15, 2006
Symposium begins
January 14, 2007

Login

First Announcement
&
Call for Papers



MACRO-2006

Polymers for advanced Technologies
9th National Conference
Organized by The Society for Polymer Science, India, Pune Chapter
December 17-20, 2006

- Home
- Patron
- Int. Advisory Committee
- National Org.Committee
- Local Org.Committee
- Invited Speakers
- Programme
- Symposium Venue
- Dates and Deadlines
- Preliminary Registration
- Manuscript Submission
- Hotel Accommodation
- Travel Information
- Correspondence
- About Pune
- Climate and Clothing
- Currency and Banking
- Exhibition

Theme

Polymer science and technology interfacing with Materials Science and Engineering, Chemistry, Physics, Biology and Medicine gave rise to a host of new polymers with unprecedented properties and immense commercial opportunities. The discovery of a variety of polymerization processes coupled with significant advances in theory led to a materials revolution that is of great importance today. Novel methods of characterization and structure-property correlations generated enough information for tailor making of polymers for specific applications. The present growth in different areas like electronics, medicine, agriculture and automobile industries demands further development in this field. The conference will focus attention on the major advances that are taking place in the field of polymer science and technology in the new millennium. It is expected to provide an international forum for leading scientists, academicians, engineers as well as industrialists to discuss the current scenario and the future developments. The conference will cover the following themes:

- Synthesis and modifications
- Characterization and structure- property relationships
- Modeling and simulation
- Rheology and processing techniques
- Blends and composites

Important Deadlines
Abstract Submission
September 30, 2006
Submission of full manuscript
October 20, 2006
Conference begins
December 17, 2006

Login

First Announcement
&
Call for Papers

RESEARCH PLANNING AND AUDIT

Research Planning & Audit Unit

Research Planning & Audit Unit (RPA) was 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. Highlights of the major activities during the year 2005 -06 are:

In-house projects

RPA is associated with the screening, evaluation and providing funding for the new projects within the lab. During the year, new proposals were invited and reviewed. In addition, monitoring and review of existing In-house research programmes was undertaken. During the year 2005-06, four review meetings / seminars were conducted to audit the technical and scientific performance of 27 ongoing projects.

Start-up grants

Two new scientists joined during the year 2005-06 were given a start up grant of Rs. 6 lakhs/year for 2 years. In addition, the start-up grants for four scientists (who joined in the previous year) were continued into the second year. The total funding to all In-house projects (including start-up grant) during 2005-06 was Rs. 73 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, to review and monitor the scientific and financial progress and provides the necessary data support for the procurement of equipments and instruments.

The highlight of the activity was the preparation of a comprehensive "Tenth Five~~-year plan~~ (2002-07)-Annual Plan document for the X Five-year plan (2002-07) projects, which included a review of all the networked and non network projects at NCL and an annual plan for 2006-07. The report was submitted to CSIR as a part of the major review by the Planning Commission.

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 projects at NCL. During the audit for 2004-05 held in June - July 2005, with the quantity and quality of information provided, many existing and outstanding objections and paras were dropped.

Research Council meetings

The unit has been involved in arranging and conducting Research Council meetings at NCL. During the last one year, two meetings were conducted and actions taken to follow-up and implement the recommendations. The unit also made presentations on the "Analysis of Major publicly funded projects during 2003-05"

Liaison with CSIR

The unit liaises with CSIR in providing timely information on many aspects of the laboratory, which may be required from time to time. Moreover, the consolidated performance reports on two major network projects and Research utilization data of NCL were sent to CSIR on a quarterly basis. This involves providing current status on the all on-going projects, highlighting the work done, major achievements in basic and applied science, outputs (patents - applied for and granted), funds generated through technical services, etc.

SAFETY MANAGEMENT

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, divisional safety committees also exist with member representations from scientific staff and research students.

During the year, three 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

To sensitize newly joined research students, project assistants and scientists, the talks were delivered at three safety orientation courses organized by the Student Academic Committee on the safety in a chemical laboratory, initiatives taken by the safety unit, information sources and facilities; their duties and responsibilities.

Fire Safety

A live demonstration and hands on practical training for tackling small fires and the use of portable fire extinguishers, was organised three times during the year and more than 350 scientists and students were trained.

Upgradation of infrastructure

The health, safety and environment is protected and the systems were 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. Fifteen new fume hoods were installed while many more labs were equipped with eye wash fountains and safety showers. The solvent storage facility was renovated and safety systems upgraded.

National Safety Day

National safety day was observed on 6th March 2006. As a part of this event, various programmes like — a live demonstration and hands-on practical training programme for tackling small fires and using portable fire extinguishers — were organized. The event was aimed particularly at new entrants to the laboratory and members of the staff who wanted to update their skill in fire fighting. A team of external experts, in coordination with NCL security, conducted the programme in three batches. It was attended by a large number of research students and project staff.

SAFETY MANAGEMENT

Mr. R. Veeraraghvan, Head, Fire Safety Department (Retd, Hindustan Petroleum Corporation Limited (HPCL), Mumbai delivered a special lecture on 'Safety and its management in a chemical laboratory'. Head, Safety management and divisional safety coordinators presented the annual safety reports and work done for upgradation of safety in respective divisions.

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 were also organized for various educational and industrial establishments.

ENGINEERING SERVICES UNIT

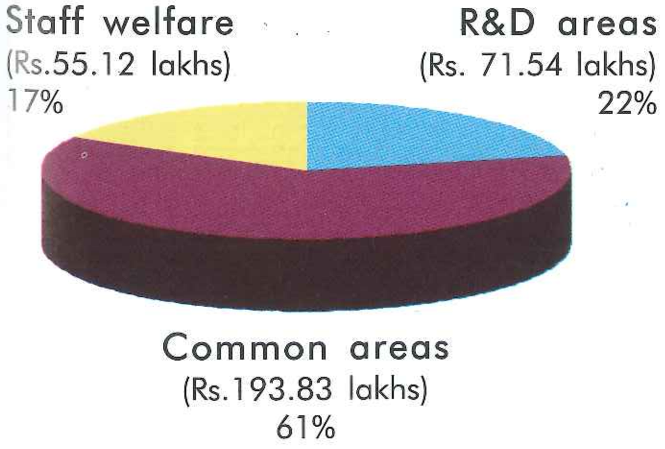
ENGINEERING SERVICES UNIT

The Unit renovated labs in Biochemical Sciences Division and Centre for Material Characterization. New labs were made for housing analytical equipments in Pilot Plant –III and for R & D work in Pilot Plant –I. Substations I and II were augmented and its load was enhanced from 2000 KVA 3000 KVA. Reading room facility was created in library. Beside the Board Room attached to the Director's office was renovated and the furniture was made as per the requirement for C & P and Accounts Section. Bins for segragation of returned material were created in auction yard of Store and Purchase Section. The glass blowing unit is renovated. The machine were painted and reconditioned. The windows were changed for better air-circulation and flooring was changed with new tiles.

As a part of colony maintenance, the works related to rewiring and water-proofing of staff quarters were completed. Maintenance of street-lighting and repair of drainage lines in residential colony was carried out.

The Glass Blowing Unit received more than 2200 job cards with each card containing up to 100 small jobs. These included special projects that required glass apparatus with innovative ideas, new fabrication work like distillation sets and filtration sets, new jobs like manufacturing of round bottom flasks, columns, viscometers, special stirrers, maintenance work like repairing of broken glasswares and various minor jobs

Total works & services handled by Engineering Services Unit in terms of value (Rs in Lakhs) during the year 2005-06



Electrical sub-station

Library reading hall

Establishment section

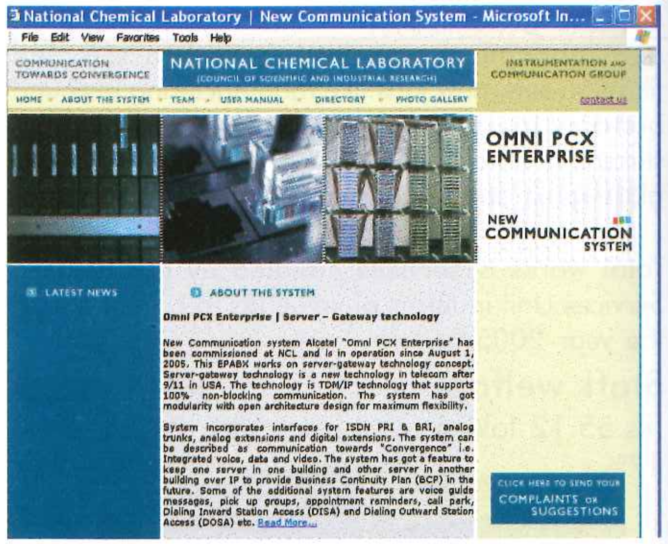
COMMUNICATION SYSTEM

COMMUNICATION SYSTEM

Commissioning of Omni PCX enterprise – a server gateway technology

New Communication system Alcatel "Omni PCX Enterprise" has been commissioned at NCL and is in operation since 1 August 2005. This EPABX works on server-gateway technology concept. Server-gateway technology is the latest technology in telecom sector. The technology is Time Division Multiplexing (TDM) / IP technology that supports 100% non-blocking communication. The system has got modularity with open architecture design for maximum flexibility. This technology is expected to have lifetime of fifteen years. NCL is the first CSIR Laboratory to commission this server-gateway EPABX technology for its communication solutions. System incorporates interfaces for ISDN PRI & BRI, analog trunks, analog extensions and digital extensions. The system can be described as communication towards "Convergence" i.e., integrated voice, data and video and has got a feature to keep two servers at a distance over IP to provide Business Continuity Plan (BCP). Some of the additional system features are voice guide messages, pick up groups, appointment reminders, Call Park, Dialing Inward Station Access (DISA) and Dialing Outward Station Access (DOSA).

System is equipped for 800 analog extensions and 64 digital extensions. Voice guide messages like "Press 5 for Call Back" have been embedded in the system hardware which is the unique feature offered by Alcatel. The system is fully equipped for 29 party multi conference facility. These parties can be the NCL extensions, parties in India or abroad. Such 13 conferences can be conducted simultaneously at NCL. The system backbone can be used for video conference solutions by using ISDN BRI hardware incorporated in the system. Omni PCX Enterprise server gateway technology is a totally modular technology and can be geared up for applications for analog extensions, digital extensions, IP phones, wireless phones and wireless IP phone and also the connectivity to mobile phones. Level DID facility with prefix number 2590 for NCL has been enabled for all extensions at NCL.



Omni PCX Enterprise | Server – Gateway technology

New Communication system Alcatel "Omni PCX Enterprise" has been commissioned at NCL and is in operation since August 1, 2005. This EPABX works on server-gateway technology concept. Server-gateway technology is a new technology in telecom after 9/11 in USA. The technology is TDM/IP technology that supports 100% non-blocking communication. The system has got modularity with open architecture design for maximum flexibility.

System incorporates interfaces for ISDN PRI & BRI, analog trunks, analog extensions and digital extensions. The system can be described as communication towards "Convergence" i.e. Integrated voice, data and video. The system has got a feature to keep one server in one building and other server in another building over IP to provide Business Continuity Plan (BCP) in the future. Some of the additional system features are voice guide messages, pick up groups, appointment reminders, call park, Dialing Inward Station Access (DISA) and Dialing Outward Station Access (DOSA) etc. Read More...

प्रशासन, वित्त एवं लेखा, भण्डार एवं क्रय

प्रशासन, वित्त एवं लेखा, भण्डार एवं क्रय

सामान्य प्रशासन

प्रशासन

वर्ष के दौरान निम्नलिखित प्रमुख कार्य सम्पादित किए गए :-

- वर्ष 2005-06 के दौरान जारी किए गए विज्ञापन हेतु वेबसाइट द्वारा ऑनलाइन भर्ती के दूसरे प्रयास में उसे (ऑनलाइन भर्ती) अधिक प्रभावी एवं सफल बनाया गया । गत वर्ष इस प्रणाली के प्रयोग में आई कठिनाइयों को देखते हुए उसमें परिवर्तन किया गया । वैज्ञानिकों के 13 पदों पर भर्ती का कार्य वेबसाइट पर आधारित प्रणाली का प्रयोग करते हुए सफलतापूर्वक पूरा किया गया ।
- प्रबंधन परिषद की बैठकों का आयोजन किया गया ।
- मूल्यांकन वर्ष 2004-05 हेतु 97 तकनीकी एवं सहायक स्टाफ का मूल्यांकन किया गया । इसके अलावा वर्ष 2003-04 के लिए 60 वैज्ञानिकों का मूल्यांकन भी पूरा किया गया ।
- वर्ष के दौरान 75 वैज्ञानिकों की विदेशों में प्रतिनियुक्ति का कार्य सम्पन्न हुआ ।
- लगभग 18, 000/- निजी दावे, छुट्टी के आवेदन एवं संबंधित दस्तावेजों पर कार्रवाई की गई । उनमें से 75 प्रतिशत दावों पर कार्रवाई करके निर्धारित समय के अन्दर उनका निपटारा किया गया।

वित्त एवं लेखा

वर्ष के दौरान निम्नलिखित प्रमुख कार्य सम्पादित किए गए :-

- स्टाफ के सभी कर्मचारियों के सामान्य भविष्य निधि/अंशदायी भविष्य निधि खातों को अद्यतन किया गया, स्टाफ को नए वित्त वर्ष के पहले दिन उनके सार्वजनिक भविष्य निधि खातों के वार्षिक विवरण जारी किए ।
- लगभग 500 बाहरी सहायता प्राप्त परियोजनाओं से संबंधित वित्त एवं लेखा का कार्य किया गया ।
- वित्तीय आंकड़े (डेटा)/ रिपोर्ट सीएसआईआर मुख्यालय, निदेशक, विभिन्न एजेंसियाँ, वैज्ञानिक आदि को प्रस्तुत किए गए ।
- सभी प्रभागों से वित्त संबंधित प्राप्त विविध प्रस्तावों जैसे- करार, कार्य-प्रस्ताव, वेतन नियतन मामले, निजी फाइलें, प्रतिनियुक्ति, कोर्ट द्वारा जब्ती आदि की जाँच-पड़ताल की गई ।
- पेंशन के मामलों का निपटारा निर्धारित अवधि में किया गया ।
- सम्पूर्ण लेखा (इम्पैक्ट) एवं संबंधित रजिस्टरों को अद्यतन रखा गया।
- विविध प्रकार के वाउचर तैयार किए गए (भुगतान 18,156, प्राप्ति, 5,481 अंतरण प्रविष्टि 380)
- वर्ष के दौरान अधिशेष निधि निवेश पर प्राप्त ब्याज से रु. 150.075 लाख का प्रयोगशाला आरक्षित निधि निर्माण किया गया था ।

निधि का उपयोग :-

(क) अग्रेनित अनुदान (30.09.2005 तक)		
परियोजना	राशि	उपयोग का प्रतिशत
I) नेटवर्क	124.674	100
II) नॉन-नेटवर्क	250.000	100

(ख) वार्षिक अनुदान (31.03.2006 तक)		
परियोजना	राशि	उपयोग का प्रतिशत
I) नेटवर्क	632.318	100
II) नॉन-नेटवर्क	4965.342	100

(ग) प्रयोगशाला आरक्षित निधि — रु. 266.409 लाख

(घ) निमिटली परियोजनाएँ — रु. 470.422 लाख

(च) बाहरी निधि-सहायता प्राप्त परियोजनाऍं — रु. 2049.933 लाख

ओबी मदों का निपटान

	(रुपए लाख में)			
वर्ष के दौरान किए गए समायोजन	सरकारी	निजी	टीए/एलटीसी	स्थानीय
	1.432	1804.835	45.871	32.201

भण्डार एवं क्रय

वर्ष के दौरान निम्नलिखित प्रमुख कार्य सम्पादित किए गए :-

- स्थानीय क्रय की बारम्बारता कम करने के लिए भण्डार के स्टॉक एवं नई मदों में बढ़ोतरी गई ।
- वर्ष 2002-03 तक की आपूर्ति की सभी बकाया का निपटान/ समायोजन किया गया ।
- विभिन्न प्रकार की अधिक मूल्य वाली मदों की प्राप्ति हेतु 10 प्रेस निविदाएँ जारी की गईं ।
- भण्डार एवं क्रय हेतु फाइलें रखने के लिए ऑप्टीमाइजर्स से युक्त एक नया अभिलेख कक्ष बनाया गया ।

प्रशासन, वित्त एवं लेखा, भण्डार एवं क्रय

भण्डार एवं क्रय : सम्पादित किए गए कार्य :-

मद	संख्या		मूल्य (रुपए करोड़ में)	
	2004-05	2005-06	2004-05	2005-06
कुल प्राप्त एवं कार्रवाई किए गए माँगपत्र	2292	2322	29.81	34.03
कुल दिए गए ऑर्डर (आयातीत)	767	763	20.73	26.72
कुल दिए गए ऑर्डर (स्वदेशी)	4275	1258(I)	9.89	8.04
कुल प्राप्त सामान्य कन्साइनमेन्ट (आयातीत)	1007	917	11.31	24.04
कुल प्राप्त सामान्य कन्साइनमेन्ट (स्वदेशी)	2376	2112	8.57	7.79
स्थानीय खरीद (ऑनलाइन आरसी सहित)	8852	8458	2.29	2.30
भण्डार द्वारा जारी की गई कुल सामग्री	**24160**	**35517**	**–**	**0.79**
वित्त वर्ष 2005-06 के दौरान समायोजित बकाया राशि			11.56	24.46
वर्ष 2005-06 के दौरान उत्पाद शुल्क की छूट से प्राप्त राशि			18.67	21.64
वर्ष 2005-06 के दौरान सीमाशुल्क की छूट से प्राप्त राशि	237	159	1.528	1.589

*ऑनलाइन दर ठेका (रेट कांट्रैक्ट छोड़कर)

ADMINISTRATION, FINANCE & ACCOUNTS, STORES & PURCHASE

Administration

Following are the major initiatives / work completed during the year:

- The web enabled online recruitment was made more effective and successful in its second attempt for the advertisement issued during the year 2005-06. The system was modified based on the problems faced in its usage last year. Recruitment for the thirteen positions of scientists was successfully completed using web based system.
- Three meetings of Management Council were convened.
- Assessment of ninety-seven technical and support staff due for the assessment year 2004-05 was completed. Further, the assessment of sixty scientists due for the year 2003-04 was also completed.
- Deputation of seventy-five scientists to foreign countries was finalized during the year.
- Around 18,000 receipts relating to personal claims, leave applications and related papers were dealt. Seventy-five per cent of the claims were processed and completed within the time target.

Finance & accounts

Following are the major initiatives / work completed during the year:

- ➢ Maintained GPF/CPF accounts of all individuals, issued annual closure statements to the staff members on the 1st day of new financial year.
- ➢ Dealt with the financing and accounting of around 500 externally funded projects.
- ➢ Financial data/ reports were submitted to the CSIR Hq, Director, various agencies, scientists, etc.
- ➢ Scrutiny of various proposals from financial angles received from all the Divisions, viz. agreements, works proposals, pay fixation cases, personal files, deputation, court attachments, etc.
- ➢ Pension cases were settled / finalized within stipulated time period.
- ➢ Full accounts (IMPACT) and related registers were maintened.
- ➢ Various types of vouchers were generated (payment, 18,156; receipt, 5,481; transfer entry, 380).
- ➢ Lab reserve of Rs. 150.075 Lakh was generated through earning of interest on investment of surplus funds during the year.

Funds utilization:

a) Carry forward grant (by 30.9.2005)

Project	Amount	% of utilization
i) Network	124.674	100
ii) Non –network	250.000	100

b) Annual Grant (by 31.3.2006)

Project	Amount	% of utilization
i) Network	632.318	100
ii) Non –network	4965.342	100

c)	Laboratory reserve	Rs. 266.409 lakh
d)	NMITLI Projects	Rs. 470.422 lakh
e)	Externally funded projects	Rs. 2049.933 lakh

Clearance of OB items (Rs. in lakh)

Adjustments made during the year			
Govt.	Private	TA/LTC	Local
1.432	1804.835	45.871	32.201

ADMINISTRATION, FINANCE & ACCOUNTS, STORES & PURCHASE

Stores & Purchase

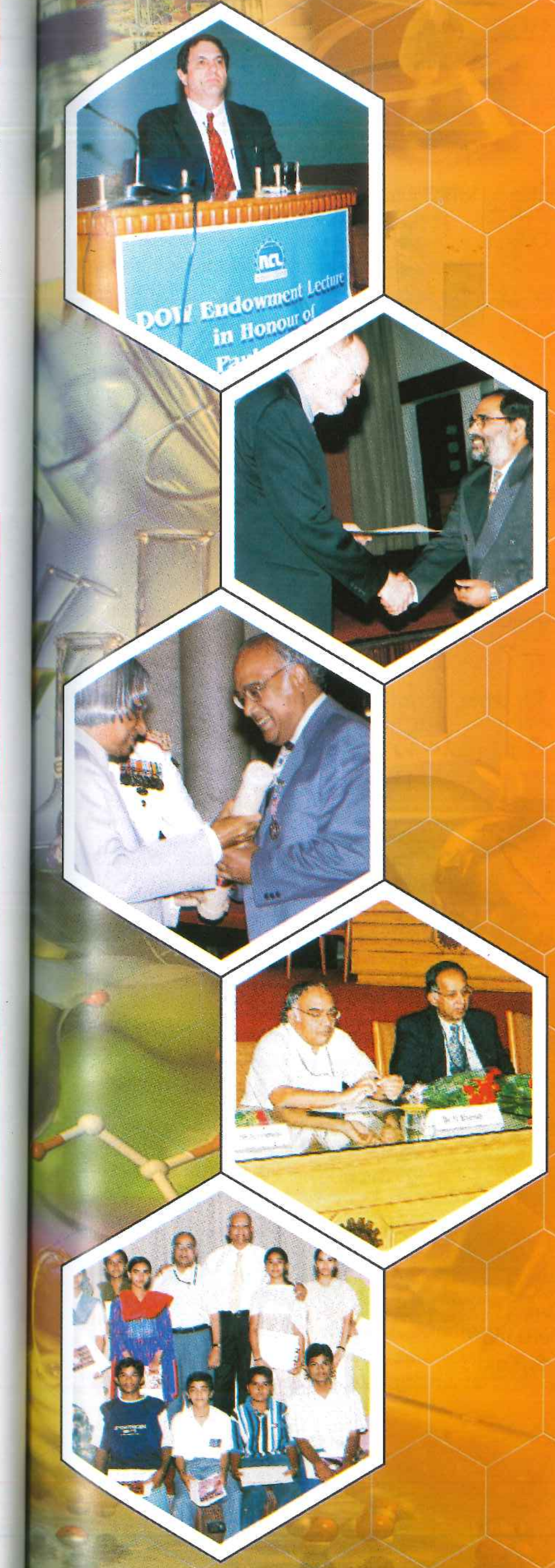
Following are the major initiatives/ work completed during the year:

- Stock at various Stores and new items added to minimise frequency of local purchases.
- All the outstanding balances against supplies up to the year 2002-2003 have been cleared / adjusted.
- Ten press tenders were issued during 2005-06 for procurement of various high value items.
- A new record room created for Stores & Purchase with optimisers for storage of files.

Stores & Purchase: Accomplishments

Item	Numbers		Value (Rs. in Crores)	
	2004-05	2005-06	2004-05	2005-06
Total indents received and processed	2292	2322	29.81	34.03
Total orders placed (imported)	767	763	20.73	26.72
Total orders placed (indigenous)	4275	1258(*)	9.89	8.04
Total consignments received (imported)	1007	917	11.31	24.04
Total consignments received (indigenous)	2376	2112	8.57	7.79
Local purchases (including on-line RC)	8852	8458	2.29	2.30
Total Stores Issues	24160	35517	-	0.79
Outstanding balance adjusted during the financial year 2005-06			11.56	24.46
Utilization of custom duty exemption during 2005-06			18.67	21.64
Utilization of excise duty exemption during 2005-06	237	159	1.528	1.589

* - excluding on-line rate contract



ANNEXURES

Annual Report 2005-06

TOP PAPERS PUBLISHED

FULL_TITLE	AUTHOR	BIBLI_DTL	IF
Conformationally constrained PNA analogues: Structural evolution toward DNA/RNA binding selectivity	Kumar, V.A.;Ganesh, K.N.	Accounts of Chemical Research, 38(5), 404(2005)	13.154
Simultaneous conversion of methane and methanol into gasoline over bifunctional Ga-, Zn-, In-, and/or Mo-modified ZSM-5 zeolites	Choudhary, V.R.;Mondal, K.C.;Mulla, S.A.R.	Angewandte Chemie - International Edition, 44(28), 4381(2005)	9.161
Nucleobases in molecular recognition: Molecular adducts of adenine and cytosine with COOH functional groups	Perumalla, S.R.;Suresh, E.;Pedireddi, V.R.	Angewandte Chemie - International Edition, 44(47), 7752(2005)	9.161
Bioleaching of sand by the fungus fusarium oxysporum as a means of producing extracellular silica nanoparticles	Bansal, V.;Sanyal, A.;Rautaray, D.;Sastry, M.;Ahmad, A.	Advanced Materials, 17(7), 889(2005)	8.079
(SR/RS)-cyclohexanyl PNAs: Conformationally preorganized PNA analogues with unprecedented preference for duplex formation with RNA	Govindaraju, T.;Kumar, V.A.;Ganesh, K.N.	Journal of the American Chemical Society, 127(12), 4144(2005)	6.903
Bacterial aerobic synthesis of nanocrystalline magnetite	Bharde, A.;Wani, A.;Shouche, Y.;Joy, P.A.;Prasad, B.L.V.;Sastry, M.	Journal of the American Chemical Society, 127(26), 9326(2005)	6.903
Identification of coding and non-coding sequences using local H÷lder exponent formalism	Kulkarni, O.C.; Vigneshwar, R.;Jayaraman, V.K.;Kulkarni, B.D.	Bioinformatics, 21(20), 3818(2005)	5.742
Synthesis and assembly of gold nanoparticles in quasi-linear lysine-keggin-ion colloidal particles	Sanyal, A.;Mandal, S.;Sastry, M.	Advanced Functional Materials, 15(2), 273(2005)	5.679
2,5-Dioxido-1,4-Benzoquinonediimine (H2L2-), A Hydrogen bonding noninnocent bridging ligand related to animated topaquinone - different oxidation-state distributions in complexes [((BPY)(2)RU)(2)(MU-H2L)(N)(N=0,+,2+,3+,4+) and [((ACAC)(2)RU)(2)(MU-H	Kar, S.;Sarkar, B.;Ghumaan, S.;Janardanan, D.;VanSlageren, J.;Fiedler, J.;Puranik, V.G.;Sunoj, R.B.;Kaim, W.;Lahiri, G.K.	Chemistry - A European Journal, 11(17), 4901(2005)	4.517

TOP PAPERS PUBLISHED

FULL_TITLE	AUTHOR	BIBLI_DTL	IF
Benzoyl transfer reactivities of racemic 2,4-di-O-acyl-myo-inositYl 1,3,5-orthoesters in the solid state: Molecular packing and intermolecular interactions correlate with the ease of the reaction	Sarmah, M.P.;Shashidhar, M.S.;Gonnade, R.G.;Bhadbhade, M.M.	Chemistry - A European Journal, 11(7), 2103(2005)	4.517
Structural rationalisation of co-crystals formed between trithiocyanuric acid and molecules containing hydrogen bonding functionality	Ahn, S.;Kariuki, B.M.;Prakashareddy, J.;Pedireddi, V.R.;Chatterjee, S.;Ranganathan, A.;Rao, C.N.R.;Harris, K.D.M.	Chemistry - A European Journal, 11(8), 2433(2005)	4.517
Structural, electronic, and bonding properties of zeolite Sn-beta: A periodic density functional theory study	Shetty, S.;Pal, S.;Kanhere, D.G.;Goursot, A.	Chemistry - A European Journal, 12(2), 518(2005)	4.517
New synthetic approach to a [1.1.6] metapara cyclophane derivative via Suzuki-Miyaura cross-coupling and ring-closing metathesis	Kotha, S.;Mandal, K.;Arora, K.K.;Pedireddi, V.R.	Advanced Synthesis and Catalysis, 347(9), 1215(2005)	4.482
Enhance super capacitor performance of organo-inorganic nanocomposite prepared by the incorporation of poly (3,4-ethylene dioxythiophen) nanoribbons into MoO3	Murugan, A.V.;Viswanath, A.K.;Gopinath, C.S.;Vijaymohanan, K.	Applied Physics Letters, 87(), 24351(2005)	4.308
Enhancement of double-layer capacitance behavior and its electrical conductivity in layered poly (3, 4-ethylenedioxythiophene)-based nanocomposites	Murugan, A.V.;Viswanath, A.K.;Campet, G.;Gopinath, C.S.;Vijayamohanan, K.	Applied Physics Letters, 87(24), 1(2005)	4.308
Diversity oriented synthesis of tricyclic compounds from glycals using the Ferrier and the Pauson-Khand reactions	Hotha, S.;Tripathi, A.	Journal of Combinatorial Chemistry, 7(6), 968(2005)	4.197
Stereospecific route to 5,11-methanomorphanthridine alkaloids via intramolecular 1,3-dipolar cycloaddition of nonstabilized azomethine ylide: Formal total synthesis of ('%)-pancracine	Pandey, G.;Banerjee, P.;Kumar, R.;Puranik, V.G.	Organic Letters, 7(17), 3713(2005)	4.195

TOP PAPERS PUBLISHED

FULL_TITLE	AUTHOR	BIBLI_DTL	IF
NaLO(4)/LIBR-mediated diastereoselective dihydroxylation of olefins - A catalytic approach to the Prevost-Woodward reaction	Emmanuel, L.;Shaikh, T.M.A.;Sudalai, A.	Organic Letters, 7(22), 5071(2005)	4.195
NBS-catalyzed hydroamination and hydroalkoxylation of activated styrenes	Talluri, S.K.;Sudalai, A.	Organic Letters, 7(5), 855(2005)	4.195
Noncovalent and nonspecific molecular interactions of polymers with multiwalled carbon nanotubes	Baskaran, D.;Mays, J.W.;Bratcher, M.S.	Chemistry of Materials, 17(13), 3389(2005)	4.103
Nature of manganese species in Ce1-xMnxO 2-? solid solutions synthesized by the solution combustion route	Murugan, B.;Ramaswamy, A.V.;Srinivas, D.;Gopinath, C.S.;Ramaswamy, V.	Chemistry of Materials, 17(15), 3983(2005)	4.103
Porous gold nanospheres by controlled transmetalation reaction - A novel material for application in cell imaging Porous gold nanospheres by controlled transmetalation reaction - A novel material for ap	Shukla, S.;Priscilla, A.;Banerjee, M.;Bhonde, R.R.;Ghatak, J.;Satyam, P.V.;Sastry, M.	Chemistry of Materials, 17(20), 5000(2005)	4.103
Direct synthesis of well-ordered and unusually reactive FeSBA-15 mesoporous molecular sieves	Vinu, A.;Sawant, D.P.;Ariga, K.;Hossain, K.Z.;Halligudi, S.B.;Hartmann, M.;Nomura, M.	Chemistry of Materials, 17(21), 5339(2005)	4.103
Synthesis, characterization, electronic structure, and photocatalytic activity of nitrogen-doped TiO2 nanocatalyst	Sathish, M.;Viswanathan, B.;Viswanath, R.P.;Gopinath, C.S.	Chemistry of Materials, 17(25), 6349(2005)	4.103
Direct observation of Ni metal impurities in lightly doped ferromagnetic polycrystalline (ZnNi)O	Deka, S.;Joy, P.A.	Chemistry of Materials, 17(26), 6507(2005)	4.103
Controlling the optical properties of lemongrass extract synthesized gold nanotriangles and potential application in infrared-absorbing optical coatings	Shankar, S.S.;Rai, A.;Sastry, M.;Ahmad, A.	Chemistry of Materials, 17(3), 566(2005)	4.103
Polymerization in surfactant liquid crystalline phases	Wadekar, M.N.;Pasricha, R.;Gaikwad, A.B.;Kumaraswamy, G.	Chemistry of Materials, 17(9), 2460(2005)	4.103

RESEARCH PAPERS PUBLISHED

RESEARCH PAPERS PUBLISHED (2005)

Biochemical Sciences

1. X-ray crystallographic studies on C-phycocyanins from cyanobacteria from *different habitats: marine and freshwater*
Satyanarayana, L.; Suresh, C.G.; Patel,A.; Mishra, S.; Ghosh, P.K.
Acta Crystallogr. Section F : Struct Biol & Cryst, F61, 844

2. Crystallization and preliminary X-ray characterization of a lectin from *Cicer arietinum (chickpea)*
Katre, U.V.; Gaikwad, S.M.; Bhagyawant, S.S.; Deshpande, U.D.; Khan, M.I.; Suresh, C.G.
Acta Crystallogr. Section F: Struct Biol & Cryst C, F61, 141

3. Cloning, purification, crystallization and preliminary structural studies of penicillin V acylase from *Bacillus subtilis*
Priya, R.; Pundle, A.V.; Prabhune, A; SivaRaman, H.; Brannigan, J.A.; Dodson, G.G.; Suresh, C.G.
Acta Crystallogr. Section F: Struct Biol & Cryst C, F61, 680

4. Cloning, preparation and preliminary crystallographic *studies of Penicillin V acylase autoproteolytic processing mutants*
Chandra, P.M.; Brannigan, J.A.; Prabhune, A.; Pundle, A.; Turkenburg, J.P.; Dodson, G.G.; Suresh, C.G.
Acta Crystallogr. Section F: Struct Biology & Cryst C, F61, 124

5. High resolution mtDNA studies of the Indian population: *implications for Palaeolithic settlement of the Indian subcontinent*
Barnabas, S.; Shouche, Y.; Suresh, C.G.
Ann. Hum. Genet., 70, 52

6. Purification and properties of a low molecular weight 1,4 D-glucan glucohydrolase having one active site for carboxymethyl cellulose and xylan from *an alkalothermophilic Thermomonospora sp.*
Jagtap, S.; Rao, M.
Biochemical and Biophysical Research Communication, 329(1), 111

7. Illustration of HIV-1 protease folding through a molten-globule-like intermediate using an experimental model that implicates *-crystallin and calcium ions*
Dash, C.; Rao, M.; Sastry, M.; Dash, C.
Biochemistry, 44(10), 3725

8. Using 2-aminopurine fluorescence to detect bacteriophage T4 DNA polymerase-*DNA complexes that are important for primer extension and proofreading reactions*
Hariharan, C.; Reha-Krantz, L.J.
Biochemistry, 44(48), 15674

9. In vivo and in vitro effect of Capsicum annum proteinase inhibitors on *Helicoverpa armigera gut proteinases*
Tamhane, V.A.; Chougule, N.P.; Giri, A.P.; Dixit, A.R.; Sainani, M.N.; Gupta, V.S.
Biochimica et Biophysica Acta - General Subjects, 1722(2), 156

10. Lignin-carbohydrate complexes from *sugarcane bagasse: Preparation, purification, and characterization*
Singh, R.; Singh, S.; Trimukhe, K.D.; Pandare, K.V.; Bastawade, K.B.; Gokhale, D.V.; Varma, A.J.
Carbohydrate Polymers, 62(1), 57

11. Unraveling biochemical properties of cockroach (Periplaneta americana) proteinases with a gel X-ray film contact print method
Hivrale, V.K.; Chougule, N.P.; Chhabda, P.J.; Giri, A.P.; Kachole, M.S.
Comparative Biochemistry and Physiology - B Bioche, 141(3), 261

12. Cataloging Indian Biota - Response
Chavan, V.S.; Watve, A.V.; Rane, N.S.; Krishnan, S.
Current Science, 88(4), 532

13. Assessing the role of FecB mutation in productivity of Indian sheep
Pardeshi, V.C.; Sainani, M.N.; Maddox, J.F.; Ghalsasi, P.M.; Nimbkar, C.; Gupta, V.S.
Current Science, 89(5), 887

14. IndCollections: Biological specimens in Indian collections [4]
Chavan, V.; Rane, N.S.; Ghate, H.V.;Krishnan,S.
Current Science, 89(9), 1454

15. Modified nucleosides and across the anticodon loop interactions in tRNA
Sonavane, U.B.; Sonawane, K.D.; Tiwari, R.P.
European Biophysics Journal, 34, 581

RESEARCH PAPERS PUBLISHED

16. PHB synthase from Streptomyces aureofaciens NRRL 2209
Ramachander, T.V.N.; Rawal, S.K.
FEMS Microbiology Letters, 242(1), 13

17. Expression of Streptomyces coelicolor alpha-galactosidase gene in Eccherichia coli and characterization
Morisaki, K.; Kim, W.D.; Kotwal, S.M.; Kaneko, S.; Kobayashi, H.Food
Science and Technology Research, 11, 207

18. Thidiazuron-induced morphogenesis in tamarind seedlings
Mehta, U.J.; Sahasrabudhe, N.; Hazra, S.
In Vitro Cellular and Developmental Biology - Plan, 41(3), 240

19. Gene expression patterns of Helicoverpa armigera gut proteases
Chougule, N.P.; Giri, A.P.; Sainani, M.N.; Gupta, V.S.
Insect Biochemistry and Molecular Biology, 35(4), 355

20. Determination of ploidy of a dimorphic zygomycetes Benjaminiella poitrasii and the occurence of meiotic division during zygospore germination
Ghormade,V.; Shastry, P.; Chiplunkar, J.; Deshpande, M.V.
Journal of Agricultural Technology, 1, 97

21. Extra/Intracellular Biosynthesis of Gold Nanoparticles by a Novel Alkalotolerant Fungus, Trichothecium sp.
Ahmad, A.; Senapati, S.; Khan, M.I.; Kumar, R.; Sastry, M.
Journal of Biomed Nanotech, 1, 47

22. Studies on the lactic-fermentation of sugar apple (Annona squamosa L.) puree
Tien, Y.-Y.; Ng, C.-C.; Chang, C.-C.; Tseng, W.-S.; Kotwal, S.; Shyu, Y.-T.
Journal of Food and Drug Analysis, 13(4), 377

23. Mitochondrial sequence reveals high levels of gene flow between breeds of domestic sheep from Asia and Europe
Meadows, J.R.S.; Li, K.; Kantanen, J.; Tapio, M.; Sipos, W.; Pardeshi, V.; Gupta, V.; Calvo, J.H.; Whan, V.; Norris, B.
Journal of Heredity,96(5), 494

24. Podborer (Helicoverpa-Armigera Hubn.) does not show specific adaptations in GUT proteinases to dietary cicer-arietinum kunitz proteinase-inhibitor
Srinivasan, A.; Chougule, N.P.; Giri, A.P.; Gatehouse, J.A.; Gupta, V.S.
Journal of Insect Physiology, 51(11), 1268

25. Characterization of two midgut proteinases of Helicoverpa armigera and their interaction with proteinase inhibitors
Telang, M.A.; Giri, A.P.; Sainani, M.N.; Gupta, V.S.
Journal of Insect Physiology, 51(5), 513

26. Fungus-mediated biosynthesis of silica and titania particles
Bansal, V.; Rautaray, D.; Bharde, A.; Ahire, K.; Sanyal, A.; Ahmad, A.; Sastry, M.
Journal of Materials Chemistry, 15(26), 2583

27. Higher accumulation of proteinase inhibitors in flowers than leaves and fruits as a possible basis for differential feeding preference of Helicoverpa armigera on tomato (Lycopersicon esculentum Mill, Cv. Dhanashree)
Damle, M.S.; Giri, A.P.; Sainani, M.N.; Gupta, V.S.
Phytochemistry, 66(22), 2659

28. A Kunitz trypsin inhibitor from chickpea (Cicer arietinum L.) that exerts anti-metabolic effect on podborer (Helicoverpa armigera) larvae Srinivasan,
A.; Giri, A.P.; Harsulkar, A.M.; Gupta, V.S.; Srinivasan, A.; Gatehouse, J.A.
Plant Molecular Biology, 57(3), 359

29. Extracellular nuclease from a thermophile, Streptomyces thermonitrificans: Production, purification and partial characterization of - Double strand preferential - Deoxyribonuclease activity
Patil, N.S.; Deshmukh, S.S.; Shankar, V.
Process Biochemistry, 40(3-4), 1271

30. Optimization and scale up of production of alkaline protease from Conidiobolus coronatus
Laxman, R.S.; Sonawane, A.P.; More, S.V.; Rao, B.S.; Rele, M.V.; Jogdand, V.V.; Deshpande, V.V.; Rao, M.B.
Process Biochemistry, 40(9), 3152

31. In ovulo rescue of hybrid embryos in Flame Seedless grapes - Influence of pre-bloom sprays of benzyladenine
Bharathy, P.V.; Karibasappa, G.S.; Patil, S.G.; Agrawal, D.C.
Scientia Horticulturae, 106(3), 353

32. Extracellular biosynthesis of bimetallic Au-Ag alloy nanoparticles
Senapati, S.; Ahmad, A.; Khan, M.I.; Sastry, M.; Kumar, R.
Small, 1(5), 517

RESEARCH PAPERS PUBLISHED

Catalysis

1. Dynamics of drop impact on solid surface: Experiments and VOF simulations
Gunjal, P.R.; Ranade, V.V.; Chaudhari, R.V.
AIChE *Journal, 51(1), 59*

2. Computational study of a single-phase flow in packed beds of spheres
Gunjal, P.R.; Ranade, V.V.; Chaudhari, R.V.
AIChE *Journal, 51(2), 365*

3. Simultaneous conversion of methane and methanol into gasoline over bifunctional Ga-, Zn-, In-,and/ or Mo-modified ZSM-5 zeolites
Choudhary, V.R.; Mondal, K.C.; Mulla, S.A.R. Angewandte *Chemie - International Edition, 44(28), 4381*

4. Highly active and selective AlSBA-15 catalysts for the vapor phase tert-butylation of phenol
Vinu, A.; Hartmann, M.; Devassy, B.M.; Halligudi, S.B.; B÷hlmann, W.
Applied Catalysis A: General, 281(1-2), 207

5. Transesterification of diethyl oxalate with phenol using MoO3/SiO2 catalyst
Biradar, A.V.; Umbarkar, S.B.; Dongare, M.K.
Applied Catalysis A: General, 285(1-2), 190

6. Biphenyl hydrogenation over supported transition metal catalysts under supercritical carbon dioxide solvent
Hiyoshi, N.; Rode, C.V.; Sato, O.; Shirai, M.
Applied Catalysis A: General, 288(1-2), 43

7. Zeolite-based organic-inorganic hybrid catalysts for phosgene-free and solvent-free synthesis of cyclic carbonates and carbamates at mild conditions utilizing CO2
Srivastava, R.; Srinivas, D.; Ratnasamy, P.
Applied Catalysis A: General, 289(2), 128

8. Vanadium-containing ordered mesoporous silicas: Synthesis, characterization and catalytic activity in the hydroxylation of biphenyl
George, J.; Shylesh, S.; Singh, A.P.
Applied Catalysis A: General, 290(1-2), 148

9. 3-Aminopropyltriethoxysilyl functionalized Na-Al-MCM-41 solid base catalyst for selective preparation of 2-phenylpropionitrile from phenylacetonitrile
Venkatesan, C.; Chidambaram, M.; Singh, A.P.
Applied Catalysis A: General, 292(1-2), 344

10. Role of a co-metal in bimetallic Ni-Pt catalyst for hydrogenation of M-dinitrobenzene to M-phenylenediamine
Telkar, M.M.; Nadgeri, J.M.; Rode, C.V.; Chaudhari, R.V.
Applied Catalysis A: General, 295(1), 23

11. In situ XPS investigations of Cu1-xNixZnAl-mixed metal oxide catalysts used in the oxidative steam reforming of bio-ethanol
Velu, S.; Suzuki, K.; Vijayaraj, M.; Barman, S.; Gopinath, C.S.; Velu, S.
Applied Catalysis B: Environmental, 55(4), 287

12. Enhance super capacitor performance of organo-inorganic nanocomposite prepared by the incorporation of poly (3,4-ethylene dioxythiophen) nanoribbons into MoO3
Murugan, A.V.; Viswanath, A.K.; Gopinath, C.S.; Vijaymohanan, K.
Applied Physics Letters, 87, 24351

13. Effect of alkali metal carbonate on the hydrohenation of 2-butyne 1,4 diolover platinum catalysts
Rode, C.V.; Telkar, M.M.; Rane, V.H.; Chaudhari, R.V.
Catal Commun, 6, 725

14. Textural/structural, stability and morphological properties of mesostructured silicas (MCM-41 and MCM-48) prepared using different silica sources
Gaydhankar, T.R.; Taralkar, U.S.; Jha, R.K.; Joshi, P.N.; Kumar, R.
Catal Commun, 6(5), 361

15. Polystyrene encapsulation of manganese porphyrins: Highly efficient catalysts for oxidation of olefins
Naik, R.; Joshi, P.; Umbarkar, S.; Deshpande, R.K.
Catal Commun, 6(2), 125

16. Influence of PdO content and pathway of its formation on methane combustion activity
Choudhary, T.V.; Banerjee, S.; Choudhary, V.R.
Catal Commun, 6(2), 97

17. Synthesis, characterization and catalytic properties of hexagonal mesoporous vanadium aluminophosphate molecular sieves
Venkatathri, N.; Srivastava, R.
Catal Commun, 6(3), 177

RESEARCH PAPERS PUBLISHED

18. Carbon-free dry reforming of methane to syngas over NdCoO3 perovskite-type mixed metal oxide catalyst
Choudhary, V.R.; Mondal, K.C.; Mamman, A.S.; Joshi, U.A.
Catalysis Letters, 100(3-4), 271

19. Hydrogen peroxide formation in the interaction of oxygen with boron-containing Pd catalysts prereduced by hydrazine in aqueous acidic medium containing bromide anions
Choudhary, V.R.; Samanta, C.
Catalysis Letters, 99(1-2), 79

20. Carbonylation of alkynes, alkenes and alcohols using metal complex catalysts
Sarkar, B.R.; Chaudhari, R.V.
Catalysis Surveys from Asia, 9(3), 193

21. A novel route for in-situ H2O2 generation from selective reduction of O2 by hydrazine using heterogeneous Pd catalyst in an aqueous medium
Choudhary, V.R.; Samanta, C.; Jana, P.
Chemical Communications, (43), 5399

22. Vapour phase oxidation of acetophenone to benzoic acid over binary oxides of V and Mo
Chumbhale, V.R.; Paradhy, S.A.; Anilkumar, M.; Kadam, S.T.; Bokade, V.V.
Chemical Engineering Research and Design, 83(1 A), 75

23. Kinetics of the complete combustion of dilute propane and methyl ethyl ketone over Cr-doped ZrO2 catalyst
Choudhary, V.R.; Deshmukh, G.M.
Chemical Engineering Science, 60(6), 1575

24. Enhanced selectivity to decalin in naphthalene hydrogenation under supercritical carbon dioxide
Hiyoshi, N.; Miura, R.; Rode, C.V.; Sato, O.; Shirai, M.
Chemistry Letters, 34(3), 424

25. Partial ring hydrogenation of naphthols over supported metal catalysts in supercritical carbon dioxide solvent
Mine, E.; Haryu, E.; Arai, K.; Sato, T.; Sato, O.; Sasaki, A.; Rode, C.V.; Shirai, M.
Chemistry Letters, 34(6), 782

26. Role of Mg ions in modulating the morphology and structure of CaCO 3 crystals grown in aqueous foams
Rautaray, D.; Kasture, M.; Sastry, M.
CrystEngComm, 7, 469

27. Low-temperature complete combustion of a dilute mixture of methane and propane over transition-metal-doped ZrO2 catalysts: Effect of the presence of propane on methane combustion
Choudhary, V.R.; Pataskar, S.G.; Deshmukh, G.M.
Environmental Science and Technology, 39(7), 2364

28. A green process for chlorine-free benzaldehyde from the solvent-free oxidation of benzyl alcohol with molecular oxygen over a supported nano-size gold catalyst
Choudhary, V.R.; Dhar, A.; Jana, P.; Jha, R.; Uphade, B.S.
Green Chemistry, 7(11), 768

29. A comparative study of the Jasad Bhasma samples obtained from various pharmaceutical campanies
Bhagwat, M.; Ramaswamy, V.
Indian Drugs, 42, 658

30. Kinetic modeling of reductive alkylation of aniline with acetone using Pd/Al2O3 catalyst in a batch slurry reactor
Roy, D.; Jaganathan, R.; Chaudhari, R.V.
Industrial and Engineering Chemistry Research, 44(14), 5388

31. Hydrodynamics of trickle-bed reactors: Experiments and CFD modeling
Gunjal, P.R.; Kashid, M.N.; Ranade, V.V.; Chaudhari, R.V.
Industrial and Engineering Chemistry Research, 44(16), 6278

32. Analysis of a gas-liquid-liquid-solid catalytic reaction: Kinetics and modeling of a semibatch slurry reactor
Roy, D.; Chaudhari, R.V.
Industrial and Engineering Chemistry Research, 44(25), 9586

33. Characterization of gas-liquid flows in stirred vessels using pressure and torque fluctuations
Khopkar, A.R.; Panaskar, S.S.; Pandit, A.B.; Ranade, V.V.
Industrial and Engineering Chemistry Research, 44(9), 3298

34. Effect of 2-(2-pyridyl)azole-based ancillary ligands (L1-4) on the electrophilicity of the nitrosyl function in [RuII(trpy)(L 1-4)(NO)]3+ [trpy = 2,2:6,2-terpyridine]. Synthesis, structures, and spectroscopic, electrochemical, and kinetic aspects
Chanda, N.; Paul, D.; Kar, S.; Mobin, S.M.; Datta, A.; Puranik, V.G.; Krishnamurthy Rao, K; Lahiri, G.K.
Inorganic Chemistry, 44(10), 3499

RESEARCH PAPERS PUBLISHED

35. Zirconia-supported 12-tungstophosphoric acid as a solid catalyst for the synthesis of linear alkyl benzenes
Devassy, B.M.; Halligudi, S.B.; Lefebvre, F.
Journal of Catalysis, 229, 576

36. Rearrangement of allyl phenyl ether over Al-MCM-41
Mathew, N.T.; Khaire, S.; Mayadevi, S.; Jha, R.; Sivasanker, S.
Journal of Catalysis, 229(1), 105

37. A MCM-41-supported platinum carbonyl cluster-derived asymmetric hydrogenation catalyst
Bhaduri, S.; Basu, S.; Paul, H.; Lahiri, G.K.; Gopinath, C.S.
Journal of Catalysis, 229(2), 298

38. Oxidative dehydrogenation of ethylbenzene over vanadia-alumina catalysts in the presence of nitrous oxide: Structure-activity relationship
Shiju, N.R.; Anilkumar, M.; Mirajkar, S.P.; Gopinath, C.S.; Rao, B.S.; Satyanarayana, C.V.
Journal of Catalysis, 230(2), 484

39. CO2 activation and synthesis of cyclic carbonates and alkyl/aryl carbamates over adenine-modified Ti-SBA-15 solid catalysts
Srivastava, R.; Srinivas, D.; Ratnasamy, P.
Journal of Catalysis, 233(1), 1

40. High-temperature stable and highly active/selective supported NiCoMgCeOx catalyst suitable for autothermal reforming of methane to syngas
Choudhary, V.R.; Mondal, K.C.; Mamman, A.S.
Journal of Catalysis, 233(1), 36

41. Vanadium-containing ordered mesoporous silicates: Does the silica source really affect the catalytic activity, structural stability, and nature of vanadium sites in V-MCM-41
Shylesh, S.; Singh, A.P.
Journal of Catalysis, 233(2), 359

42. Formation of nanosized zirconia-supported 12-tungstophosphoric acid in mesoporous silica SBA-15: A stable and versatile solid acid catalyst for benzylation of phenol
Sawant, D.P.; Vinu, A.; Jacob, N.E.; Lefebvre, F.; Halligudi, S.B.
Journal of Catalysis, 235(2), 341

43. Zirconia-supported heteropoly acids: characterization and catalytic behaviour in liquid-phase veratrole benzoylation
Devassy, B.M.; Halligudi, S.B.
Journal of Catalysis, 236(2), 313

44. Effect of NaBr, KCl, KBr, and MgCl2 on viscosities of aqueous glycine and L-alanine solutions at 298.15 K
Badarayani, R.; Satpute, D.B.; Kumar, A.
Journal of Chemical and Engineering Data, 50(3), 1083

45. Highly active and reusable catalyst from Fe-Mg-hydrotalcite anionic clay for Friedel-Crafts type benzylation reactions
Choudhary, V.R.; Jha, R.; Choudhari, P.A.
Journal of Chemical Sciences, 117(6), 635

46. Low temperature complete combustion of dilute toluene and methyl ethyl ketone over Mn-doped ZrO2 (cubic) catalysts
Choudhary, V.R.; Deshmukh, G.M.; Pataskar, S.G.
Journal of Chemical Technology and Biotechnology, 80(8), 934

47. Mannich reaction in Bronsted acidic ionic liquid : A facile synthesis of beta-amino carbonyl compounds
Sahoo, S.; Joseph, T.; Halligudi, S.B.
Journal of Molecular Catalysis A : Chem, 244,179

48. Synthesis of monoallyl guaiacol via allylation using HY zeolite
Kumbhar, S.M.; Shanbhag, G.V.; Halligudi, S.B.
Journal of Molecular Catalysis A : Chem, 244,278

49. Selective synthesis of N,N-dimethyl aniline derivatives using dimethyl carbonate as a methylating agent and onium salt as a catalyst
Shivarkar, A.B.; Gupte, S.P.; Chaudhari, R.V.
Journal of Molecular Catalysis A: Chemical, 226(1), 49

50. Synthesis, characterization and photo catalytic degradation of aqueous eosin over Cr containing Ti/MCM-41 and SiO2-TiO2 catalysts using visible light
Awate, S.V.; Jacob, N.E.; Deshpande, S.S.; Gaydhankar, T.R.; Belhekar, A.A.
Journal of Molecular Catalysis A: Chemical, 226(2), 149

51. Factors affecting activation and utilization of carbon dioxide in cyclic carbonates synthesis over Cu and Mn peraza macrocyclic complexes
Srivastava, R.; Bennur, T.H.; Srinivas, D.
Journal of Molecular Catalysis A: Chemical, 226(2),199

52. Epoxidation of styrene by anhydrous hydrogen peroxide over boehmite and alumina catalysts with continuous removal of the reaction water
Choudhary, V.R.; Patil, N.S.; Chaudhari, N.K.; Bhargava, S.K.
Journal of Molecular Catalysis A: Chemical, 227(1 2), 217

RESEARCH PAPERS PUBLISHED

53. Oxidation of norbornene over vanadium-substituted phosphomolybdic acid catalysts and spectroscopic investigations
Raj, N.K.K.; Ramaswamy, A.V.; Manikandan, P.
Journal of Molecular Catalysis A: Chemical, 227(1-2), 37

54. Oxyfunctionalization of limonene using vanadium complex anchored on functionalized SBA-15
Joseph, T.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 229(1-2), 241

55. Zirconia-supported phosphotungstic acid as catalyst for alkylation of phenol with benzyl alcohol
Devassy, B.M.; Shanbhag, G.V.; Halligudi, S.B.; Lefebvre, F.; B÷hringer, W.; Fletcher, J.
Journal of Molecular Catalysis A: Chemical, 230(1-2), 113

56. An insight into the mechanism of selective mono-N-methylation of aniline on Cu1-xZnxFe2O4: A DRIFTS study
Vijayaraj, M.; Murugan, B.; Umbarkar, S.; Hegde, S.G.; Gopinath, C.S.
Journal of Molecular Catalysis A: Chemical, 231(1-2), 169

57. Hydroformylation of 1-hexene using Rh/TPPTS complex exchanged on anion exchange resin: Kinetic studies
Diwakar, M.M.; Deshpande, R.M.; Chaudhari, R.V.
Journal of Molecular Catalysis A: Chemical, 232(1-2), 179

58. Silicotungstate-modified zirconia as an efficient catalyst for phenol tert-butylation
Devassy, B.M.; Shanbhag, G.V.; Mirajkar, S.P.; Halligudi, S.B.; B÷hringer, W.; Fletcher, J.
Journal of Molecular Catalysis A: Chemical, 233(1-2), 141

59. Br÷nsted acidic ionic liquids: A green, efficient and reusable catalyst system and reaction medium for Fischer esterification
Joseph, T.; Sahoo, S.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 234(1-2), 107

60. Vapor phase oxidation of 4-fluorotoluene over vanadia-titania catalyst
Maurya, S.K.; Gurjar, M.K.; Patil, P.; Umbarkar, S.B.; Dongare, M.; Rudiger, S.; Kemnitz, E.
Journal of Molecular Catalysis A: Chemical, 234(12), 51

61. Catalyzing Henry reactions in chloroaluminate ionic liquids
Kumar, A.; Pawar, S.S.
Journal of Molecular Catalysis A: Chemical, 235(1-2), 244

62. tert-Butylation of p-cresol over WOx/ZrO2 solid acid catalysts
Sarish, S.; Devassy, B.M.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 235(1-2), 44

63. Bis(2-[Alpha hydroxyethyl]benzimidazolato)copper(II) anchored onto chloromethylated polystyrene for the biomimetic oxidative coupling of 2-aminophenol to 2-aminophenoxazine-3-one
Maurya, M.R.; Sikarwar, S.; Joseph, T.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 236(1-2), 132

64. Copper(II) ion-exchanged montmorillonite as catalyst for the direct addition of NH bond to CC triple bond
Joseph, T.; Shanbhag, G.V.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 236(1-2), 139

65. Synthesis of linear alkyl benzenes over zirconia-supported 12-molybdophosphoric acid catalysts
Devassy, B.M.; Lefebvre, F.; B÷hringer, W.; Fletcher, J.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 236(1-2), 162

66. Alkylation of benzene with Alpha-olefins over zirconia supported 12-silicotungstic acid
Sawant, D.P.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 237(1-2), 137

67. Immobilization of metallporphyrins on polystyrene: Efficient catalysts for aerobic oxidation of alcohols
Naik, R.; Joshi, P.; Deshpande, R.K.
Journal of Molecular Catalysis A: Chemical, 238(1-2), 46

68. Influence of silica source in the catalytic activity and heterogenity of mesoporous vanadosilicates
Shylesh, S.; Mirajkar, S.P.; Singh, A.P.
Journal of Molecular Catalysis A: Chemical, 239(1-2), 57

69. In-Mg-hydrotalcite anionic clay as catalyst or catalyst precursor for Friedel-Crafts type benzylation reactions
Choudhary, V.R.; Jha, R.; Narkhede, V.S.
Journal of Molecular Catalysis A: Chemical, 239(1 2), 76

70. Liquid-phase alkylation of phenol with long-chain olefins over WO x/ZrO2 solid acid catalysts
Sarish, S.; Devassy, B.M.; B÷hringer, W.; Fletcher, J.; Halligudi, S.B.
Journal of Molecular Catalysis A: Chemical, 240(1-2), 123

RESEARCH PAPERS PUBLISHED

71. Synthesis, characterization and catalytic activity of Mn(III)- and Co(II)-salen complexes immobilized mesoporous alumina
Chaube, V.D.; Shylesh, S.; Singh, A.P.
Journal of Molecular Catalysis A: Chemical, 241(1-2), 79

72. Isolation and characterization of an iodide bridged dimeric palladium complex in carbonylation of methanol
Tonde, S.S.; Kelkar, A.A.; Chaudhari, R.V.; Bhadbhade, M.M.
Journal of Organometallic Chemistry, 690(6), 1677

73. Preparation and characterization of a copper based Indian traditional drug: Tamra bhasma
Wadekar, M.P.; Rode, C.V.; Bendale, Y.N.; Patil, K.R.; Prabhune, A.A.
Journal of Pharmaceutical and Biomedical Analysis, 39(5), 951

74. A molecular beam study of the NO + CO reaction on Pd(111) surfaces
Thirunavukkarasu, K.; Thirumoorthy, K.; Libuda, J.; Gopinath, C.S.
Journal of Physical Chemistry B, 109(27), 13272

75. Isothermal kinetic study of nitric oxide adsorption and decomposition on Pd(111) surfaces: Molecular beam experiments
Thirunavukkarasu, K.; Thirumoorthy, K.; Libuda, J.; Gopinath, C.S.
Journal of Physical Chemistry B, 109(27), 13283

76. Molecular origins of wettability of hydrophobic poly(vinylidene fluoride) microporous membranes on poly(vinyl alcohol) adsorption: Surface and interface analysis by XPS
Gholap, S.G.; Badiger, M.V.; Gopinath, C.S.
Journal of Physical Chemistry B, 109(29), 13941

77. Synthesis of high silica content silicoaluminophosphate-5 (SAPO-5) from non-aqueous medium using hexamethyleneimine template
Venkatathri, N.
Journal of Scientific and Industrial Research, 64(7), 509

78. Conversion of fly-ash AN environmentally detrimental waste to zeolite-beta (BEA) for commercial catalytic application
Kasture, M.W.; Bokade, V.V.; Joshi, P.N.
Journal of the Americal Ceramic Society, 88(11), 3260

79. Synthesis and characterization of a novel extra large pore aluminophosphate molecular sieve, NCL-6
Venkatathri, N.
Journal of the Indian Chemical Society, 82(1), 77

80. Benzylation of benzene and other aromatics by benzyl chloride over mesoporous AlSBA-15 catalysts
Vinu, A.; Sawant, D.P.; Halligudi, S.B.; Ariga, K.; Hartmann, M.
Microporous and Mesoporous Materials, 80(1-3), 195

81. Novel, benign, solid catalysts for the oxidation of hydrocarbons
Ratnasamy, P.; Raja, R.; Srinivas, D.
Philosophical Transactions: Mathematical, Physical, 363(1829), 1001(20

82. Synthesis and analysis of ZnO and CdSe nanoparticles
Ashtaputre, S.S.; Deshpande, A.; Marathe, S.; Wankhede, M.E.; Chimanpure, J.; Pasricha, R.; Urban, J.; Haram, S.K.; Gosavi, S.W.; Kulkarni, S.K.
Pramana - Journal of Physics, 65(4 SPE), 615

83. Synthesis, characterization and catalytic potentials of polymer anchored copper(II), oxovanadium(IV) and dioxomolybdenum(VI) complexes of 2-(-hydroxymethyl)benzimidazole
Maurya, M.R.; Sikarwar, S.; Joseph, T.; Manikandan, P.; Halligudi, S.B.
Reactive and Functional Polymers, 63(1), 71

84. Incorporation of tin into mesoporous silics SBA-15 molecular sieves
Ramaswamy, A.V.; Pasricha, R.; Ramaswamy, V.
Studies in Surface Science and Catalysis, 154, 870

85. Use of N, N-Diisopropylethylamine for faster synthesis of AlPo-5 and MgAPO-5 molecular sieves and their characterization
Murugan, B.; Ramaswamy, V.
Studies in Surface Science and Catalysis, 154, 971

86. Immobilized molybdovanadophosphoric acids on SBA-15 for selective oxidation of alkenes
Raj, N.K.K.; Deshpande, S.S.; Ingle, R.H.; Raja, T.; Manikandan, P.
Studies in Surface Science and Catalysis, 156, 769

87. Influence of Sn- and Al- metal sources on post-synthesis modification of mesoporous SBA-15 molecular sieves
Shah, P.; Ramaswamy, A.V.; Ramaswamy, V.
Studies in Surface Science and Catalysis, 158, 565

88. Molecular dynamics simulations of H2O with sites of Cu I-FAU and CuII-FAU
Berthomieu, D.; Krishnamurty, S.; Heine, T.; Goursot, A.
Studies in Surface Science and Catalysis, 158, 655

89. Characterization of nanocrystalline anatase titania: An in situ HTXRD study
Jagtap, N.; Bhagwat, M.; Awati, P.; Ramaswamy, V.
Thermochimica Acta, 427(1-2), 37

90. Pressure dependence of the dissociation of acetic, benzoic, mandelic and succinic acids at 298.15 K
Kumar, A.
Thermochimica Acta, 439(1-2), 154

91. Ti-oxo radicals and product selectivity in olefin oxidations over titanosilicate molecular sieves
Shetti, V.N.; Srinivas, D.; Ratnasamy, P.
Zeitschrift fur Physikalische Chemie, 219(7), 905

Engineering Science

1. Performance assessment of HCFC-22 window air conditioner retrofitted with R-407C
Devotta, S.; Padalkar, A.S.; Sane, N.K.
Applied Thermal Engineering, 25(17-18), 2937

2. Soft-sensor development for fed-batch bioreactors using support vector regression
Desai, K.; Badhe, Y.; Tambe, S.S.; Kulkarni, B.D.
Biochemical Engineering Journal, 27(3), 225(2006)

3. Identification of coding and non-coding sequences using local H÷lder exponent formalism
Kulkarni, O.C.; Vigneshwar, R.; Jayaraman, V.K.; Kulkarni, B.D.
Bioinformatics, 21(20), 3818

4. Modeling a continuous multistage liquid phase cyclohexane oxidation reactor network
Bhattacharya, A.
Chemical Engineering and Processing, 44(5), 567

5. Modeling of rotary desiccant wheels
Harshe, Y.M.; Utikar, R.P.; Ranade, V.V.; Pahwa, D.
Chemical Engineering and Technology, 28(12), 1473

6. Characterization of gas-liquid flows in rectangular bubble columns using conductivity probes
Buwa, V.V.; Ranade, V.V.
Chemical Engineering Communications, 192(7-9), 1129

7. A general kinetic model framework for the interpretation of adiabatic calorimeter rate data
Bhattacharya, A.
Chemical Engineering Journal, 110(1-3), 67

8. Regression models using pattern search assisted least square support vector machines
Patil, N.S.; Shelokar, P.S.; Jayaraman, V.K.; Kulkarni, B.D.
Chemical Engineering Research and Design, 83(8 A), 1030

9. Matched asymptotic solution for flow in a semi-hyperbolic die
Subramanian, G.; Nagarkar, S.; Lele, A.; Ranade, V.
Chemical Engineering Science, 60(11), 3107

10. Modeling of vaporization and cracking of liquid oil injected in a gas-solid riser
Nayak, S.V.; Joshi, S.L.; Ranade, V.V.
Chemical Engineering Science, 60(22), 6049

11. Comment on "prediction of viscosity of mixed electrolyte solutions based on the Eyring's absolute rate theory and the equations of Patwardhan and Kumar by Y.-F. Hu" (chemical engineering science 2003,59,2457-2464)
Kumar, A.
Chemical Engineering Science, 60(6), 1793

12. Gas-liquid flow generated by a Rushton turbine in stirred vessel: CARPT/CT measurements and CFD simulations
Khopkar, A.R.; Ranade, V.V.; Rammohan, A.R.; Dudukovic, M.P.
Chemical Engineering Science, 60(8-9 S), 2215

13. A novel local singularity distribution based method for flow regime identification: Gas-liquid stirred vessel with Rushton turbine
Jade, A.M.; Jayaraman, V.K.; Kulkarni, B.D.; Khopkar, A.R.; Ranade, V.V.; Sharma, A.
Chemical Engineering Science, 61(2), 688(2006)

14. Characterization of gas-solid fluidization regimes: Using wall pressure fluctuations technique
Ippalpalli, S.R.; Ranade, V.V.; Bapat, J.D.
Chemical Engineering World, 40(4), 66

15. Knowledge incorporated support vector machines to detect faults in Tennessee Eastman Process
Kulkarni, A.; Jayaraman, V.K.; Kulkarni, B.D.
Computers and Chemical Engineering, 29(10), 2128

---

16. Kinetics of the complete combustion of dilute propane and toluene over iron-doped ZrO2 catalyst
Choudhary, V.R.; Choudhary, V.R.; Deshmukh, G.M.; Mishra, D.P.
Energy and Fuels, 19(1), 54

17. New route for the synthesis of propylene glycols via hydroformylation of vinyl acetate
Borole, Y.L.; Chaudhari, R.V.
Industrial and Engineering Chemistry Research, 44(25), 9601

18. Integrated fuel cell processor for a 5-kW proton-exchange membrane fuel cell
Ratnamala, G.M.; Shah, N.; Mehta, V.; Rao, P.V.; Devotta, S.
Industrial and Engineering Chemistry Research, 44(5), 1535

19. Microchannel reactors: Applications and use in process development
Gokhale, S.V.; Jayaraman, V.K.; Tayal, R.K.; Kulkarni, B.D.
International Journal of Chemical Reactor Engineer, 3, 0

20. Performance assessment of HC-290 as a drop-in substitute to HCFC-22 in a window air conditioner
Devotta, S.; Padalkar, A.S.; Sane, N.K.
International Journal of Refrigeration, 28(4), 594

21. Lilliputian hardware platform for scientific applications
Iyer, N.; Khatavkar, R.; Joshi, B.; Upadhye, V.
International Journal of Software Engineering and, 15(2), 189

22. Vapor-liquid equilibria of ammonia + water + potassium hydroxide and ammonia + water + sodium hydroxide solutions at temperatures from (293.15 to 353.15) K
Salavera, D.; Chaudhari, S.K.; Esteve, X.; Coronas, A.
Journal of Chemical and Engineering Data, 50(2), 471

23. Morphology and chain dynamics during collapse transition of pnipam gels studied by combined imaging, relaxometry and Xe-129 spectroscopy techniques
kariyo, S.; Kuppers, M.; Badiger, M.V.; Prabhakar, A.; Jagdeesh, B.; Stapf, S.; Blumich, B.
Magnetic Resonance Imaging, 23(2), 249

24. An SVM classifier incorporating simultaneous noise reduction and feature selection: Illustrative case examples
Kumar, R.; Jayaraman, V.K.; Kulkarni, B.D.
Pattern Recognition, 38(1), 41

25. Measuring organizational scientific productivity: A study at NCL
Mehta, N.
Current Science, 88(2), 223i

26. Encoding and decoding graphical chemical structures as two-dimensional (PDF417) barcodes
Karthikeyan, M.; Bender, A.
Journal of Chemical Information and Modeling, 45(3), 572

27. General melting point prediction based on a diverse compound data set and artificial neural networks
Karthikeyan, M.; Glen, R.C.; Bender, A.
Journal of Chemical Information and Modeling, 45(3), 581i

RESEARCH PAPERS PUBLISHED

Materials Chemistry

1. Recent applications of chloroaluminate ionic liquids in promoting organic reactions
Sarma, D.; Kumar, A.
ACS Symposium Series, 902, 350

2. (E)-1-(2-Hydroxy-3,4-dimethoxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one
Krishna, J.R.; Kumar, N.J.; Krishnalah, M.; Rao, C.V.; Rao, Y.K.; Puranik, V.G.
Acta Crystallographica Section E: Structure Report, 61(5), 1323

3. Synthesis and assembly of gold nanoparticles in quasi-linear lysine-keggin-ion colloidal particles
Sanyal, A.; Mandal, S.; Sastry, M.
Advanced Functional Materials, 15(2), 273

4. Bioleaching of sand by the fungus fusarium oxysporum as a means of producing extracellular silica nanoparticles
Bansal, V.; Sanyal, A.; Rautaray, D.; Sastry, M.; Ahmad, A.
Advanced Materials, 17(7), 889

5. Enhancement of double-layer capacitance behavior and its electrical conductivity in layered poly (3, 4-ethylenedioxythiophene)-based nanocomposites
Murugan, A.V.; Viswanath, A.K.; Campet, G.; Gopinath, C.S.; Vijayamohanan, K.
Applied Physics Letters, 87(24), 1

6. Deposition of PTFE thin films by RF plasma sputtering on 1 0 0 silicon substrates
Bodas, D.S.; Mandale, A.B.; Gangal, S.A.
Applied Surface Science, 245(1-4), 202

7. Deposition of indium nitride films by activated reactive evaporation process - A feasibility study
Patil, S.J.; Bodas, D.S.; Gangal, S.A.; Mandale, A.B.
Applied Surface Science, 245(1-4), 73

8. Free-standing nanogold membranes as supports for the growth of calcium phosphate crystals
Rautaray, D.; Sastry, M.
Biotechnology Progress, 21(6), 1759

9. Silver nanoparticles of variable morphology synthesized in aqueous foams as novel templates
Manual, S.; Arumugam, S.K.; Pasricha, R.; Sastry, M.
Bulletin of Material Science, 28(5), 503

10. Preparation of nanocrystalline ferroelectric BaNb2O6 by citrate gel method
Gaikwad, S.P.; Ravi, V.; Samuel, V.; Pasricha, R.
Bulletin of Materials Science, 28(2), 121

11. A coprecipitation technique to prepare ZnNb2O6 powders
Deshpande, V.V.; Patil, M.M.; Navale, S.C.; Ravi, V. *Bulletin of Materials Science, 28(3), 205*

12. Preparation of ultrafine LiTaO3 powders by citrate gel method
Navale, S.C.; Samuel, V.; Ravi, V.
Bulletion of Material Science, 28(5), 391

13. Synthesis of Ce0.75Zr0.25O2 at 100 °C
Dhage, S.R.; Gaikwad, S.P.; Ravi, V.; Muthukumar, P.
Ceramics International, 31(1), 211

14. Co-precipitation method for the preparation of fine ferroelectric BaBi 2Nb2O9
Gaikwad, S.P.; Potdar, H.S.; Ravi, V.; Samuel, V.
Ceramics International, 31(3), 379

15. Synthesis of bismuth oxide nanoparticles using bismuth nitrate and urea
Jha, R.K.; Pasricha, R.; Ravi, V.
Ceramics International, 31(3), 495

16. Synthesis of nanocrystalline rutile
Samuel, V.; Pasricha, R.; Ravi, V.
Ceramics International, 31(4), 555

17. Preparation of nanocrystalline ferroelectric CaBi2Ta 2O9 by the urea method
Gaikwad, S.P.; Pasricha, R.; Ravi, V.
Ceramics International, 31(6), 773

18. Synthesis of bismuth oxide nanoparticles by citrate gel method
Anilkumar, M.; Pasricha, R.; Ravi, V.
Ceramics International, 31(6), 889

19. Wet-chemical templateless assembly of metal nanowires from nanoparticles
Maddanimath, T.; Kumar, A.; D'Arcy-Gall, J.; Ganesan, P.G.; Ramanath, G.; Maddanimath, T.; Vijayamohanan, K.
Chemical Communications, (11), 1435

20. Hollow gold and platinum nanoparticles by a transmetallation reaction in an organic solution
Selvakannan, P.R.; Sastry, M.
Chemical Communications, (13), 1684

21. On the single root approach within the framework of coupled-cluster theory in fock space
Horny, L.; Schaefer, H.F.; Hubac, I.; Pal, S.
Chemical Physics, 315(3), 240

22. 2,5-Dioxido-1,4-Benzoquinonediimine (H2L2-), A Hydrogen bonding noninnocent bridging ligand related to animated topaquinone - different oxidation-state distributions in complexes [((BPY)(2)RU)(2)(MU-H2L)(N) (N=0,+,2+,3+,4+) and [((ACAC)(2)RU)(2)(MU-H
Kar, S.; Sarkar, B.; Ghumaan, S.; Janardanan, D.; VanSlageren, J.; Fiedler, J.; Puranik, V.G.; Sunoj, R.B.; Kaim, W.; Lahiri, G.K.
Chemistry - A European Journal, 11(17), 4901

23. Benzoyl transfer reactivities of racemic 2,4-di-O-acyl-myo-inositol 1,3,5-orthoesters in the solid state: Molecular packing and intermolecular interactions correlate with the ease of the reaction
Sarmah, M.P.; Shashidhar, M.S.; Gonnade, R.G.; Bhadbhade, M.M.
Chemistry - A European Journal, 11(7), 2103

24. Structural, electronic, and bonding properties of zeolite Sn-beta: A periodic density functional theory study
Shetty, S.; Pal, S.; Kanhere, D.G.; Goursot, A.
Chemistry - A European Journal, 12(2), 518

25. Nature of manganese species in Ce1-xMnxO 2- solid solutions synthesized by the solution combustion route
Murugan, B.; Ramaswamy, A.V.; Srinivas, D.; Gopinath, C.S.; Ramaswamy, V.
Chemistry of Materials, 17(15), 3983

26. Porous gold nanospheres by controlled transmetalation reaction - A novel material for application in cell imaging Porous gold nanospheres by controlled transmetalation reaction - A novel material for ap
Shukla, S.; Priscilla, A.; Banerjee, M.; Bhonde, R.R.; Ghatak, J.; Satyam, P.V.; Sastry, M.
Chemistry of Materials, 17(20), 5000

27. Direct synthesis of well-ordered and unusually reactive FeSBA-15 mesoporous molecular sieves
Vinu, A.; Sawant, D.P.; Ariga, K.; Hossain, K.Z.; Halligudi, S.B.; Hartmann, M.; Nomura, M.
Chemistry of Materials, 17(21), 5339

28. Synthesis, characterization, electronic structure, and photocatalytic activity of nitrogen-doped TiO2 nanocatalyst
Sathish, M.; Viswanathan, B.; Viswanath, R.P.; Gopinath, C.S.
Chemistry of Materials, 17(25), 6349

29. Direct observation of Ni metal impurities in lightly doped ferromagnetic polycrystalline (ZnNi)O
Deka, S.; Joy, P.A. Chemistry of Materials, 17(26), 6507

30. Controlling the optical properties of lemongrass extract synthesized gold nanotriangles and potential application in infrared-absorbing optical coatings
Shankar, S.S.; Rai, A.; Sastry, M.; Ahmad, A.
Chemistry of Materials, 17(3), 566

31. Polymerization in surfactant liquid crystalline phases
Wadekar, M.N.; Pasricha, R.; Gaikwad, A.B.; Kumaraswamy, G.
Chemistry of Materials, 17(9), 2460

32. Electronic spectra and ionization potentials of halogen oxides using the fock space coupled-cluster method
Vaval, N.; Manohar, P.; Pal, S.
Collection of Czechoslovak Chemical Communications, 70(7), 851

33. Corrosion protective poly(o-toluidine) coatings on copper
Shinde, V.; Patil, P.P.; Sainkar, S.R.
Corrosion Science, 47(6), 1352

34. Biological synthesis of stable vaterite crystals by the reaction of calcium ions with germinating chickpea seeds
Rautaray, D.; Sanyal, A.; Bharde, A.; Sastry, M.; Ahmad, A.
Crystal Growth and Design, 5(2), 399

35. Short S=OC=O contacts associate diastereomers of, 2,4(6)-di-O-benzoyl-6(4)-O-[(1S)-10-camphorsulfonyl]-myo-inositol 1,3,5-orthoformate in their inclusion complexes
Manoj, K.; Sureshan, K.M.; Gonnade, R.G.; Bhadbhade, M.M.; Shashidhar, M.S.
Crystal Growth and Design, 5(3), 833

36. Identical molecular strings woven differently by intermolecular interactions in dimorphs of myo-inositol 1,3,5-orthobenzoate
Bhosekar, G.; Murali, C.; Gonnade, R.G.; Shashidhar, M.S.; Bhadbhade, M.M.
Crystal Growth and Design, 5(5), 1977

37. DNA and PNA as templates for building nanoassemblies via electrostatic complexation with gold nanoparticles
Gourishankar, A.; Ganesh, K.N.; Shukla, S.; Pasricha, R.; Sastry, M.
Current Applied Physics, 5(2), 102

38. Interfacing biology with nanoparticles
Mandal, S.; Phadtare, S.; Sastry, M.
Current Applied Physics, 5(2), 118

39. Calcite growth in Cissus quadrangularis plant extract, a traditional Indian bone-healing aid
Sanyal, A.; Ahmad, A.; Sastry, M.
Current Science, 89(10), 1742

40. Gradual transitions in morphology of diamond films grown by using N 2 admixtures of CH4+H2 gas in a hot filament assisted chemical vapour deposition system
Kshirsagar, S.T.; Kshirsagar, R.B.; Patil, P.S.; Kulkarni, A.V.; Mandale, A.B.; Gaikwad, A.B.; Gokhale, S.P.
Diamond and Related Materials, 14(2), 232

41. Electrochemical studies of poly (3,4-ethylenedioxythiophene) PEDOT/VS 2 nanocomposite as a cathode material for rechargeable lithium batteries
Murugan, A.V.; Gopinath, C.S.; Vijayamohanan, K.
Electrochemistry Communications, 7(2), 213

42. Using the dynamic, expanding liquid-liquid interface in a Hele-Shaw cell in crystal growth and nanoparticle assembly
Rautaray, D.; Kavathekar, R.; Sastry, M.
Faraday Discussions, 129, 205

43. Rapid microwave -hydrothermal (MH) synthesis of Ba1-xSrxTiO3 (BST) powders and their characterization
Deshpande, S.B.; Khollam, Y.B.; Potdar, H.S.
Ferroelectrics, 327(1), 39

44. Oriented growth of nanocrystalline gamma ferric oxide in electrophoretically deposited films
Bhave, T.M.; Balasubramanian, C.; Nagar, H.; Kulkarni, S.; Pasricha, R.; Bakare, P.P.; Date, S.K.; Bhoraskar, S.V.
Hyperfine Interaction, 160(1-4), 199

45. Destructive adsorption of methyl parathion over nanocrystalline MgO
Prasad, R.; Gupta, R.K.; Chumbale, V.R.; Reddy, V.S.; Radheshyam, A.; Dwivedi, R.
Indian Journal of Chemistry - Section A Inorganic,, 44(2), 251

46. Improved synthesis of an energetic material, 1,3,3-trinitroazetidine (TNAZ) exploiting 2-iodoxy benzoic acid (IBX) as an oxidising agent
Singh, A.; Sikder, N.; Sikder, A.K.
Indian Journal of Chemistry - Section B Organic an, 44(12), 2560

47. Unusual monodentate binding mode of 2,2-dipyridylamine (L) in isomeric trans-(acac)2RuII(L)2, trans-[(acac)2RuIII(L)2]ClO4, and cis-(acac)2RuII(L)
Kar, S.; Chanda, N.; Mobin, S.M.; Lahiri, G.K.; Urbanos, F.A.; Jimenez-Aparicio, R.; Niemeyer, M.; Puranik, V.G.
Inorganic Chemistry, 44(5), 1571

48. Novel method for the synthesis of siloxane nanowires and filaments using gold nanoparticle catalysts
Prasad, B.L.V.; Stoeva, S.; Sorensen, C.M.; Klabunde, K.J.; Zaikovskii, V.
International Journal of Nanoscience, 4(5-6), 1007

49. Dimorphism in Benjaminiella poitrasii: Light, fluorescence and scanning electron microscopy studies of the vegetative and reproductive forms with special reference to the Glutamate Dehydrogenase, a Novel fungicidal Target
Ghormade, V.; Sainkar, S.; Joshi, C.; Doiphode, N.; Deshpande, M.V.
J. Mycol Plant Pathol, 35, 1

50. Magnetic properties of superparamagnetic lithium ferrite nanoparticles
Verma, S.; Joy, P.A.
Journal of Applied Physics, 98(12), 1

51. Electrochemical synthesis and corrosion protection properties of poly(o-toluidine) coatings on low carbon steel
Shinde, V.; Patil, P.P.; Sainkar, S.R.
Journal of Applied Polymer Science, 96(3), 685

52. Determination of 13C CSA tensors: Extension of the model-independent approach to an RNA kissing complex undergoing anisotropic rotational diffusion in solution
Ravindranathan, S.; Kim, C.-H.; Bodenhausen, G.
Journal of Biomolecular NMR, 33(3), 163

53. Analytically continued Fock space multireference coupled-cluster theory: Application to the 2g shape resonance in e-N 2 scattering
Sajeev, Y.; Santra, R.; Pal, S.
Journal of Chemical Physics, 122(23), 34320

54. Correlated complex independent particle potential for calculating electronic resonances
Sajeev, Y.; Santra, R.; Pal, S.
Journal of Chemical Physics, 123(20), 4110

55. Separability of local reactivity descriptors
Tanwar, A.; Pal, S.
Journal of Chemical Sciences, 117(5), 497

56. Phase transfer of oleic acid capped NicoreAgshell nanoparticles assisted by the flexibility of oleic acid on the surface of silver
Bala, T.; Swami, A.; Prasad, B.L.V.; Sastry, M.
Journal of Colloid and Interface Science, 283(2), 422

57. Cure characteristics and dielectric properties of magnetic composites containing strontium ferrite
Soloman, M.A.; Kurian, P.; Anantharaman, M.R.; Joy, P.A.
Journal of Elastomers and Plastics, 37(2), 109

58. Co-precipitation method for the preparation of nanocrystalline ferroelectric SrBi2Nb2O9 ceramics
Gaikwad, S.; Dhage, S.; Potdar, H.; Ravi, V.; Samuel, V.
Journal of Electroceramics, 14(1), 83

59. Characterization of Barium-Titanate BaTiO3 (BT) ceramics prepared from SOL-Gelderived BT powders
Deshpande, S.B.; Godbole, P.D.; Khollam, Y.B.; Potdar, H.S.
Journal of Electroceramics, 15(2),103

60. Photoluminescent core-shell particles of organic dye in silica
Ethiraj, A.S.; Hebalkar, N.; Kharrazi, S.; Urban, J.; Sainkar, S.R.; Kulkarni, S.K.
Journal of Luminescence, 114(1), 15

61. Increasing the sensitivity of 2-D high-resolution NMR methods applied to quadrupolar Nuclei
Amoureux, J.P.; Delevoye, L.; Steuernagel, S.; Gan, Z.; Ganapathy, S.; Montagne, L.
Journal of Magnetic Resonance, 172(2), 268

62. New approaches to the synthesis of anisotropic, core-shell and hollow metal nanostructures
Sastry, M.; Swami, A.; Mandal, S.; Selvakannan, P.R.
Journal of Materials Chemistry, 15(31), 3161

63. Synthesis of gold, silver and their alloy nanoparticles using bovine serum albumin as foaming and stabilizing agent
Singh, A.V.; Bandgar, B.M.; Kasture, M.; Prasad, B.L.V.; Sastry, M.
Journal of Materials Chemistry, 15(48), 5115

64. Entrapment of poly(3,4-ethylenedioxythiophene) between VS2 layers to form a new organic-inorganic intercalative nanocomposite
Murugan, A.V.; Quintin, M.; Delville, M.-H.; Campet, G.; Vijayamohanan, K.
Journal of Materials Chemistry, 15(8), 902

65. Study of correlation of structural and surface properties with electrochemical behaviour in carbon aerogels
Hebalkar, N.; Arabale, G.; Sainkar, S.R.; Pradhan, S.D.; Mulla, I.S.; Vijayamohanan, K.; Ayyub, P.; Kulkarni, S.K.
Journal of Materials Science, 40(14), 3777

66. Co-precipitation method for the preparation of ferroelectric CaBi4Ti4O15 Gaikwad, S.P.; Dhage, S.R.; Ravi, V. Journal of Materials Science: Materials in Electro, 16(4), 229

67. Effects of conjugation length and donor-acceptor functionalization on the non-linear optical properties of organic push-pull molecules using density functional theory
Datta, A.; Pal, S.; Datta, A.
Journal of Molecular Structure: THEOCHEM, 715(1-3), 59

68. Biosynthesis of gold and silver nanopartivles using Emblica Officcinalis fruit extract, their phase transfer and transmetallation in an organic solution
Ankamwar, B.; Damle, C.; Ahmad, A.; Sastry, M.
Journal of Nanoscience and Nanotechnology, 5(10), 1665

69. Synthesis of gold nanospheres and nanotriangles by the Turkevich approach
Shankar, S.S.; Bhargava, S.; Sastry, M.
Journal of Nanoscience and Nanotechnology, 5(10), 1721

70. Recent advances in biodegradable nanocomposites
Pandey, J.K.; Kumar, A.P.; Misra, M.; Mohanty, A.K.; Drzal, L.T.; Singh, R.P.
Journal of Nanosciences and Nanotechnology, 5(4), 497

71. Synthesis and intramolecular nitrile oxide cycloaddition of 3,5'-ether-linked psudooligosaccharide derivatives - An approach to chral macrooxacycles
Sengupta, J; Mukhopadhyay, R.; Mhattacharjya, A.; Bhadbhade, M.M.; Bhosekar, G.V.
Journal of Organic Chemistry, 70(21), 8579

72. Reassessment of the binary, ternary, and quaternary interactions in mixed electrolytes from thermodynamic quantities: The systems with uncommon ions containing hydrophobice character
Kumar, A.
Journal of Physical Chemistry B, 109(23), 11743

RESEARCH PAPERS PUBLISHED

73. Effect of RuO_2 in the shape selectivity of submicron-sized SnO_2structures
Ramgir, N.S.; Mulla, I.S.; Vijayamohanan, K.P.
Journal of Physical Chemistry B, 109(25), 12297

74. Optimization of nonlinear optical properties by substituent position, geometry and symmetry of the molecule: An ab initio study
Davis, D.; Sreekumar, K.; Sajeev, Y.; Pal, S.
Journal of Physical Chemistry B, 109(29), 14093

75. Layered inorganic-organic clay-like nanocomposites rearrange to form silsesquioxanes on acid treatment
Kumarswamy, G.; Deshmukh, Y.; Agarwal, V.V.; Rajmohanan, P.
Journal of Physical Chemistry B, 109(33), 16034

76. Transmetalation reaction between hydrophobic silver nanoparticles and aqueous chloroaurate ions at the air-water interface
Pasricha, R.; Swami, A.; Sastry, M.
Journal of Physical Chemistry B, 109(42), 19620

77. Temperature-induced phase transitions of the ordered superlattice assembly of Au nanoclusters
Chaki, N.K.; Vijayamohanan, K.P.
Journal of Physical Chemistry B, 109(7), 2552

78. Preparation and characterization of composite electrodes of coconut-shell-based activated carbon and hydrous ruthenium oxide for supercapacitors
Dandekar, M.S.; Arabale, G.; Vijayamohanan, K.
Journal of Power Sources, 141(1), 198

79. Formation of $BaCrO_4$ nano crystallites within thermally evaporated sodium BIS-2-Ethylhexyl-sufosuccinate and stearic-acid thin-films
Rautaray, D.; Sinha, K.; Sainkar, S.R.; Pasricha, R.; Pavaskar, N.R.; Sastry, M.
Journal of the American Ceramic Society, 88(1), 24

80. A novel low-temperature synthesis of nanosized NIZN ferrite
Verma, S.; Pradhan, S.D.; Pasricha, R.; Sainkar, S.R.; Joy, P.A.
Journal of the American Ceramic Society, 88(9), 2597

81. Bacterial aerobic synthesis of nanocrystalline magnetite
Bharde, A.; Wani, A.; Shouche, Y.; Joy, P.A.; Prasad, B.L.V.; Sastry, M.
Journal of the American Chemical Society, 127(26), 9326

82. Studies on effect of silane coupling agent on the mechanical properties of clay filled natural rubber
Alkadasi, N.A.N.; Sarwade, B.D.; Kapadi, U.R.; Hundiwale, D.G.
Journal of the Indian Chemical Society, 82(11), 985

83. Thermal, magnetic and spectral studies of metal-quinone complexes: Part III. Radical coordination and hydrogen bonding mediated exchange interaction in copper-hydroxyquinone complex
Salunke-Gawali, S.; Salunke-Gawali, S.; Boukheddaden, K.; Codjovi, E.; Linares, J.; Varret, F.; Rane, S.Y.; Bakare, P.P.
Journal of Thermal Analysis and Calorimetry, 79(3), 669

84. Durability of natural fiber-reinforced composites of ethylene-propylene copolymer under accelerated weathering and composting conditions
Kumar, A.P.; Depan, D.; Singh, R.P.
Journal of Thermoplastic Composite Materials, 18(6), 489

85. Synthesis of hydroxyapatite crystals using amino acid-capped gold nanoparticles as a scaffold
Rautaray, D.; Mandal, S.; Sastry, M.
Langmuir, 21(11), 5185

86. Heavy-metal remediation by a fungus as a means of production of lead and cadmium carbonate crystals
Sanyal, A.; Rautaray, D.; Bansal, V.; Ahmad, A.; Sastry, M.
Langmuir, 21(16), 7220

87. Gold nanoparticle networks with photoresponsive interparticle spacings
Sidhaye, D.S.; Kashyap, S.; Sastry, M.; Hotha, S.; Prasad, B.L.V.
Langmuir, 21(17), 7979

88. Reversible transformations of gold nanoparticle morphology
Stoeva, S.I.; Zaikovski, V.; Prasad, B.L.V.; Stoimenov, P.K.; Sorensen, C.M.; Klabunde, K.J.
Langmuir, 21(23), 10280

89. Cobalt and magnesium ferrite nanoparticles: Preparation using liquid foams as templates and their magnetic characteristics
Bala, T.; Sankar, C.R.; Baidakova, M.; Osipov, V.; Enoki, T.; Joy, P.A.; Prasad, B.L.V.; Sastry, M.
Langmuir, 21(23), 10638

RESEARCH PAPERS PUBLISHED

90. Biocompatibility of gold nanoparticles and their endocytotic fate inside the cellular compartment: A microscopic overview
Shukla, R.; Bansal, V.; Chaudhary, M.; Basu, A.; Bhonde, R.R.; Sastry, M.
Langmuir, 21(23), 10644

91. Solvent-adaptable silver nanoparticles
Prasad, B.L.V.; Arumugam, S.K.; Bala, T.; Sastry, M.
Langmuir, 21(3), 822

92. Keggin ion mediated synthesis of hydrophobized Pd nanoparticles for multifunctional catalysis
Mandal, S.; Das, A.; Sastry, M.; Srivastava, R.
Langmuir, 21(6), 2408

93. Effect of connectivity and terminal functionality on mesophase behaviour of thermotropic liquid crystals containing biphenyl units
Ranganathan, T.; Ramesh, C.; Kumar, A.
Liquid Crystals, 32(4), 499

94. Growth-kinetics and thermodynamic stability of Octadecyltrichlorosilane self-assembled monolayer on Si (100) substrate
Kulkarni, S.A.; Mirji, S.A.; Mandale, A.B.; Gupta, R.P.;Vijayamohanan, K.P.
Material Letters, 59(29-30), 3890

95. Low-temperature synthesis of $MGTA_2O_6$ powders
Navale, S.C.; Samuel, V.; Ravi, V.
Material Letters, 59(29-30), 3926

96. Simple oxalate precursor route for the preparation of barium-strontium titanate: $Ba_{1-x}Sr_xTiO_3$ powders
Khollam, Y.B.; Deshpande, S.B.; Potdar, H.S.; Bhoraskar, S.V.; Sainkar, S.R.; Date, S.K.
Materials Characterization, 54(1), 63

97. A coprecipitation technique to prepare $SrNb_2O_6$
Ravi, V.
Materials Characterization, 55(1), 92

98. Self-assembly of nanostructured PbS for solar photovoltaic applications
Hawaldar, R.R.; Mulik, U.P.; Amalnerkar, D.P.; Kanade, K.G.; Patil, K.R.; Sathaye, S.D.
Materials Chemistry and Physics, 91(2-3), 447

99. PVA stabilized gold nanoparticles by use of unexplored albeit conventional reducing agent
Khanna, P.K.; Gokhale, R.; Subbarao, V.V.V.S.; Vishwanath, A.K.; Das, B.K.; Satyanarayana, C.V.V
Materials Chemistry and Physics, 92(1), 229

100. Nanostructured tin oxide: Synthesis and gas-sensing properties
Niranjan, R.S.; Hwang, Y.K.; Kim, D.-K.; Jhung, S.H.; Chang, J.-S.; Mulla, I.S.
Materials Chemistry and Physics, 92(2-3), 384

101. Synthesis of fine PbE (E = S, Se) powder from direct in situ reduction of sulphur or selenium
Khanna, P.K.; Subbarao, V.V.V.S.; Wagh, M.; Jadhav, P.; Patil, K.R.
Materials Chemistry and Physics, 93(1), 91

102. Synthesis of $Sr_{0.5}Ba_{0.5}Nb_2O_6$ by citrate gel method
Pasricha, R.; Ravi, V.
Materials Chemistry and Physics, 94(1), 34

103. Preparation of ferroelectric $BaNb_2O_6$ by the urea method
Dhage, S.R.; Ravi, V.; Pasricha, R.
Materials Letters, 59(14-15), 1929

104. Deposition and characterization of silver nano-films by a novel solid liquid interface reaction technique (SLIRT)
Godbole, P.D.; Mitra, A.; Pasricha, R.; Mandale, A.B.; Patil, K.R.
Materials Letters, 59(14-15), 1958

105. Preparation of nanocrystalline $MgNb_2O_6$ by citrate gel method
Ravi, V.; Pasricha, R.
Materials Letters, 59(17), 2146

106. Preparation of nanocrystalline $LiNbO_3$ by citrate gel method
Navale, S.C.; Samuel, V.; Ravi, V.
Materials Letters, 59(19-20), 2476

107. Synthesis of bismuth oxide nanoparticles at 100 °c
Patil, M.M.; Deshpande, V.V.; Dhage, S.R.; Ravi, V.
Materials Letters, 59(19-20), 2523

108. Low-temperature synthesis of nanocrystalline powders of lithium ferrite by an autocombustion method using citric acid and glycine
Verma, S.; Karande, J.; Patidar, A.; Joy, P.A.
Materials Letters, 59(21), 2630

109. Synthesis of rutile from ATO and stearic acid
Patil, M.M.; Deshpande, V.V.; Desphande, S.B.; Samuel, V.; Ravi, V.
Materials Letters, 59(21), 2673

RESEARCH PAPERS PUBLISHED

110. Synthesis and characterization of microwave-hydrothermally derived Ba 1-xSrxTiO3 powders
Deshpande, S.B.; Sainkar, S.R.; Potdar, H.S.; Khollam, Y.B.; Bhoraskar, S.V.; Date, S.K.
Materials Letters, 59(2-3), 293

111. Synthesis of chromium substituted nano particles of cobalt zinc ferrites by coprecipitation
Sharma, R.K.; Suwalka, O.; Lakshmi, N.; Venugopalan, K.; Banerjee, A.; Joy, P.A.
Materials Letters, 59(27), 3402

112. Synthesis of bismuth titanate by the urea method
Anilkumar, M.; Dhage, S.R.; Ravi, V.; Anilkumar, M.
Materials Letters, 59(4), 514

113. Novel polymer-inorganic solid-state reaction for the synthesis of CdS nanocrystallites
Kanade, K.G.; Hawaldar, R.R.; Seth, T.; Mulik, U.P.; Kale, B.B.; Amalnerkar, D.P.; Pasricha, R.; Radhakrishnan, S.
Materials Letters, 59(5), 554

114. Synthesis of fine particles of ZnO at 100 ^{o}c
Dhage, S.R.; Ravi, V.; Pasricha, R.
Materials Letters, 59(7), 779

115. Synthesis of Sr0.5Ba0.5Nb2O6 by urea method
Dhage, S.R.; Ravi, V.; Pasricha, R.
Materials Letters, 59(8-9), 1053

116. Synthesis of nanocrystalline Mn3O4 at 100 ^{o}c
Anilkumar, M.; Ravi, V.; Anilkumar, M.
Materials Research Bulletin, 40(4), 605

117. X-ray photoelectron spectroscopic investigations of Cu2O nanoparticles
Nikesh, V.V.; Mahamuni, S.; Mandale, A.B.; Patil, K.R.
Materials Research Bulletin, 40(4), 694

118. Synthesis and NMR characterization of SAPO-35 from non-aqueous systems using hexamethyleneimine template
Venkatathri, N.
Materials Research Bulletin, 40(7), 1157

119. Growth of PbS nanopyramidal particulate films for potential applications in quantum-dot photovoltaics and nanoantennas
Hawaldar, R.; Mulik, U.; Patil, K.; Pasricha, R.; Sathaye, S.; Lewis, A.; Amalnerkar, D.
Materials Research Bulletin, 40(8), 1353

120. TiO2 ceramic varistor modified with Tantalum and Barium
Gaikwad, A.B.; Navale, S.C.; Ravi, V.
Materials Science and Engineering B - Solid state, 123(1), 50

121. Preparation of nanocrystalline ferroelectric CaBi2Ta 2O9 by citrate gel method
Gaikwad, S.P.; Ravi, V.; Pasricha, R.
Materials Science and Engineering B: Solid-State M, 117(2), 159

122. A coprecipitation technique to prepare BaNb2O6
Natarajan, N.; Ravi, V.; Samuel, V.; Pasricha, R.
Materials Science and Engineering B: Solid-State M, 117(2), 169

123. A rapid hydrothermal synthesis route for nanocrystalline SrZrO3 using reactive precursors
Athawale, A.A.; Bapat, M.; Chandwadkar, A.; Karandikar, P.
Materials Science and Engineering B: Solid-StateM, 119(1),87

124. Preparation of fine MgTa2O6 and Mg4Ta 2O9 powders by chemical methods
Navale, S.C.; Ravi, V.
Materials Science and Engineering B: Solid-State M, 119(2), 189

125. Zincoaluminophosphate molecular sieves with AFI and ATS topologies: Synthesis by dry-gel conversion methods and their catalytic properties in the isopropylation of biphenyl
Saha, S.K.; Maekawa, H.; Waghmode, S.B.; Mulla, S.A.R.; Komura, K.; Kubota, Y.; Sugi, Y.; Cho, S.J.
Materials Transactions, 46(12), 2659

126. Influence of hydrothermal pretreatment on acidity and activity of H-GaAlMFI zeolite for the propane aromatization reaction
Choudhary, T.V.; Kinage, A.; Banerjee, S.; Choudhary, V.R.
Microporous and Mesoporous Materials, 87(1), 23

127. Synthesis, characterization and catalytic application of Ru II-ethylenediamine complex-mesoporous silica as heterogeneous catalyst system in chemo-selective hydrogenation of alpha, beta-unsaturated carbonyl compounds
Ghosh, A.; Kumar, R.
Microporous and Mesoporous Materials, 87(1), 33

128. A general formalism of the Fock space multireference coupled cluster method for investigating molecular electronic resonances
Sanjeev, Y.; Pal, S.
Molecular Physics, 103(15-16), 2267

129. Controlled growth of nanocrystallites in silicon oxide matrix using 150 MeV Ag ion irradiation
Chaudhari, P.S.; Bhave, T.M.; Pasricha, R.; Singh, F.; Kanjilal, D.; Bhoraskar, S.V.
Nuclear Instru Methods in Phys Res Sec. B, 239(3), 185

RESEARCH PAPERS PUBLISHED

130. Superspin glass behavior of a nonstoichiometric lanthanum manganite LaMnO3.13
Sankar, C.R.; Joy, P.A.
Physical Review B - Condensed Matter and Materials, 7213(13), 2407(200

131. Magnetic properties of the self-doped Lanthanum Manganites LA1-XMnO3-Art.No.024405
Joy, P.A.
Physical Review B, 7202(2), 4405

132. Effect of disorder on the magnetic properties of LaMn0.5Fe0.5O3 - Art. No. 054426
Bhame, S.D.; Joly, V.L.J.; Joy, P.A.
Physical Review B, 7205(5), 4426

133. Tetrazine derived mononuclear RuII(acac)2(L) (1), [RuII(bpy)2(L)](ClO4)2 (2) and [RuII(bpy)(L)2](ClO4)2 (3) (L = 3-amino-6-(3,5-dimethylpyra
Nayak, A.; Patra, S.; Ghumaan, S.; Lahiri, G.K.; Sarkar, B.; Kaim, W.; Puranik, V.G.
Polyhedron, 24(2), 333

134. Brewster Angle Microscope - An excellent tool for Nanoscience Researchers
Iyer, N.; Joshi, B.; Khatavkar, R.
Proc of Int Conference on Nanomaterials NANO2005

135. Actuation behavioral studies on polyaniline-cllophane based electroactive paper
Deshpande, S.D.; Kim, J.; Song, C.; Li, Q.
Proc of SPIE - The Int Society for Optical Engg, 5759, 431

136. Surface disorder in c-Si induced by swift heavy ions
Bogle, K.A.; Gokhale, S.P.; Bhoraskar, V.N.
Radiation Effects and Defects in Solods, 160(6),207

137. A room temperature nitric oxide sensor actualized from Ru-doped SnO 2 nanowires
Ramgir, N.S.; Mulla, I.S.; Vijayamohanan, K.P.
Sensors and Actuators, B: Chemical, 107(2), 708

138. Studies on conducting polymer electroactive paper actuators: Effect of humidity and electrode thickness
Deshpande, S.D.; Kim, J.; Yun, S.-R.
Smart Materials and Structures, 14(4), 876

139. Influence of process pressure on HW-CVD deposited A-Si-H films
Jadkar, S.R.; Sali, J.V.; Kshirsagar, S.T.; Takwale, M.G.
Solar Energy materials and Solar Cells, 85(3), 301

140. Electronic structure and ferromagnetism of polycrystalline Zn 1-xCoxO (0x0.15)
Deka, S.; Joy, P.A.
Solid State Communications, 134(10), 665

141. Green nanocomposites from renewable resources: Effect of plasticizer on the structure and material properties of clay-filled starch
Pandey, J.K.; Singh, R.P.
Starch/Staerke, 57(1), 8

142. Characterization of 'ARE' deposited silicon nitride films and their feasibility as antireflection coating
Patil, S.J.; Mohite, K.C.; Mandale, A.B.; Takwale, M.G.; Gangal, S.A.
Surface and Coatings Technology, 200(7), 2058

143. Gold nanotriangles biologically synthesized using tamarind leaf extract and potential application in vapor sensing
Ankamwar, B.; Chaudhary, M.; Sastry, M.
Synthesis & Reactivity in Inorg and Metal-Org Chem, 35(1), 19

144. Sulfonate protecting groups. Synthesis of O- and C-methylated inositols: D- and L-ononitol, D- and L-laminitol, mytilitol and scyllo-inositol methyl ether
Sarmah, M.P.; Shashidhar, M.S.; Sureshan, K.M.; Gonnade, R.G.; Bhadbhade, M.M.
Tetrahedron, 61(18), 4437

145. Phase transitions in octanethiol-capped Ag nanocluster microfilm assemblies
Ellis, A.V.; D'Arcy-Gall, J.; Vijayamohanan, K.; Goswami, R.;Ganesan, P.G.; Ramanath, G.; Ellis, A.V.; Ryu, C.
Thermochimica Acta, 426(1-2), 207

146. Corrosion protection of low carbon steel by poly (O-toluidine) electrosynthesized from tartrate solution
Shinde, V.; Sainkar, S.R.; Patil, P.P.
Transactions of the SAEST (Society for Advancement, 40(3), 81

147. DNA-binding studies of mixed ligand cobalt(III) complexes
Barve, A.C.; Ghosh, S.; Kumbhar, A.A.; Kumbhar, A.S.; Puranik, V.G.
Transition Metal Chemistry, 30(3), 312

148. Metalloantitubercular compounds Part 3: Synthesis, crystal structure, spectroscopy, electrochemistry and antimycobacterial activity of the copper(II) ciproploxacin (cfH) complex and its phenanthroline adduct
Saha, D.K.; Patitungkho, S.; Padhye, S.; Deobagkar, D.N.; Ozarkar, A.; Bhadbhade, M.M.;Gonnade, R.G.
Transition Metal Chemistry, 30(3), 334

RESEARCH PAPERS PUBLISHED

Organic Chemistry

1. Conformationally constrained PNA analogues: Structural evolution toward DNA/RNA binding selectivity
Kumar, V.A.; Ganesh, K.N.
Accounts of Chemical Research, 38(5), 404

2. O-HO-bridged dimers linked via C-HO and C-H interactions in 4,6-di-O-benzyl-myo-inositol 1,3,5-orthoformate
Manoj, K.; Devaraj, S.; Gonnade, R.G.; Bhadbhade, M.M.; Shashidhar, M.S.
Acta Crystallographica Section C: Crystal Structur, 61(11), 628

3. Isopropyl 2,5-anhydro-3,4-di-O-tert butyldiphenylsilyl-L-ribonate
Glawar, A.F.G.; Watkin, D.J.; Sanjayan, G.J.; Tranter, G.E.; Edwards, A.A.; Fleet, G.W.J.
Acta Crystallographica Section E: Structure Report, 61(8), 0

4. New synthetic approach to a [1.1.6] metapara cyclophane derivative via Suzuki-Miyaura cross-coupling and ring-closing metathesis
Kotha, S.; Mandal, K.; Arora, K.K.; Pedireddi, V.R.
Advanced Synthesis and Catalysis, 347(9), 1215

5. A quantitative method for normalization of transfection efficiency using enhanced green fluorescent protein
Dandekar, D.H.; Kumar, M.; Ladha, J.S.; Ganesh, K.N.; Mitra, D.
Analytical Biochemistry, 342(2), 341

6. Nucleobases in molecular recognition: Molecular adducts of adenine and cytosine with COOH functional groups
Perumalla, S.R.; Suresh, E.; Pedireddi, V.R.
Angewandte Chemie - International Edition, 44(47), 7752

7. Catalytic transesterification of -ketoesters with zeolite H-FER under solvent free conditions
Chavan, S.P.; Pasupathy, K.; Shengule, S.; Shinde, V.; Anand, R.
Arkivoc, 2005(13), 162

8. Efficient and selective cleavage of the tert butoxycarbonyl (Boc) group under basic condition
Mohapatra, D.K.; Durugkar, K.A.
Arkivoc, 2005(14), 20

9. Asymmetric total synthesis of eicosanoid
Mohapatra, D.K.; Yellol, G.S.
Arkivoc, 2005(3), 144

10. Ring-closing metathesis mediated total synthesis of microcarpalide and herbarumin III
Gurjar, M.K.; Nagaprasad, R.; Ramana, C.V.; Karmakar, S.; Mohapatra, D.K.
Arkivoc, 2005(3), 237

11. An asymmetric dihydroxylation route to (R)-(-)-octopamine, (R)-(-)-tembamide and (R)-(-)-aegeline
Sadyandy, R.; Fernandes, R.A.; Kumar, P.
Arkivoc, 2005(3), 36

12. Novel enzymatic route for kinetic resolution of 1,4-benzodioxan- 2-carboxylic acid
Kasture, S.M.; Varma, R.; Kalkote, U.R.; Nene, S.; Kulkarni, B.D.
Biochemical Engineering Journal, 27(1), 66

13. Response of trichogramma-chilonis to infochemicals - An SEM and Electrophysisological investigation
Sen, A.; Raina, R.; Joseph, M.; Tungikar, V.B.
Biocontrol, 50(3), 429

14. Hydrogen bond mediated open-frame networks in coordination polymers: Supramolecular assemblies of Pr(III) and 3,5-dinitro-4 methylbenzoic acid with aza-donor compounds
Varughese, S.; Pedireddi, V.R.
Chemical Communications, (14), 1824

15. PNA C-C+ i-motif: superior stability of PNA TC8 tetraplexes compared to DNA TC8 tetraplexes at low pH
Sharma, N.K.; Ganesh, K.N.
Chemical Communications, (34), 4330

16. Concomitant dimorphs of tri-O-[p-halobenzoyl]-myo-inositol 1,3,5-orthoformates with different halogen bonding contacts: First order crystal-to-crystal thermal phase transition of kinetic form to the thermodynamic form
Gonnade, R.G.; Bhadbhade, M.M.; Shashidhar, M.S.; Sanki, A.K.
Chemical Communications, (47), 5870

17. Backbone-extended pyrrolidine peptide nucleic acids (bepPNA): Design, synthesis and DNA/RNA binding studies
Govindaraju, T.; Kumar, V.A.
Chemical Communications, 11(4), 495

RESEARCH PAPERS PUBLISHED

18. Structural rationalisation of co-crystals formed between trithiocyanuric acid and molecules containing hydrogen bonding functionality
Ahn, S.; Kariuki, B.M.; Prakashareddy, J.; Pedireddi, V.R.; Chatterjee, S.; Ranganathan, A.; Rao, C.N.R.; Harris, K.D.M.
Chemistry - A European Journal, 11(8), 2433

19. Larvicidal activity of Acacia nilotica extracts and isolation of D-pinitol - A bioactive carbohydrate
Chaubal, R.; Pawar, P.V.; Hebbalkar, G.D.; Tungikar, V.B.; Puranik, V.G.; Deshpande, V.H.; Deshpande, N.R.
Chemistry and Biodiversity, 2(5), 684

20. Poly(pseudo)rotaxane-like network mediated by hydrogen bonds in the solid-state structure of 1,7-phenanthroline
Arora, K.K.; Pedireddi, V.R.
Crystal Growth and Design, 5(4), 1309

21. BisPNA targeting to DNA: Effect of neutral loop on DNA duplex strand invasion by aepPNA-N7G/aepPNA-c substituted peptide nucleic acids
Shirude, P.S.; Kumar, V.A.; Ganesh, K.N.
European Journal of Organic Chemistry, (24), 5207

22. Synthesis of isoflavones containing naturally occurring substitution pattern by oxidative rearrangement of respective flavanones using thallium(III) p-tosylate
Singh, O.V.; Muthukrishnan, M.; Sunderavadivelu, M.
Indian Journal of Chemistry - Section B, 44(12), 2575

23. Enantioselective synthesis of (S)-arylpropionic acids via Pd-catalyzed kinetic resolution of benzylic alcohols
Thakur, V.V.; Sudalai, A.
Indian Journal of Chemistry - Section B, 44(3), 557

24. Stereoselective synthesis of (2R, 3S, 22R, 23E)-6, 6-ethylenedioxy-22- hydroxy- 2, 3-isopropylidenedioxy-24-methyl-5-cholest-23-ene: An intermediate for the synthesis of castasterone, dolichosterone and brassinolide
Hazra, B.G.; Kumar, T.P.; Pore, V.S.
Indian Journal of Chemistry - Section B, 44(3), 611

25. Titanium superoxide catalyzed selective oxidation of phenols to p-quinones with aq. H2O2
Dewkar, G.K.; Shaikh, T.M.; Pardhy, S.; Kulkarni, S.S.; Sudalai, A.
Indian Journal of Chemistry - Section B, 44(7), 1530

26. Pd-catalyzed oxidative kinetic resolution of 2-azido-1-arylethanols
Sayyed, I.A.; Kumar, N.S.C.R.; Sudalai, A.
Indian Journal of Chemistry - Section B, 44(7), 1533

27. Microwave promoted solvent-free one-pot synthesis of N,N- disubstituted urea derivatives
Jadhav, V.H.; Deshpande, S.S.; Borate, H.B.; Wakharkar, R.D.
Journal of Chemical Research, (3), 205

28. The synthesis of substituted tetrahydro-1H-xanthen 1-ones and xanthenes
Patil, M.L.; Borate, H.B.
Journal of Chemical Research, (7), 454

29. Diversity oriented synthesis of tricyclic compounds from glycals using the Ferrier and the Pauson-Khand reactions
Hotha, S.; Tripathi, A.
Journal of Combinatorial Chemistry, 7(6), 968

30. Absence of food aversion learning in the polyphagous noctuid, Spodoptera litura (F.) following intoxication by deleterious chemicals
Ghumare, S.S.; Mukherjee, S.N.
Journal of Insect Behavior, 18(1), 105

31. Asymmetric synthesis of both the enantiomers of trans-3-hydroxypipecolic acid
Kumar, P.; Bodas, M.S.
Journal of Organic Chemistry, 70(1), 360

32. Total synthesis of microcarpalide
Kumar, P.; Naidu, S.V.
Journal of Organic Chemistry, 70(10), 4207

33. Copper- and ligand-free Sonogashira reaction catalyzed by Pd(0) nanoparticles at ambient conditions under ultrasound irradiation
Gholap, A.R.; Venkatesan, K.; Pasricha, R.; Daniel, T.; Lahoti, R.J.; Srinivasan, K.V.
Journal of Organic Chemistry, 70(12), 4869

34. Self-assembly with degenerate prototropy
Baruah, P.K.; Gonnade, R.; Phalgune, U.D.; Sanjayan, G.J.
Journal of Organic Chemistry, 70(16), 6461

35. trans-5-aminopipecolyl-aegPNA chimera: Design, synthesis, and study of binding preferences with DNA/RNA in duplex/triplex mode
Lonkar, P.S.; Kumar, V.A.
Journal of Organic Chemistry, 70(17), 6956

36. A diastereoselective and general route to 5-amino-5-deoxysugars: Influence of C-3 substitution on the addition of amines to C-5 of vinyl sulfone-modified Hex-5-enofuranosyl carbohydrates
Das, I.; Pathak, T.; Suresh, C.G.
Journal of Organic Chemistry, 70(20), 8047

37. A carbohydrate-based approach for the total synthesis of 1,3-polyol/-pyrone antifungal natural products
Ramana, C.V.; Srinivas, B.; Puranik, V.G.; Gurjar, M.K.
Journal of Organic Chemistry, 70(20), 8216

38. Synthesis of eupomatilone-6 and assignment of its absolute configuration
Gurjar, M.K.; Karumudi, B.; Ramana, C.V.
Journal of Organic Chemistry, 70(23), 9658

39. Preorganizing linear (self-complementary) quadruple hydrogen-bonding arrays using intramolecular hydrogen bonding as the sole force
Prabhakaran, P.; Puranik, V.G.; Sanjayan, G.J.
Journal of Organic Chemistry, 70(24), 10067

40. 1,3-Dipolar cycloaddition reaction of D-glucose-derived nitrone with allyl alcohol: Synthesis of 2-hydroxy-1-deoxycastanospermine analogues
Karanjule, N.S.; Markad, S.D.; Dhavale, D.D.; Sharma, T.; Sabharwal, S.G.; Puranik, V.G.
Journal of Organic Chemistry, 70(4), 1356

41. Diastereoselective amidoalkylation of (3S,7aR)-6-benzyl-7-hydroxy-3- phenyltetrahydro-5H-imidazo[1,5-c][1,3]thiazol-5-one: A short and highly efficient synthesis of (+)-biotin
Chavan, S.P.; Chittiboyina, A.G.; Ravindranathan, T.; Kamat, S.K.; Kalkote, U.R.
Journal of Organic Chemistry, 70(5), 1901

42. Efficient total synthesis of sapinofuranone B
Kumar, P.; Naidu, S.V.; Gupta, P.
Journal of Organic Chemistry, 70(7), 2843

43. Synthesis, structure, electrochemistry and ROMP-activity of new ferrocenyl analog of Grubbs' metathesis catalyst
Maishal, T.K.; Sarkar, A.; Mondal, B.; Lahiri, G.K.; Puranik, V.G.; Wadgaonkar, P.P.
Journal of Organometallic Chemistry, 690(4), 1018

44. (SR/RS)-cyclohexanyl PNAs: Conformationally preorganized PNA analogues with unprecedented preference for duplex formation with RNA
Govindaraju, T.; Kumar, V.A.; Ganesh, K.N.
Journal of the American Chemical Society, 127(12), 4144

45. Facile oxidation of flavanones to flavones using [hydroxy(tosyloxy)iodo] benzene in an ionic liquid
Muthukrishnan, M.; Patil, P.S.; More, S.V.; Joshi, R.A.
Mendeleev Communications, (3), 100

46. A new bis-andrographolide ether from Andrographis paniculata nees and evaluation of anti-HIV activity
Reddy, V.L.N.; Reddy, S.M.; Ravikanth, V.; Krishnaiah, P.; Goud, T.V.; Rao, T.P.; Venkateswarlu, Y.; Ram, T.S.; Gonnade, R.G.; Bhadbhade, M.
Natural Product Research, 19(3), 223

47. Aziridine carboxylate from D-glucose: Synthesis of polyhydroxylated piperidine, pyrrolidine alkaloids and study of their glycosidase inhibition
Dhavale, D.D.; Kumar, K.S.A.; Chaudhari, V.D.; Sharma, T.; Sabharwal, S.G.; Prakashareddy, J.
Organic and Biomolecular Chemistry, 3(20), 3720

48. Stereospecific route to 5,11-methanomorphanthridine alkaloids via intramolecular 1,3-dipolar cycloaddition of nonstabilized azomethine ylide: Formal total synthesis of pancracine
Pandey, G.; Banerjee, P.; Kumar, R.; Puranik, V.G.
Organic Letters, 7(17), 3713

49. NaLO(4)/LIBR-mediated diastereoselective dihydroxylation of olefins - A catalytic approach to the Prevost-Woodward reaction
Emmanuel, L.; Shaikh, T.M.A.; Sudalai, A.
Organic Letters, 7(22), 5071

50. NBS-catalyzed hydroamination and hydroalkoxylation of activated styrenes
Talluri, S.K.; Sudalai, A.
Organic Letters, 7(5), 855

51. Synthesis and characterization of ferrocenylchalcogenopropargyl complexes [Fe(5-C5H4EICH 2C=CH)2] (EI = Se, S) and their reactions to form unusual ferrocenyl-containing met
Mathur, P.; Srinivasu, C.; Trivedi, R.; Bhunia, A.K.; Mathur, P.; Mobin, S.M.; Puranik, V.G.; Singh, V.K.
Organometallics, 24(3), 367

52. Proceedings of the National Conference on Nanoscience and Technology Part - I National Chemical Laboratory, Pune 7-8 March 2005 - Foreword
Sood, A.K.; Ganesh, K.N.; Sundar, C.S.; Raychaudhuri, A.K.
Pramana - Journal of Physics, 65(4), 547

---

53. Proceedings of the National Conference on Nanoscience and Technology Part - II - Foreword
Sood, A.K.; Ganesh, K.N.; Sundar, C.S.; Raychaudhuri, A.K.
Pramana - Journal of Physics, 65(5), 3

54. Mesityllithium
Mhaske, S.B.; Mhaske, S.B.
Synlett, (1), 184

55. Synthesis of bile acid dimers linked with 1,2,3-triazole ring at C-3, C-11, and C-24 positions
Aher, N.G.; Pore, V.S.
Synlett, (14), 2155

56. An efficient synthesis of 2,3-aziridino-lactones from azetidin-2-ones
Kale, A.S.; Deshmukh, A.R.A.S.
Synlett, (15), 2370

57. Sodium methylsulfinylmethylide: A versatile reagent
Mondal, M.
Synlett, (17), 2697

58. A facile regioselective decomposition of tosylhydrazones: An application towards the synthesis of -lipoic acid
Chavan, S.P.; Kale, R.R.; Pasupathy, K.
Synlett, (7), 1129

59. 2-Iodoxybenzoic acid (IBX): A versatile reagent
Kumar, I.
Synlett, (9), 1488

60. A facile synthesis of rubrolide E1
Kar, A.; Argade, N.P.
Synthesis-Stuttgart, (14), 2284

61. A concise account of recent SN2 Grignard coupling reactions in organic synthesis
Kar, A.; Argade, N.P.
Synthesis-Stuttgart, (18), 2995

62. A simple synthesis of sarkomycin
Kar, A.; Argade, N.P.
Synthesis-Stuttgart, (8), 1234

63. Simplistic expedient and practical synthesis of lipoic acid
Chavan, S.P.; Shivsankar, K.; Pasupathy, K.
Synthesis-Stuttgart, (8), 1297

64. A novel one-pot synthesis of 2-aryl-4(3H)-quinazolinones using room temperature ionic liquid as reaction medium as well as promoter
Potewar, T.M.; Nadaf, R.N.; Daniel, T.; Lahoti, M.J.; Srinivasan, K.V.
Synthetic Communications, 35(2), 231

65. Wittig-Horner approach for the synthesis of tamoxifen
Pandey, R.K.; Wakharkar, R.D.; Kumar, P.
Synthetic Communications, 35(21), 2795

66. A simple, concise, stereocontrolled synthesis of (8E,10Z)-pentadecadien-1- ol acetate
Chavan, S.P.; Kharul, R.K.; Kamat, S.K.; Kalkote, U.R.; Kale, R.R.
Synthetic Communications, 35(7), 987

67. New electro-active paper actuator using conducting polypyrrole: Actuation behaviour in LiClO4 acetonitrile solution
Deshpande, S.D.; Kim, J.; Yun, S.-R.; Deshpande, S.D.
Synthetic Metals, 149(1), 53

68. Activity of azadirachtin against the potato tuber moth Phthorimaea operculella (Zeller) (Lepidoptera: Gelechiidae)
Adu-Acheampong, R.; Sen, A.; Joshi, S.P.; Tungikar, V.B.; Mukherjee, S.N.
Tests of Agrochemicals and Cultivars, (26), 10

69. A simple and practical approach to enantiomerically pure (S)-3-hydroxy-butyrolactone: Synthesis of (R)-4-cyano-3-hydroxybutyric acid ethyl ester
Kumar, P.; Deshmukh, A.N.; Upadhyay, R.K.; Gurjar, M.K.
Tetrahedron Asymmetry, 16(16), 2717

70. Asymmetric synthesis of (-)-conhydrine
Kandula, S.R.V.; Kumar, P.
Tetrahedron Asymmetry, 16(19), 3268

71. An asymmetric aminohydroxylation route to (+)-L-733,060
Kandula, S.R.V.; Kumar, P.
Tetrahedron Asymmetry, 16(21), 3579

72. A convenient synthesis of the enantiomerically pure -blocker (S)-betaxolol using hydrolytic kinetic resolution
Joshi, R.A.; Garud, D.R.; Muthukrishnan, M.; Joshi, R.R.; Gurjar, M.K.
Tetrahedron Asymmetry, 16(23), 3802

73. Stereoselective synthesis of (2S,7S)-7-(4-phenoxymethyl)-2-(1-N- hydroxyureidyl-3-butyn-4-yl)oxepane: A potential anti-asthmatic drug candidate
Gurjar, M.K.; Krishna, L.M.; Rao, B.V.; Chorghade, M.S.; Ley, S.V.
Tetrahedron Asymmetry, 16(5), 935

RESEARCH PAPERS PUBLISHED

74. Synthetic studies toward tricyclic cembranoids: A modular approach for the construction of the tricyclic framework of eunicin
Gurjar, M.K.; Nayak, S.; Ramana, C.V.
Tetrahedron Letters, 46(11), 1881

75. Stereoselective synthesis of (-)-microcarpalide
Chavan, S.P.; Praveen, C.
Tetrahedron Letters, 46(11), 1939

76. Stereoselective synthesis of (+)-boronolide
Naidu, S.V.; Gupta, P.; Kumar, P.
Tetrahedron Letters, 46(12), 2129

77. A novel supramolecular assembly of 3,5-dinitro-4-methylbenzoic acid and trans-1,2-bis(4-pyridyl)ethene
Varughese, S.; Pedireddi, V.R.
Tetrahedron Letters, 46(14), 2411

78. A carbohydrate-based approach for the total synthesis of strictifolione
Ramana, C.V.; Raghupathi, N.; Gurjar, M.K.; Chorghade, M.S.
Tetrahedron Letters, 46(23), 4073

79. Stereoselective syntheses of (+)-alpha-conhydrine and (-)-beta-conhydrine from L-aspartic acid
Pandey, S.K.; Kumar, P.
Tetrahedron Letters, 46(23), 4091

80. Niobium(V) chloride catalyzed microwave assisted synthesis of 2,3-unsaturated O-glycosides by the Ferrier reaction
Hotha, S.; Tripathi, A.
Tetrahedron Letters, 46(27), 4555

81. Expedient synthesis of 1,2,3-triazole-fused tetracyclic compounds by intramolecular Huisgen ('click') reactions on carbohydrate-derived azido-alkynes
Hotha, S.; Anegundi, R.I.; Natu, A.A.
Tetrahedron Letters, 46(27), 4585

82. [6+3] Cycloaddition of fulvenes with 3-oxidopyrylium betaine: A novel methodology for the synthesis of fused cyclooctanoid natural products
Radhakrishnan, K.V.; Krishnan, K.S.; Bhadbhade, M.M.; Bhosekar, G.V.
Tetrahedron Letters, 46(28), 4785

83. An efficient stereoselective synthesis of (2S,4S,5R)-(-)- and (2R,4R,5S)-(+)-bulgecinine
Chavan, S.P.; Praveen, C.; Sharma, P.; Kalkote, U.R.
Tetrahedron Letters, 46(3), 439

84. Stereoselective synthesis of spiroannulated cyclopentenones by the Pauson-Khand reaction on carbohydrate derived enynes
Hotha, S.; Maurya, S.K.; Gurjar, M.K.
Tetrahedron Letters, 46(32), 5329

85. NaIO4-mediated C-H activation of alkylbenzenes and alkanes with LiBr
Shaikh, T.M.; Sudalai, A.
Tetrahedron Letters, 46(33), 5589

86. Stereoselective syntheses of (+)-proto, (-)-gala quercitols and carba-l-rhamnose from d-(-)-quinic acid
Murugan, A.; Yadav, A.K.; Gurjar, M.K.
Tetrahedron Letters, 46(37), 6235

87. An expeditious convergent synthesis of a dibromotyrosine alkaloid inhibitor of mycothiol-S-conjugate amidase
Chanda, B.M.; Sulake, R.S.
Tetrahedron Letters, 46(38), 6461

88. Enantioselective synthesis of tarchonanthuslactone via iterative hydrolytic kinetic resolution
Gupta, P.; Naidu, S.V.; Kumar, P.
Tetrahedron Letters, 46(38), 6571

89. Efficient total synthesis of iso-cladospolide B and cladospolide B
Pandey, S.K.; Kumar, P.
Tetrahedron Letters, 46(39), 6625

90. Chiral 2-C-methylene glycosides and carbohydrate-derived pyrano[2,3-B][1] benzopyrans - synthesis via incl3 catalyzed stereoselective ferrier rearrangement of 2-C-Acetoxymethyl glycal derivatives
Chakraborty, A.; Maiti, D.K.; Puranik, V.G.
Tetrahedron Letters, 46(46), 8047

91. A facile direct conversion of aldehydes to esters and amides using acetone cyanohydrin
Raj, I.V.P.; Sudalai, A.
Tetrahedron Letters, 46(48), 8303

92. Convenient synthesis of 5-methylene-4-substituted-2(5H)-furanones
Mahajan, V.A.; Shinde, P.D.; Borate, H.B.; Wakharkar, R.D.
Tetrahedron Letters, 46(6), 1009

93. Asymmetric synthesis of aryloxypropanolamines via OsO4-catalyzed asymmetric dihydroxylation
Sayyed, I.A.; Thakur, V.V.; Nikalje, M.D.; Dewkar, G.K.; Kotkar, S.P.; Sudalai, A.
Tetrahedron, 61(11), 2831

RESEARCH PAPERS PUBLISHED

94. Room temperature ionic liquid promoted improved and rapid synthesis of 2,4,5-triaryl imidazoles from aryl aldehydes and 1,2-diketones or -hydroxyketone
Siddiqui, S.A.; Narkhede, U.C.; Palimkar, S.S.; Daniel, T.; Lahoti, R.J.; Srinivasan, K.V.
Tetrahedron, 61(14), 3539

95. An efficient method for the synthesis of methyl 11-amino-3, 7-diacetoxy-12-oxo-5-cholan-24-oate
Salunke, D.B.; Hazra, B.G.; Pore, V.S.; Gonnade, R.G.; Bhadbhade, M.M.
Tetrahedron, 61(14), 3605

96. First enantiospecific synthesis of (+)-herbertenol
Chavan, S.P.; Thakkar, M.; Kharul, R.K.; Pathak, A.B.; Bhosekar, G.V.; Bhadbhade, M.M.
Tetrahedron, 61(15), 3873

97. Synthesis of naturally-occuring bioactive butyrolactones - maculalactones A-C and nostoclide-I
Kar, A.; Gogoi, S.; Argade, N.P.
Tetrahedron, 61(22), 5297

98. Chelation controlled regiospecific O-substitution of myo-inositol orthoesters: Convenient access to orthogonally protected myo-inositol derivatives
Devaraj, S.; Shashidhar, M.S.; Dixit, S.S.
Tetrahedron, 61(3), 529

99. Stereoselectivity ratios in a simple Diels-Alder reaction in aqueous salt solutions of alcohols
Deshpande, S.S.; Kumar, A.
Tetrahedron, 61(33), 8025

100. An unusual stereochemical outcome of radical cyclization: Synthesis of (+)-biotin
Chavan, S.P.; Chittiboyina, A.G.; Ramakrishna, G.; Tejwani, R.B.; Ravindranathan, T.; Kamat, S.K.; Rai, B.; Sivadasan, L.; Balakrishnan, K.; Ramalingam, S.
Tetrahedron, 61(39), 9273

101. Pyridine mediated supramolecular assemblies of 3,5-dinitro substituted benzoic acid, benzamide and benzonitrile
Arora, K.K.; PrakashaReddy, J.; Pedireddi, V.R.
Tetrahedron, 61(45), 10793

102. Synthesis of cis bis-lactams via Staudinger cycloaddition reaction using C2-symmetric 1,2-diamines
Shaikh, A.L.; Deshmukh, A.R.A.S.; Puranik, V.G.
Tetrahedron, 61(9), 2441

103. Molecular mapping of stem and leaf rust resistance in wheat
Khan, R.R.; Bariana, H.S.; Dholkia, B.B.; Naik, S.V.; Lagu, M.D.; Rathjen, A.J.; Bhavani, S.; Gupta, V.S.
Theoretical and Applied Genetics, 111(5), 846

RESEARCH PAPERS PUBLISHED

Polymer Science

1. Enzymatic hydrolysis of delignified bagasse polysaccharides
   Adsul, M.G.; Ghule, J.E.; Shaikh, H.; Singh, R.; Bastawde, K.B.; Gokhale, D.V.; Varma, A.J.
   Carbohydrate Polymers, 62(1), 6

2. Noncovalent and nonspecific molecular interactions of polymers with multiwalled carbon nanotubes
   Baskaran, D.; Mays, J.W.; Bratcher, M.S.
   Chemistry of Materials, 17(13), 3389

3. Pyrazole-tethered heteroditopic ligands and their transition metal complexes: Synthesis, structure, and reactivity
   Mukherjee, A.; Sarkar, A.; Subramanyam, U. Mohandas, T.P.; Puranik, V.G.
   European Journal of Inorganic Chemistry, (7), 1254

4. Benzoylation of polyphenylene oxide: Characterization and gas permeability investigations
   Bhole, Y.S.; Kharul, U.K.; Somani, S.P. Kumbharkar, S.C.
   European Polymer Journal, 41(10), 2461

5. Nitrogen ligands: The transition metal catalyzed reaction of aryl halides with olefins (Mizoroki-Heck), phenylboronic acid (Suzuki coupling) and Buchwald-Hartwig amination, new catalysts and effect of co-catalysts - Aryl halide activation - Part I
   Iyer, S.; Kulkarni, G.M.; Ramesh, C.; Sattar, A.K.
   Indian Journal of Chemistry - Section B Organic an, 44(9), 1894

6. Poly(acrylonitrile) ultrafiltration membranes I. Polymer -salt-solvent interactions
   Phadke, M.A.; Musale, D.A.; Kulkarni, S.S.; Karode, S.K.
   J Polym Sci B, 43(15), 2061

7. Poly(acrylonitrile) ultrafiltration membranes II. membrane morphology and permeation characteristics
   Phadke, M.A.; Kulkarni, S.S.; Karode, S.K.; Musale, D.A.
   J Polym Sci B, 43(15), 2074

8. Synthesis and characterization of Aromatic Copolyesters containing Siloxane Linkages in the Polymer Backbone
   Waghmare, P.B.; Idage, S.B.; Menon, S.K.; Idage, B.B.
   Journal of Applied Polymer Science Poly, 100(4), 3224

9. Preparation, characterization, and water-sorption study of polyvinyl alcohol based hydrogels with grafted hydrophilic and hydrophobic segments
   Shukla, S.; Bajpai, A.K.; Kulkarni, R.A.
   Journal of Applied Polymer Science, 95(5), 1129

10. Swelling behavior and diffusion studies of high-water-retaining acrylamide/potassium methacrylate hydrogels
    Mohan, Y.M.; Murthy, P.S.K.; Raju, K.M.; Rao, K.M.; Sreeramulu, J.
    Journal of Applied Polymer Science, 96(4), 1153

11. Comparison of the pervaporation separation of a water-acetonitrile mixture with zeolite-filled sodium alginate and poly(vinyl alcohol)-polyaniline semi-interpenetrating polymer network membranes
    Naidu, B.V.K.; Bhat, S.D.; Sairam, M.; Wali, A.C.; Sawant, D.P.; Halligudi, S.B.; Mallikarjuna, N.N.; Aminabhavi, T.M.
    Journal of Applied Polymer Science, 96(5), 1968

12. Miscibility of chitosan-hydroxyethylcellulose blends in aqueous acetic acid solutions at 35°C
    Wali, A.C.; Naidu, B.V.K.; Mallikarjuna, N.N.; Sainkar, S.R.; Halligudi, S.B.; Aminabhavi, T.M.
    Journal of Applied Polymer Science, 96(5), 1996

13. Functional copolymers of p-cumyl phenyl methacrylate and glycidyl methacrylate: Synthesis, characterization, and reactivity ratios
    Ratnaprabha, K.; Daliya, P.K.
    Journal of Applied Polymer Science, 97(1), 336

14. Aromatic polyimides from m-phenylene diamines containing pendant groups: Synthesis and characterization
    Pal, R.R.; Patil, P.S.; Dere, R.T.; Salunkhe, M.M.; Maldar, N.N.; Wadgaonkar, P.P.
    Journal of Applied Polymer Science, 97(3), 1377

15. Thermal degradation kinetics of polyesters containing mesogenic aromatic diols
    Mule, S.A.; Ghadage, R.S.; Jacob, N.E.; Rajan, C.R.; Ponrathnam, S.
    Journal of Applied Polymer Science, 97(3), 784

16. Transparent chiral polymers for optical applications
    Pujari, N.S.; Kulkarni, M.R.; Large, M.C.J.; Basset, I.M.; Ponarathnam, S.
    Journal of Applied Polymer Science, 98(1), 58

17. Crystallization of polymers from stressed melts
    Kumarswamy, G.
    Journal of Macromolecular Science - Polymer Review, C 45(4), 375

RESEARCH PAPERS PUBLISHED

18. Synthesis, characterization, and performance evaluation of polymeric HALS in ethylene-propylene-diene terpolymer (EPDM)
    Lonkar, S.P.; Rana, S.; Singh, R.P.; Lacoste, J.; Gardette, J.L.; Jestin, F.; Brocord, E.
    Journal of Macromolecular Science - Pure and Appli, 42 A(8), 1037(2005

19. Photodegradation of ethylene/propylene/polar monomers co- and terpolymers. I - Prepared by group 4 catalyst systems
    Fernandes, S.; Correia, S.; Prasad, A.V.; Reddy, K.R.; Rana, S.; Lonkar, S.P.; Marques, M.M.; Singh, R.P.
    Journal of Macromolecular Science - Pure and Appli, 42 A(9), 1259(2005

20. Synthesis and biodegradability of polyaspartic acid: A critical review
    Thombre, S.M.; Sarwade, B.D.
    Journal of Macromolecular Science - Pure and Appli, 42 A(9), 1299(2005

21. Highly-active new alpha-dimine Nickel-catalyst for the polymerization of alpha-olefins
    Liu, H.R.; Gomes, P.T.; Costa, S.I.; Durate, M.T.; Branquinho,R.; Fernandes, A.C.; Chien, J.C.W.; Singh, R.P.; Marques, M.M.
    Journal of Organometallic Chemistry, 690(5), 1314

22. Structure of poly(L-lactic acid)s prepared by the dehydropolycondensation of L-lactic acid with organotin catalysts
    Shyamroy, S.; Garnaik, B.; Sivaram, S.
    Journal of Polymer Science, Part A: Polymer Chemis, 43(10), 2164

23. In situ polymerization of ethylene with bis(imino)pyridine iron(II) catalysts supported on clay: The synthesis and characterization of polyethylene-clay nanocomposites
    Ray, S.; Galgali, G.; Lele, A.; Sivaram, S.
    Journal of Polymer Science, Part A: Polymer Chemis, 43(2), 304

24. A novel tridentate nitrogen donor as ligand in copper catalyzed ATRP of methyl methacrylate
    Mittal, A.; Sivaram, S.
    Journal of Polymer Science, Part A: Polymer Chemis, 43(21), 4996

25. Design, syntheses, and characterization of New thermoplastic polyureas based on 3,4-ethylenedioxythiophene
    Ojha, U.P.; Ramesh, C.; Kumar, A.
    Journal of Polymer Science, Part A: Polymer Chemis, 43(23), 5823

26. Main chain thermotropic liquid crystalline polyurethanes containing biphenyl mesogens based on novel AB-type self-polycondensation route: FT-IR and XRD studies
    Ranganathan, T.; Gowd, E.B.; Ramesh, C.; Kumar, A.
    Journal of Polymer Science, Part A: Polymer Chemis, 43(9), 1903

27. Studies on characterization of nano CaCO3 prepared by the in situ deposition technique and its application in PP-nano CaCO3 composites
    Mishra, S.; Sonawane, S.H.; Singh, R.P.
    Journal of Polymer Science, Part B: Polymer Physic, 43(1), 107

28. Synthesis, characterization, and performance evaluation of novel stabilized TDI-based polyurethane coatings under accelerated weathering
    Kumar, A.P.; Reddy, K.R.; Rana, S.; Lonkar, S.P.; Raut, K.G.; Singh, R.P.
    Journal of Vinyl and Additive Technology, 11(1), 13

29. Hydrophobically modified poly(acrylic acid) using 3- pentadecylcyclohexylamine: Synthesis and rheology
    Shedge, A.S.; Lele, A.K.; Wadgaonkar, P.P.; Hourdet, D.; Perrin, P.; Chassenieux, C.; Badiger, M.V.
    Macromolecular Chemistry and Physics, 206(4), 464

30. Studies on the crystallization behavior of nylon-6 in the presence of layered silicates using variable temperature WAXS and FTIR
    Nair, S.S.; Ramesh, C.
    Macromolecules, 38(2), 454

31. Thermoreversible behaviour of associating polymer-solutions - thermothinning versus thermothickening
    Hourdet, D.; Gadgil, J.; Podhajecka, K.; Badiger, M.V.; Brulet, A.; Wadgaonkar, P.P.
    Macromolecules, 38(20), 8512

32. Degradability of composites, prepared from ethylene-propylene copolymer and jute fiber under accelerated aging and biotic environments
    Kumar, A.P.; Singh, R.P.; Sarwade, B.D.
    Materials Chemistry and Physics, 92(2-3), 458

33. Synthesis of novel polyurethanes for nonlinear optical applications
    Vohra, V.; Suresh, S.; Ponrathnam, S.; Rajan, C.R.; Rau, I.; Kajzar, F.
    Nonlinear Optics Quantum Optics, 33(3-4), 285

RESEARCH PAPERS PUBLISHED

34. An overview on the degradability of polymer nanocomposites
Pandey, J.K.; Raghunatha Reddy, K.; Pratheep Kumar, A.; Singh, R.P.
Polymer Degradation and Stability, 88(2), 234

35. Synthesis and characterization of aromatic polyamides containing an s-triazine ring with thiophenoxy linkages
Pal, R.R.; Patil, P.S.; Salunkhe, M.M.; Maldar, N.N.; Wadgaonkar, P.P.
Polymer International, 54(3), 569

36. Synthesis of poly(1-hexene)s end-functionalized with phenols
Yanjarappa, M.J.; Sivaram, S.
Polymer International, 54(9), 1310

37. Synthesis and characterization of polyimides and co-polyimides having pendant benzoic acid moiety
Kulkarni, M.; Kothawade, S.; Kulkarni, R.A.; Vernekar, S.P.; Arabale, G.; Wagh, D.; Vijayamohanan, K.
Polymer, 46(11), 3669

38. Morphological consequences of interchange reactions during solid state copolymerization in poly(ethylene terephthalate) and polycarbonate oligomers
Gowd, E.B.; Ramesh, C.
Polymer, 46(18), 7443

39. Polycondensation in liquid crystalline phases of nonionic surfactants. Kinetics and morphology
Kumaraswamy, G.; Wadekar, M.N.; Agrawal, V.V.; Pasricha, R.
Polymer, 46(19 SP), 7961

40. Synthesis and swelling behaviour of hydrophobically modified responsive polymers in dilute aqueous solutions Padmanabha Iyer, N.; Hourdet, D.; Badiger, M.V.; Chassenieux, C.; Perrin, P.; Wadgaonkar, P.P. Polymer, 46(26), 12190

41. Role of non-linear processes in conducting polymer blends for piezo-sensors: Part 2: Studies on polyaniline/SBS blends
Radhakrishnan, S.; Kar, S.B.
Sensors and Actuators, A: Physical, 120(2), 474

FOREIGN PATENTS GRANTED

FOREIGN PATENTS GRANTED
(1-1-2005 TO 31-12-2005)

Sr. No.	Title	Inventor(s)	Country (Patent No)
1	Oligomers and preparation thereof	Kulkarni, M.G., Khandare, J.J.	US 6,977,285
2	Process for the preparation of aqueous urethane dispersions	Ramanathan, L.S., Raut, K.G., Srinivasan, S.R., Sivaram, S.	EP 982331
3	A process for the preparation of 1-[cyano(aryl)methyl] cyclohexanol	Chavan, S.P., Kamat, S.K., Sivadasan, L., Balakrishnan, K., Khobragade, D.A., Ravindranathan, T., Gurjar, M.K., Kalkote, U.R.	EP 1238967
4	A process for the preparation of 1-[2-dimethylamino-(4-methoxyphenyl) -ethyl] cyclohexanol	Chavan, S.P., Kamat, S.K., Sivadasan, L., Balakrishnan, K., Khobragade, D.A., Ravindranathan, T., Gurjar, M.K., Kalkote, U.R.	EP 1238965
5	Process for the preparation of a polyesteramide	Kelkar, A.A., Kulkarni, S.M., Chaudhari, R.V.	EP 1229065
6	Process for preparation of cyclic carbonate	Manikandan, P., Sankar, M.	US 6,924,379
7	Diol functionalised antioxidant and process for their preparation	Solanki. S.S., Desai, S.M., Singh, R.P.	US 6,916,960
8	Process for the preparation of ultrafiltration membranes of polyacrylonitrile, using malic acid as an additive	Kulkarni, S.S., Shinde, M.H., Musale, D.A.	US 6,858,141
9	Process for preparing alkyl/aryl chloroformates	Deshmukh, A.R.A.S., Gumaste, V.K.	US 6,919,471
10	Process for the epoxidation of liquid olefinic organic compound using a supported nano-gold catalyst	Choudhary, V.R., Patil, N.S., Uphade, B.S., Prabhas, J.	US 6,933,397
11	Process for the conversion of phenol to hydroquinone and quinones	Dewkar, G.K., Thakur, V.V., Pardhy, S.A., Sudalai, A., Devotta, S.	US 6,872,857
12	A novel catalytic formulation and its preparation	Mahajan, A.N., Chaudhari, R.V.	EP GB2389324
13	Process for the synthesis of	Naik, R.H., Joshi, P.L.	US 6,852,864
14	Process for the preparation of Dimethyl cumenes	Patra, C.R., Rajiv Kumar Dipyrromethanes	US 6,921,843

INDIAN PATENTS GRANTED

Sr. No.	Title	Inventors	Patent No (Appln. No.)
15.	An improved process for simultaneous preparation of sex specific and gender neutral semi synthetic amplicons useful for sex determination	Ranjekar, P.K., Parasnis, A.S., Gupta, V.S.	193289(2377/DEL/ 1998)
16.	A process for the preparation of dimer of 4-methodxy-5(mercaptomethyl)-1,3-bis (phenylmethyl)-2-imidazolidinone, D(+)-biotin intermediate	Chavan, S.P., Kamat, S.K., Rai, B., Sivadasan, L., Balakrishnan, K., Ramalingam, S., Gopal, C.A., Deshpande, V.H., Ravindranathan, T.	192297(910/DEL/ 2000)
17.	A process for the preparation of cellulase free alkali tolerant xylanase	Ahmad, A., Lachke, A., Sathivel, C., Kinhikar, A.	192501(230/DEL/ 2001)
18.	An improved process for the preparation of meta-chlorotoluene	Singh, A.P., Kale, S.M.	193312(569/DEL/ 2000)
19.	An improved process for the preparation of 2-aryl propionic acids	Chaudhari, R.V., Seayad, A., Seayad, J.	192841(570/DEL/ 1999)
20.	A process for the preparation of substituted 2-Heptyne, 4-OL-1-(Arylmethoxy)	Wakharkar, R.D., Barhate, N.B.	193287(1564/DEL/ 1999)
21.	An improved process for the preparation of cycloalkylphenols	Phukan, P., Dalavoy, V.S., Sudalai, A.	192844(1561/DEL/ 1999)
22.	A process for the preparation of mycolytic enzymes containing mainly chitosanase	Deshpande, M., Patil, R., Chitnis, M., Laxman, R.Seeta	193300(279/DEL/ 2001)
23.	An improved process for the preparation of keto-isophorone	Halligudi, S.B., Deshpande, S.S., Degaonkar, M.P.	193309(302/DEL/ 2000)
24.	A process for the preparation of 3-sulfanyl cyclic ketones	Ravindranathan, T., Wakharkar, R.D., Borate, H.B., Shinde, P.D., Mahajan, V.A., Tillu, V.H., Ghumare, S.S., Jagtap, H.S.	192827(299/DEL/ 2000)
25.	A new process for the preparation of (2R, 3S, 22S, 23S)-2, 3, 22, 23-tetraacetoxy -B-homo-7-oxastigmastan-6-one	Massey, A.P., Pore, V.S., Hazra, B.G.	192836(727/DEL/ 2000)
26.	A process for the extraction of penicillin G acylase from enzyme extract of escherichia coli.	Ghadge, V.B., Ponrathnam, S., Rajan, C.R., Mujawar, S.K., Shewale, J.G.	192969(1060/ DEL/2000)
27.	A process for the purified penicillinase	Ghadge, V.B., Ponrathnam, S., Rajan, C.R., Deshpande, B.S., Sudhakaran, V.K., Shewale, J.G.	192740(1062/ DEL/2000)

INDIAN PATENTS GRANTED

Sr. No.	Title	Inventors	Patent No (Appln. No.)
28.	An improved process for the single step hydrogenation of nitrobenzene to p-aminophenol	Rode, C.V., Vaidya, M.J., Chaudhari, R.V.	193298(164/DEL/ 2001)
29.	A process for the preparation of a novel cis, cis-3-hydroxy-5-methylcarbonyloxy-cyclohexylacetate useful as an intermediate for 6-hydroxymethyl-4-(tert-butyldimethylsilyloxy)-(4R, 6S)-tetrahydro-2H-2-pyranone	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	192849(92/DEL/ 2001)
30.	A process for the preparation of a novel 3-tetrahydro-2H-2-pyranyloxy-5-(tert.butyldimethylsilyloxy)-(1S,3R,5R)-cyclohexan-1-one useful as an intermediate for 6-hydroxymethyl-4-(tert-butyldimethylsilyloxy)-(4R,6S)-tetrahydro-2H-2-pyranone	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	192170(80/DEL/ 2001)
31.	An improved process for preparation of N substituted carabamates	Gupte, S.P., Chaudhari, R.V., Shivarkar, A.B., Mulla, S.A.R.	192391(376/DEL/ 2002)-

BOOKS / CHAPTER IN BOOKS

Books

Chemistry of Natural Products, Sivakumar, Meenakshi; Nagasampagi, Bhimsen A.; Bhat, Sujata V. , Narosa Publishing House Pvt Ltd , New Delhi, 2005, pp. XXXI+840.

Chapter in books

Biodegradable Polymers from Sugars, Dr. A.J. Varma in Biodegradable Polymers for Industrial Applications, Ed. Smith Roy, CRC and WP, Cambridge, England, pp. 165- 188.

Fungal Biotechnology: Opportunities In Pulp and Paper Manufacturing, Dr. Absar Ahmad, Dr. A.H. Lachke, and Dr. R.S. Vyas in Fungi: Diversity and Biotechnology, Ed. M.K. Rai and S.K. Deshmukh, Scientific Publisher (India), Jodhpur, pp. 1-30

Enzymes for pulp and paper manufacturing towards sustainable development, Dr. A.H. Lachke, and Dr. R.S. Vyas in Chemistry for green environment, Ed. M. M. Srivastava and Rashmi Sanghi, Narosa Publishng House, New Delhi, pp. 170-184.

ACADEMIC COLLABORATIONS

ACADEMIC COLLABORATIONS

NCL and its scientists have many collaborative projects with leading academic and scientific institutes and also with individual researchers. NCL as an institute has entered into Memorandum of Understandings with University of Science and Technology, Lille (USTL) and the National Institute for Applied Sciences, Lyon (INSA, Lyon), both from France, National Center for Cell Science and Vasantdada Sugar Institute, both from Pune. NCL scientists individually or as a team also have many collaborative programmes with various leading research groups from India and abroad.

Prof. J-S, Lee, Department of Materials Science & Engineering, GIST and Dr. S. Sivaram, Director, NCL exchanging the MoU.

Institute to Institute Collaborations:

External Institute	Field(s) of Collaboration Scientist (S)	NCL Nodal
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
Center of Excellence in Polymer Science, Karnatak University, Dharwad	Polymer Science	Dr. M.G. Kulkarni
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
University of Kansas, Lawrence, USA	Environmentally benign catalysis, oxidation and hydroxy formylation reaction in super critical CO_2 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
Vasantdada Sugar Institute,Pune	Zeolite assisted Ethanolic Fermentation	Dr. Archana Pundle

ACADEMIC COLLABORATIONS

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, 38054GrenobleCedex 9,France
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 Graduate	Dr. C. Ramesh	Prof. K. Tashiro, Department of Macromolecular Science, School of Science, Osaka University, Japan
Design, synthesis & biological evaluation of cationised PNAs as antisense agents ex vivo and in vivo	Dr. Ganesh K.N./ Dr. (Mrs.) V.A. Kumar	Prof. Bernard LebleuUniversite Montpellier 2UMR-CNRS 5241Montpellier
Development of a mycoinsecticide against Helicoverpa armigera 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
Development of novel biopesticides based on fungi/ bacteria exhibiting dual antagonistic activity against plant pathogenic fungal and insect pests	Dr. M. V. Deshpande	Prof. A. Lobanok Director Institute of Microbiology, Belarus Academy of Sciences,Minsk, Belarus
Microbial Control of pest: Entomopathogenic fungi as mycoinsecticides	Dr. M. V. Deshpande	Dr. Mounir Hassani Directeur general ATLAS AGRO, Zurich, Switzerland Dr. Keller Siegfried, Swiss Federal Research Station for Agroecology and Agriculture, Zurich-Reckenholz, Switzerland
Polyamines, dimorphism in Yarrowia lipolytica and the petroleum oil degradation in marine environment	Dr. M. V. Deshpande	Prof. J.Ruiz-Herrera Unidad Irapuato, Apartado Postal #629 Irapuato, Guanajuato 36500 Mexico.
Catalytic reaction engineering using ionic liquids	Dr. R. M. Deshpande	Prof. Henri Delmas ENSIACET, Toulouse, France
Evaluation and improvement of the durability in a composite insulator: study of the degradation/stabilization of epoxy fiber glass composites coated with elastomers	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 Merces Marques, Instituto Superior Technico, Centro de Qumica Estrutural IILisboa Cedex, Portugal
Comparative study on the development of solid acid for alkylation of phenolics	Dr. S. B. Halligudi	Prof. Jack CQ Fletcher, Associate ProfessorDirector, Catalysis Research catalysts UnitDepartment of Chemical EngineeringUniversity of Capetown, Pvt. Bag 7701 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 (Arachis hypogaea L) by protoplast fusion	Dr. Sulekha Hazra	Dr. Maria-Teresa Scarano, Instituto di Genetica Vegetale - Sezione di Palermo Consiglio Nazionale delle Ricerche,Palermo, Italy
Studies on the structure and function of metal in mesoporous materials	Dr. Veda Ramaswamy	Dr. Zdenek Sobalik, J. Heyrovsky Institute of Physical Chemistry, Dolejskova, Czech Republic
Improved productivity, profitability & sustainability of sheep production in Maharashtra, India 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 BiotechnologySchool of Veterinary Science University of Melbourne, Victoria 3010 AUSTRALIA
Increasing the efficiency of production and nutritional value of chickpea	Dr. Vidya Gupta	Fred J. Muehlbauer USDA-ARS303 Johnson HallWashington State UniversityPullman, WA 99164-6434, USA John Gatehouse, Reader in Biological Sciences, School of iological and Biomedical Sciences, University of Durham,South Road, Durham DH1 3LE, UK.
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	TJ Higgins Deputy Chief CSIRO Plant Industry Prof. Beat KellerInstitute of Plant Biology University of Zurich,Zollikerstr,107, CH-8008, ZurichSwitzerland

DEPUTATION ABROAD

DEPUTATION

Business Development Activity

Dr. A. A. Natu (Switzerland & Germany): 15 - 28 Aug. 2005

Dr. K. Guruswamy (USA): 21 – 30 Mar 2005

Dr. K. Guruswamy (USA & UK): 1- 9 Feb. 2006

Dr. K.N. Ganesh (USA): 21 – 23 Dec. 2005

Dr. M.K. Gurjar (USA): 17 – 30 Apr. 2005

Dr. M.K. Gurjar (USA): 6 – 14 Nov. 2005

Dr. D.K. Mohapatra (USA): 09 – 21 May 2005

Dr. P. G. Shukla (USA): 17 – 28 Nov. 2005

Dr. R.V. Chaudhari (UK & Switzerland): 19 – 26 April 2005

Dr. R.V. Chaudhari (USA & UK): 5 – 17 Feb. 2006

Dr. Rajiv Kumar (USA): 26 Sept. – 6 Oct. 2005

Dr. S. Ponrathnam (USA): 3 – 16 Oct. 2005

Dr. S.S. Joshi (UK): 19 – 23 April 2005

Dr. Upendra Natarajan (USA): 24 – 26 May 2005

Dr. V.V. Ranade (UK): 06 – 12 March 2006

Bilateral/ collaborative/ exchange programmes

Dr. B.L.V. Prasad (UK): To explore and identify specific areas of common interest for collaborative research, 23 – 29 Oct. 2005

Dr. M.V. Badiger (France): To carry out research work under the IFCPAR project, 11 – 15 May 2005

Dr. C. Ramesh (Thailand): Indo-Thai project, 27 Mar – 9 Apr 2005

Dr. C.S. Gopinath (Japan): To attend the 3rd JSPS Symposium on surfaces and interfaces for nanomaterials under a DST-JSPS Program, 6 – 14 Nov. 2005

Dr. M.K. Dongare (Germany & France): To review the work carried out under the ongoing project CSIR-FZj Indo-German Collaborative project with Humboldt-University Berlin and visit to Lille University, France on the invitation of Prof. Edmond Payen to explore the possibility for future collaboration, 09 – 29 May 2005

DEPUTATION ABROAD

Dr. M.V. Deshpande (Switzerland): To visit project partners for discussion concerning future of the joint research project, 26 – 31 July 2005

Dr. M.V. Deshpande (México): Under Indo-Mexican Project, 1 - 8 Aug 2005

Dr. P. Manikandan (UK): Under Joint Scientific Project between NCL and the Davy Faraday Research laboratory at the Royal Institution, 5 – 18 Oct. 2005

Dr. R.M. Deshpande (France): IFCPAR, 16 Mar – 5 Apr 2006

Dr. R.P. Singh (Portugal and France): Under Indo-Portuguese Collaborative Research Project and for discussion on ongoing project and future planning of collaborative programmes, 17 – 23 Oct 2005

Dr. Rajiv Kumar (Japan): To attend the 3rd JSPS Symposium on surfaces and interfaces for nanomaterials under a DST-JSPS Program, 6 – 14 Nov. 2005

Dr. S.B. Halligudi (South Africa): Indo-South Africa Joint Research Project, 1 - 23 Feb. 2006

Dr. R.P Singh (France): To carry out research work under the IFCPAR project, 1 – 30 May 2005

Dr. Sourav Pal (Germany): To visit BASF in connection with Joint Project, 18 – 22 July 2005

Dr. Sourav Pal (Germany): Joint project, 12 – 18 Feb. 2006

Dr. T. Raja (Germany): DST-DAAD, 7 – 28 Feb. 2006

Dr. Vincent Paul Swamy (South Africa): Indo-South African Co-operation in S&T, 18 Mar – 9 Apr 2005

Dr. Vincent Paul Swamy (South Africa): Under Indo-South African Co-operation in S&T to carry out project work, 20 Jan – 11 Feb 2006

Extra - ordinary leave

Dr. A. Murugan (USA): Post Doctoral Res. Associate, 20 Jun 2005 – 19 June 2006

Dr. Ashok P. Giri (Germany): To avail an offer of Professor Ian Baldwin, Director, MPI, 15 – 17 Apr 2005

Dr. B.B. Idage (South Korea): As an International Fellow at, KRICT, 7 June 2005 – 6 June 2006

Dr. H.S. Potdar (South Korea): To take up an assignment as an International Fellow, 1 Feb 2006 – 31 Jan. 2007

Dr. M. Srisailas (USA): Extension of EOL, 27 Oct.2005 – 26 Oct. 2006

Dr. S.G. Kumbhar (USA): EOL – Extension, 08 Jan. 2005 – 31 Aug. 2006

Dr.(Ms.) Moneesha D'Costa (Germany): EOL - Extension 07 Oct. 2005 – 01 Sep. 2006

DEPUTATION ABROAD

Dr.(Ms.) Moneesha D'Costa (Germany): Post-Doctoral Research Fellowship - Extension of EOL, 10 Jan. – 09 Jul 2006

Dr. Ajit Singh Mamman (South Korea): To Take up an assignment as an International Fellow, 10 Jan. 2006 – 9 Jan. 2007

Fellowships / sabbatical leave

Dr. V. Premnath (UK): Sabbatical Leave Extension, 07 Jan – 31 Aug. 2005

Dr. (Ms) Nayana Vaval (Germany): To avail Alexander Von Humboldt Fellowship, 1 June 2005 – 31 May 2006

Dr. Ashok P. Giri (Germany): To avail the Alexander vonHumboldt Foundation Research, 9 Dec. 2005 – 8 Dec. 2006

Meetings

Dr. A.J. Varma (Italy): To attend UNIDO Expert Group Meeting, 5 – 6 Dec. 2005

Dr. K.N. Ganesh (China): To attend 40th IUPAC Divisional Committee Meeting & to deliver invited lectures, 13 – 21 Aug. 2005

Dr. M.K. Gurjar (China): Member of CSIR Delegation to China, 13 – 21 Mar 2006

Dr. N.P. Argade (Thailand): To participate in Expert Group meeting, 29 Jun. – 1 July 2005

Dr. N.P. Argade (Italy): To participate in the Expert Group Meeting, 12 - 13 Dec. 2005

Shri V.S. Chavan (Germany): To participate in the meeting of Experts for Ocean Biogeographic Information System, 3 – 7 Nov. 2005

Shri V.S. Chavan (Belgium): Science Planning Meeting including the meeting of Outreach and capacity building science sub-committee of GBIF, 21 – 24 Apr 2005

Shri V.S. Chavan (USA): To participate in the ICOMM Informatics and Data Management Working Group 25 – 26 Sept. 2005

Training

Mrs. Renu Pasricha (Belgium): To attend summer School ELCRYST 2005, 2 - 9 Sept 2005

Dr. Dhiman Sarkar (USA): Training on HTS Based assays on botanicals & Skin-care, 26 Mar – 2 Apr 2005

DEPUTATION ABROAD

Conferences/ seminars/ symposia/ workshops

Dr. (Mrs.) Ramaswamy. V (USA): To attend the 19th North American Catalysis Society Meeting, 22 – 27 May 2005

Dr. B.L.V. Prasad (Japan): 3rd Japan-India Workshop, 16 Feb. – 3 March 2006

Dr. C. Ramesh (France & Germany): To participate in the Indo-French Seminar on Fibrillar Networks as Advanced Materials by IFCPAR, 20 – 26 Sept. 2005

Dr. C.V.V. Satyanarayana (Singapore): To present paper at 3rd ICMAT, 3 – 7 July 2005

Dr. K.N. Ganesh (USA): To deliver a lecture at the PACIFICHEM 2005, 15 – 20 Dec., 2005

Dr. K.N. Ganesh (USA): PNA Symposium & Visit to Universities, 24 –27 Mar 2006

Dr. K.P. Vijayamohanan (Korea): International Conference on Nanoscience and Nano Technology, 10 – 1 Nov. 2005

Dr. K.V. Srinivasan (Austria): To participate in International Congress on Ionic Liquids, 19 – 22 Jun 2005

Dr. M. Karthikeyan (France, The Netherlands and UK): To visit BIOCHEMICS Consulting, to attend the 7th International Conference on Chemical Structures at the Netherlands and to deliver talk in the Unilever Centre, UK, 1 – 13 Jun 2005

Dr. M.K. Dongare (Singapore): 3rd ICMAT - To present paper, 3 – 7 July 2005

Dr. M.K. Gurjar (USA): To attend Organic Process Research and Development Conference, 15 – 18 Nov. 2005

Dr. M.V. Badiger (France & Germany): To participate in the Indo-French Seminar on Fibrillar Networks as Advanced Materials by IFCPAR, 20 – 26 Sept. 2005

Dr. Murali Sastry (Taiwan): Member of Indian Delegation of the Indo-Taiwan Nanomaterials workshop, 9 – 12 Mar 2005

Dr. Murali Sastry (South Africa): South African Nano Technology Conference, 18 – 21 Apr 2005

Dr. Murali Sastry (USA): To attend the 79th Colloid and Surface science symposium of American Chemical Society, 12 – 15 Jun 2005

Dr. R. Tewari (France): To attend International Biophysics Congress, 27 Aug. – 1 Sept. 2005

Dr. R.V. Chaudhari (Slovenia and USA): 5th International Symposium on CAMURE -5 and Green Chemistry Conference, to visit centre for environmentally beneficial Catalysis, 15 Jun – 10 July 2005

Dr. Rajesh Gonnade (Italy): To participate in the XX Congress of International Union of Crystallography, 23 – 31 Aug. 2005

DEPUTATION ABROAD

Dr. Sourav Pal (Germany): To attend 6th Demon Workshop as a speaker, 29 Mar – 7 Apr 2005

Dr. Sourav Pal (Greece & Germany): International conference on computational methods in science and engineering, 21 – 29 Oct. 2005

Dr. Thomas Daniel (Austria): To participate in International Congress on Ionic Liquids, 19 – 22 Jun 2005

Dr. V.R. Pedireddi (France): To participate in the Indo-French Seminar on Fibrillar Networks as Advanced Materials by IFCPAR, 20 – 23 Sept. 2005

Dr. V.R. Pedireddi (Japan): 3rd Japan-India Workshop, 16 – 18 Feb. 2006

Shri V.S. Chavan (Taiwan): To participate in the 2005 International Workshop on integrated Bio-diversity Databases & Forum of Species 20000 Asia-Oceania, 30 Sept. – 2 Oct. 2005

Dr. V.V. Ranade (Italy): 19 – 24 June 2005

Dr. K. Vijaymohanan (UK): To attend the G8 Energy Research & Innovation Workshop 11 – 12 May 2005

Dr.(Mrs.) A.A. Prabhune (Australia & Singapore): To participate & present paper in International Thermophiles Conference, & to Deliver Lectures and Discuss future Collaborations, 18 – 26 Sept. 2006

Dr.(Mrs.) Mala Rao (Australia & Singapore): To participate & present paper in International Thermophiles Conference & to Deliver Lectures and Discuss future Collaborations, 18 – 26 Sept. 2006

Shri Siddharth Paralikar (Mexico): To participate in GBIF Data Modelling workshop, 04 – 08 Apr 2005

Shri Rajesh Gonnade (Italy): To participate in the International Union of Crystallographic congress at Florence, 24 Aug. 2005

Students' participation in conference/ research projects

Shri Amit Singh (USA): To work under collaborative research project at North Eastern University, Boston, 28 March – 1 July 2005

Ms Anupa R. Menjoge (USA): To present poster at conference, Florida, 18 – 22 June 2005

Shri Debdut Roy (Slovenia): To participate in the International Symposium CAMURE–5 and ISMR-4, 15 – 18 June 2005

Ms Sophy (Germany): To participate in Demon Developer's Workshop at Dresden, 30 March – 3 April 2005

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

LECTURES / SEMINARS DELIVERED BY VISITORS

Date	Topic	Speaker and affiliation
07-04-2005	Engaging Zwittrions in Carbon-Carbon Bond Foring Reactions : A Promising Synthetic Strategy	Dr. Vijay Nair, Regional Research Laboratory, Thiruvananthapuram (Dr. Sukh Dev Endowment Lecture)
13-04-2005	Chemistry of Azaphospholes	Prof. Raj Kumar Bansal, Dept. of Chem. Rajasthan University, Jaipur
20-04-2005	Synthesis of plant self-sustenance agents: allelochemicals from cultivar	Prof. R. V. Venkateswaran, Department of Organic Chemistry, IACS, Kolkata
25-04-2005	Conjugated polymers for photonic applications	Dr. Satish Patil, Department of Chemistry and Biochemistry, UCLA, USA
27-04-2005	Synthesis of Modified Nucleic Acids for Their Structural Studies by EPR	Dr. Nivrutti Barhate, University of Washington Department of Chemistry Box 351700 Seattle, WA 98195-1700 USA
28-04-2005	Electronic absorption from first-principle calculation	Dr. Anirban Hazra, Department of Chemistry, Princeton University, New Jersey, USA
06-05-2005	Heat Setting of Polymeric Fibres	Prof. V. B. Gupta, IIT Delhi
17-05-2005	Weak Interaction in Protein Structures	Prof. Pinak Chakrabarti, Dept. of Biochemistry, Bose Institute, Kolkata
18-05-2005	Nanostructured organic field effect transistors and functional systems: towards the integration of fluid fabrication and solid state devices	Prof. Fabio Biscarini, Institute for Nanostructured Materials, Italy
30-05-2005	Microanalytical Characterization of Polymers	Anuya Harkare, GE-India Technology Centre, Bangalore
07-07-2005	Green Process Design, Industrial Ecology & Sustainability	Dr. Urmila Diwekar, Chemical & Industrial Engg. Dept., University of Illinois at Chicago (UIC), USA
07-07-2005	Sulphur and nitrogen tolerance of noble metal catalysts for deep hydrotreating	Prof. J. Lercher, Technische Universität München , Garching, Germany
12-07-2005	Mechanistic insights in to the Chain Elongation, Branching,	Dr. H.V. Thulasiram, University of Utah, USA

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

Date	Topic	Speaker and affiliation
14-07-2005	Photo Chemical Fixation of Hexagonal Cylinder Nanostructures in Cinnanoyl-Based Lieuid Crystalline Black Co-polymer Thin Films	Dr. A.V.S. Sainath, Chemical Resources Laboratory, Tokyo Institute of Technology, Japan
15-07-2005	Green Chemistry: Environmentally friendly Tools for Chemical Processes	Raveendran Poovathinthodiyil, Supercritical Fluid Research Center, National Institute of Advanced Ind. Sci. & Tech, Sendai, Japan
18-07-2005	From Sensors to Microsystems: The blossoming of MEMS and Nanotechnology	Prof. Shekhar Bhansali, Department of Electrical Engineering, Nanomaterials and Nanomanufacturing Research Center, University of South Florida Tampa FL 33620, USA
02-08-2005	Medical Polymers: Challenges Ad Libitum	Dr. A. Jayakrishnan, Srichitra Tirumal Institute, Trivandrum
05-08-2005	Courses for the horses: how to pin a target electronic state	Prof. Sadhan Basu Memorial Lecture of Indian National Science Academy, Professor Debashis Mukherjee, Director, IACS, Kolkata
18-08-2005	Conformational Control of Synthetic Polymers	Prof. S. Ramakrishnan, IISc, Bangalore
30-08-2005	Diabetes epidemic in Indians: Is it different than diabetes in Westerners?	Dr C S Yajnik, Director, KEM Hospital Research Center, Pune
30-08-2005	Einstein's Work on the Brownian Motion and Recent Developments	Prof. Sushanta Dattagupta, S.N. Bose National Centre for Basic Science, Kolkata
05-09-2005	Mechanistic Investigations of Samarium (II) Based Reductions and Oligothia Dendrimers for the Formation of Gold Nanoparticles	Dr. Edamana Prasad, Department of Chemistry, Lehigh University, Bethlehem, Pennsylvania, USA
22-09-2005	'Artemisinin-based broad-spectrum antiparasitic agents	Dr. Muraleedharan, University of Mississippi, USA
28-09-2005	Microwave Activation of Electrochemical Processes	Dr. Ujjal Kumar Sur, Department of Chemistry, Loughborough University, UK

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

Date	Topic	Speaker and affiliation
29-09-2005	In-site Spectroscopy in Heterogeneous Catalysis	Prof. Michael Hunger, Institute of Chemical Technology, University of Stuttgart, D-70550, Germany
04-10-2005	"Solid-state 13C NMR studies of novel thermotropic liquid crystals"	Dr. Narasimha Swamy, CLRI, Chennai
17-10-2005	Synthesis and Characterization of catalysts and electrocatalysts using combinatorial methods	Dr. Ramanathan, Department of Chemistry, Texas A&M University, USA
19-10-2005	Soluble-polymer supported organic synthesis : the role of poly (ethylene glycol) (PEG)	Dr Frédéric Lamaty, Laboratoire des Aminoacides, Peptides et Protéines (LAPP), France
20-10-2005	Anionic Polymerization of Styrenic Macromonomers (sMM)	Prof. Nikos Hadjichristidis, University of Athens, Greece
21-10-2005	Nucleation and crystallization kinetics of biodegradable PPDX-b-PCL diblock copolymers	Prof. Alejandro J. Müller, USB Polymer Group, Materials Science Department, Universidad Simón Bolívar (USB), Caracas, Venezuela
27-10-2005	New Chemical tools for proteomic and study of the inhibition: New Insights in Asymmetric catalysis	Dr J-C Florent and Dr V. Vidal, University de Paris-Sud Orsay, France, ENSCP, Paris, France
31-10-2005	Modulating Solid-State Behaviour in Molecular Compounds: A Synthetic Perspective	Dr. Prasanna Ghalsasi, University of Wyoming, USA
31-10-2005	Multicomponent nanostructured materials by atom transfer radical polymerization	Prof. Krzysztof Matyjaszewski, Carnegie Mellon University, Pittsburgh, USA
08-11-2005	In the search for bio-inspired catalysts for redox and hydrolytic chemistry: the importance of a dinuclear unit	Dr. Stephane Menage, CEA, Grenoble, France
28-11-2005	Current Method Development Techniques and New Applications in Chiral LC	Dr. Denise Wallworth, Advanced Separation Technologies Ltd. (Astec), UK
28-11-2005	Time resolved in-situ energy dispersive X-ray diffraction (EDXRD) investigations of chemical reactions	Prof. W. Bench, University of Kiel, Germany

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

Date	Topic	Speaker and affiliation
29-11-2005	Synthesis, Structures and Properties of New Transition Metal Coordination Polymers	Dr. Christian Näther, University of Kiel, Germany
06-12-2005	The Nanomaterials and Their Applications	Prof. Ru-Shi Liu, Department of Chemistry, National Taiwan University, Taiwan
08-12-2005	Co-evolution of transfer RNA and tRNA modification enzymes	Prof. Henri Grosjean, Director of Research, CNRS Laboratory of Structural Enzymology and Biochemistry, Gif-sur-Yvette, France
09-12-2005	Transfer RNA Modification in the yeast S. cerevisiae	Prof. Henri Grosjean, Director of Research, CNRS Laboratory of Structural Enzymology and Biochemistry
12-12-2005	Membrane Electrode Assembly (MEA) for Direct Methanol Fuel Cell (DMFC) using Sulfonic acid containing Mesoporous Silica (SMS)	Dr. N. K Mal, Sony Corp., Okada, Japan
12-12-2005	Nobel Prize in Chemistry 2005	Prof. S. Kotha, IIT, Bombay
14-12-2005	Novel Concepts in 1-D, 2-D, and 3-D Nanomaterials for Functional and Structural Applications	Prof. Nitin P. Padture, Department of Materials Science and Engineering, The Ohio State University, USA
27-12-2005	Topics from polymer physics: Diblock copolymer in an electric field and Dynamics of polymer solution	Dr. B. Ashok, Instituut-Lorentz, LION, Universiteit Leiden, The Netherlands
28-12-2005	Courses for the horses:how to pin a target electronic state	Prof. Sadhan Basu Memorial Lecture 2004, Prof. D. Mukherjee, Director, IACS, Kolkata
04-01-2006	NMR studies of the structure and Mg2+ binding properties of a conserved RNA motif of EMCV picornavirus IRES element	Dr. Vasudevan Ramesh, School of Chemistry, University of Manchester, UK
04-01-2006	Protein-carbon nanotube conjugates as functional nanomaterials	Sandeep S. Karajanagi, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute, New York, USA
05-01-2006	Recognition of nucleic acids by carbohydrates	Dr. Dev P. Arya, Associate Professor, Bioorganic & Medicinal Chemistry , Clemson University, USA

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

Date	Topic	Speaker and affiliation
12-01-2006	si RNA therapeutics of Hepatitis	Dr. Vasant Jadhav, siRNA Therapeutics, Denver, Colorado, USA
19-01-2006	Chemistry in Supercritical Water	Dr. Joan Fraga-Dubreuil, University of Nottingham, UK
20-01-2006	Synthesis of novel therapeutic agents against tuberculosis	Dr. (Ms.) Henrietta Forintos, University of Nottingham, UK
24-01-2006	Fabrication of microfluidic devices & macroporous microchannels using transparent polysilazane glasses, protein pattering on polysilazane glasses and cell free protein synthesis in pdms reactor	Dr. Amit Asthana, Dept. of Fine Chem. Eng. & Chem., College of Engineering, Chungnam National University, Daejeon, South Korea
25-01-2006	High Strength Fibres from Polyolefin/ Organoclay Composites	Dr. Taweechai Amornsakchai, Department of Chemistry, Faculty of Science, Mahidol University, Thailand
08-02-2006	RSC Publishing: Why, where and how?	Dr. Vikki Allen, Editor of Organic & Biomolecular Chemistry, UK
14-02-2006	Ensuring the viability and business success of green initiatives	Prof. Leo Gajsler, DuPont, USA
15-02-2006	Immobilization of ionic liquids and their application	Dr. Michael H. Valkenberg, Chemical Technology and Heterogeneous Catalysis, Worringerweg 1, 52074 Aachen, Germany
17-02-2006	Synthesis of organic compounds for screening against pathogenic protozoa	Dr. Somnath Mondal, Department of Biochemistry, University of Washington-School of Medicine, Seattle, USA
21-02-2006	Seminar on tescom pressure regulators	Mr. Tomek Wolfgang, MD, Tescom Europe , Germany
22-02-2006	Multifunctional Nanoparticles- from Bioimaging to Photovoltaics?	Dr. Yudhisthir Sahoo, Institute for Lasers, Photonics, and Biophotonics, University at Buffalo, The State University of New York, USA
24-02-2006	Role of Decapping Enzyme, Dcp2, in mRNA Regulation	Dr. Mandar V. Deshmukh, Pharmaceutical Chemistry, S-516, Genentech Hall, UCSF, San Francisco, CA, USA

LECTURES / SEMINARS GIVEN AT NCL BY VISITORS

Date	Topic	Speaker and affiliation
24-02-2006	Modelling the complex dynamics of photoinduced molecular processes: a quantum perspective	Prof. Horst Koeppel, Physical Chemistry Institute, University of Heidelberg, Germany
27-02-2006	Supramolecular Synthesis on the Diffractometer: Some do it, others don't!	Prof. Roland Boese, University of Essen, Germany
28-02-2006	Two topics of nano science for organic chemistry: buckybowls and Au nanocluster	Prof. Hidehiro Sakurai, Research Center for Molecular-Scale Nanoscience, Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan
06-03-2006	Synthetic Studies and Commercial utility of dendrimers	Dr. Thatavarthy Rama Krishna, CNRS, Toulouse, France
06-03-2006	Safety and its Management in a Chemical Laboratory	Mr. R. Veeraraghvan, Retd., Fire & Safe Officer, HPCL Mumbai
14-03-2006	Ionic exchange resin as a acid catalyst in the organic synthesis	Prof. Wolfgang Hoelderich, Department of Chemical Technology and Heterogeneous Catalysis University of Aachen, Aachen, Germany,
22-03-2006	Branched Glycopolymers	Dr. Sharmila Muthukrishnan, University of Bayreuth, Germany
30-03-2006	Chemical Nanotechnology: From Molecules to Applications	Dr. Sanjay Mathur, Head, Division of CVD Technology, Leibniz-Institut fur Neue Materialien, Saarbrue, Germany

INVITED TALKS / LECTURES DELIVERED BY NCL SCIENTISTS

INVITED TALKS / LECTURES DELIVERED BY NCL SCIENTISTS

Dr. Ahmad, Absar

Enzyme mediated synthesis of inorganic nanoparticles using microbes, International Conference on Microbial Diversity: Current Perspectives and Potential Applications, Department of Microbiology University of Delhi, South Campus, Delhi, 17 April 2005

Biosynthesis of gold and silver nanoparticles using extremophilic *Actinomycete*, *Thermomonospora* sp, National Conference on Frontiers in Environmental Sciences and Engineering, Department of Environmental Sciences, Bharthiar University, Coimbatore, 15 September 2005

In vitro synthesis of inorganic nanoparticles using enzymes and proteins from microbes, National Seminar on Nanobiotechnology: The Road Ahead, National Botanical Research Institute, Lucknow, 17 November 2005

In vitro synthesis of nanomaterials using enzymes and proteins from fungi and actinomycetes, National Seminar on Nanoscience and Nanobiotechnology, Department of Bioinformatics Pondichery University, Pondichery, 6 December 2005

Enzyme mediated synthesis of inorganic nanoparticles using fungi and actinomycetes, International Interdisciplinary Conference on Sustainable Technologies for Environmental Protection "Probing the Boundaries", Coimbatore Institute of Technology, Coimbatore, Tamil Nadu, 7 January 2006

Bioinspired nanomaterials synthesis and its application in hyoperthermia and drug delivery, International Conference on Ethnopharmacology and Alternative Medicine & 5th Annual Conference of National Society of Ethnopharmacology, Amala Cancer Research Centre , Thrissur, 21 January 2006

Bioinspired nanomaterials synthesis and its applications, Indo-French Symposium on Nanotechnology, National Institute of Oceanography, Goa, 24 January 2006

Bioinspired Intracellular/ extracellular nanomaterials synthesis, National Seminar on Fungal Biodiversity, Biotechnology & Bioinformatics, Shri Bhagawan Mahaveer Jain College, Bangalore, 3 February 2006

Dr. Gadre, Ramchandra Vitthal

Bioreactor designing, Mohite College, Bharati Vidyapeeth, Paud Road, Pune, 25 February 2006

Dr. Ganesh, K.N.

Conformationally constrained PNA analogs: Structural evolution towards DNA/RNA binding selectivity, Symposia on Organic Synthesis and Process Chemistry, IICT, Hyderabad, 2 April 2005

The tale of two prolines: The role of 4-substituted prolines in collagen structure, ETH, Zurich, Switzerland, 27 May 2005

Peptide nucleic acids: Conformationally constrained PNA analogs for DNA/RNA binding selectivity, Organic Colloqium, ETH, Zurich, Switzerland, 13 June 2005

Peptide nucleic acids: Conformationally constrained analogues towards selective DNA / RNA binding, Syngenta Chemistry Lectureship, Syngenta Crop Protection AG, Basel, Switzerland, 23 June 2005

Peptide nucleic acids: Conformationally constrained analogues, Department of Chemistry, University of Bern, Switzerland, 27 June 2005

Conformationally constrained PNA analogs: Structural evolution towards DNA/RNA binding selectivity, IUPAC Congress on Innovation in Chemistry, Beijing, China, 15 August 2005

Peptide nucleic acids: Some recent exciting results from NCL, Chemistry Department, Indian Institute of Technology, Madras, 22 September 2005

DNA/RNA structure: Molecular recognition, JNCASR Lectures on Frontiers in Chemistry, Banaras Hindu University, Benaras, 17 October 2005

Chemistry Excitements: The new age of molecules, JNCASR Lectures on Frontiers in Chemistry, Banaras Hindu University, Benaras, 17 October 2005

Dr. Gokhale, S.P.

Environmental applications of Raman spectroscopy, Refresher Course, Ahmednagar College, Ahmednagar, 16 January 2006

Fuel cell technology: A promising power alternative, Refresher Course, Ahmednagar College, Ahmednagar, 16 January 2006

Dr. Gopinath, C S

Molecular origins of wettability of hydrophobic poly(vinylidene fluoride) microporous membranes on poly(vinyl alcohol) adsorption: Retchembic 2005, VHNSN College, Virudunagar, Tamil Nadu, 22 July 2005

Synthesis, characterization, electronic structure and photocatalytic activity of nitrogen doped TiO2 nanocatalyst, University of Tokyo, Department of Chemical Systems Engineering, 9 November 2005

Isothermal kinetic study of nitric oxide adsorption and decomposition on Pd(111) Surfaces: A molecular beam study, Third DST-JSPS workshop on surface and interfaces of nanomaterials including catalysis, The University of Tokyo, Department of Chemistry, Japan, 11 November 2005

An introduction to photoelectron spectroscopy: Physics and chemistry of solids, Emerging Trends in the Chemistry of Materials, Goa University, Goa, 18 March 2006

Dr. Grover, Gursharn Singh

Disaster management in a chemical warfare / accident scenario, Senior Officers Course 2005, College of Military Engineering, Pune, Pune, 19 October 2005

Dr Kulkarni, B.D.

Challenges in Bioseparations, A.C. Tech Annai University, Chennai, 02 March 2006

"Mathematical modelling of electrochemical engineering systems" and "Modelling paradigms and their applications", Central Electrochemical Research Institute, Karaikudi, 03 March 2006

Asymptotic methods - The beauty and the benefits. University of Pune, 13 March2006

Dr. Kulkarni, Mahesh Jagadish

Applications of mass spectrometry in biological research, Agharkar Research Institute, Pune, 18 January 2006

Dr. (Mrs) Nadgauda, Rajani S.

Agricultural biotechnology in and for Maharashtra, South Asia Biosafety Programme, USAID / USA, Aurora Tower, Pune, 20 September 2005

Biotechnological approaches for forestry improvement: Emerging trends in applied botany, seed science and technology, University of Mysore, Mysore, 5 October 2005

Dr. (Mrs) Ramaswamy, Veda

Photocatalytic decomposition of methylene blue on nanocrystalline titania prepared by different routes, Indo-Italian Brain Storming Workshop on Technology Transfer for Industrial Application of Novel Methods for Environmental Problems, Bharathi Vidhyapeeth Deemed University, College of Engineering, Pune, 5 December 2005

Encapsulation of metal phthalocyanine in alumina pillared clays, Indo-Italian Brain Storming Workshop on Technology Transfer for Industrial Application of Novel Methods for Environmental Problems, Bharathi Vidhyapeeth Deemed University, College of Engineering, Pune, 6 December 2005

Dr. (Mrs) Rao, Mala

Molecular characterization and biotechnological application of cellulases from thermophilic *Thermomonospora* sp., International Symposium on Thermophilic Cellulases, Griffith University, Queensland, Australia, 19 September 2005

Aspartic protease inhibitors: Role in drug development, Bioinformatics Institute, \ Singapore, 26 September 2005

Aspartic protease inhibitor: Biomedical and Agricultural application, National Symposium on Recent Trends in Molecular Biology, Pune University, Pune, 16 March 2006

Dr. Mukherjee, Samindra Nath

Environmental management of mosquito vectors, Refresher Course in Environmental Science for College & University Teachers of Pune University, New Arts, Commerce & Science College, Ahmednagar, 6 April 2005

Effects of sublethal concentrations of flufenoxuron on the biology of the red flour beetle, G. B. Pant University of Agriculture & Technology, Pantnagar, 21 September 2005

Environmental Impact of Biotechnologically Modified Crops, Biopesticide Conference-Biopesticides Emerging Trends, IHBT, Palampur, 11 November 2005

Dr. Mulla, Imtiyaz S.

Smart materials, *Vidnyan parichay*, All India Radio, Pune, 19 February 2006

Dr. Natu, A.A.

Newer developments in drug discovery, Science Expo-2005, Nehru Science Centre, Mumbai, 25 November 2005

Dr. Poddar, Pankaj

Magnetism in nanomaterials, Indo-UK Workshop, British Council, New Delhi, 15 March 2006

Dr. Prasad, B.L.V.

Current trends in nanoscience & technology, Science Expo-2005, Nehru Science Centre, Mumbai, 26 November 2005

Dr. Radhakrishnan, Subramanian

Sensors based on conducting polymers for detection of explosive vapours and toxic gases, DRDO Training, Institute of Armament Technology, Pune, 15 September 2005

Dr. Ranade, Vivek Vinayak

Reactor, process and product engineering via CFD, BHR group lunchtime seminar series, BHR Group, Cranfield, United Kingdom, 7 March 2006

Reactor, process and product engineering, PSE Seminar, process system enterprise Ltd, London, United Kingdom, 10 March 2006

Dr. Sivaram, S.

Controlled synthesis of functional polymers, Central Electrochemical Research Institute, Karaikudi, 24 May 2005

Organic - inorganic hybrids: Polymer-clay nanocomposites, Vikram Sarabhai Space Centre, Thiruvananthapuram, 28 June 2005

Organic - Inorganic hybrids: polymer-clay nanocomposites, 3rd International Conference on Materials for Advanced Technologies (ICMAT 2005), Singapore, Singapore, 5 July 2005

Organic – Inorganic hybrids: polymer-clay nanocomposites, Indian Institute of Technology, Madras, 2 September 2005

Advances in polyolefin catalysts and manufacturing technologies, Seminar on Latest Developments in the Production and Characterization of Olefin Polymers, New Delhi, New Delhi, 17 September 2005

CSIR's R&D capabilities in polymer science, CSIR-Industry Meet 2005, New Delhi, CSIR, New Delhi, 7 October 2005

Process of Innovation, URDIP, Pune, 23 November 2005

INVITED TALKS / LECTURES DELIVERED BY NCL SCIENTISTS

Innovations in polymer materials: applying knowledge in development, Dhirubhai Ambani Commemoration Day Oration, Mumbai, 25 December 2005

Nanoscience and technology: reality or science fiction, Rotary Club of Poona Downtown, Pune, 16 March 2006

Dr. Tewari, Ravindra

Modified nucleosides and across the anticodon loop interactions in tRNA, World Biophysics (IUPAB) Congress, Montpellier, France, 15th IUPAB & 5th EBSA Organized by French Biophysical Society & French National Committee for Biophysics, Montpellier, France, 27 August 2005

Dr. Varma, Anjani Jyotiprasad

Starch and cellulose based products Emerging trends in chemical technology, Second National Seminar on Root and Tuber Crops, Central Tuber crops Research Institute, Thiruvananthapuram, 19 July 2005

CONFERENCES / SYMPOSIA / WORKSHOPS ORGANISED

CONFERENCES / SYMPOSIA / WORKSHOPS ORGANISED

- 7-8 May 2005: Symposium on science education Emerging trends in Teaching and Learning organised by The Maharashtra Science Teachers Association
- 18-21 July 2005: Workshop on New Solid State NMR Methods and Materials Characterisation
- 12-14 Aug. 2005: Workshop on Termite and Mosquito Management
- 29-31 Aug. 2005: Workshop on CSIR E-Journals Consortium – User Interface
- 22 Sept. 2005: Interactive Meet with Seed Industry
- 16-18 Oct. 2005: Workshop on Curriculum Planning (Indian Institute of Science Education and Research)
- 23-28 Oct. 2005: International Symposium on Ionic Polymerization
- 25-26 Nov. 2005: Royal Society of Chemistry-West India Section Students Symposium 2005
- 5-6 Jan. 2006: Workshop on Design and Scale-up of Catalytic Multiphase Reactors
- 7-9 Jan. 2006: Joint International Conference on Building Bridges, Forging Bonds for 21st Century Organic Chemistry and Chemical Biology (ACS-CSIR OCCB 2006)
- 30 Jan. -2 Feb. 2006: Symposium on National Biodiversity and Ecosystem Information Infrastructure: Challenges and Potentials
- 21 Feb. 2006: Workshop on RoCKS: Rotary Cement Kiln Simulator

AWARDS / RECOGNITIONS

• Padmashree (Science and Engineering) • Shri Dhirubhai Ambani Oration Award by the Indian Institute of Chemical Engineers for the year 2005	Dr. S. Sivaram
• Third World Academy Science (TWAS) Prize in Chemistry for the year 2005 • JC Bose National Fellowship	Dr. K. N. Ganesh
CSIR Technology Awards for the Chemical Technology along with IICT, Hyderabad (2005)	Mr. Prashant P. Barve, Mr. Shrikant Ghike, Mr. Milind Y. Gupte, Mr. Ravindra W. Shinde, Mr. R. V. Naik, Dr. J. G. Wadkar, Dr. S. Devotta, Dr. (Mrs.) A.N. Bote, Dr. R. A. Kulkarni, and Mr. C.N. Joshi
Materials Research Society of India (MRSI) medal (2006)	Dr. Upendra Natarajan
CSIR Young Scientist Award in Engineering Sciences. (2005)	Dr. K. Guruswamy
Prof. N. S. Narasimhan Award	Dr. S. P. Chavan
Prof. G. V. Bakore Memorial Award of Indian Chemical Society for the year 2003	Dr. R. V. Chaudhari
Fellow of Royal Society of Chemistry (FRSC)	Dr. V. R. Pedireddi
LABDHI-RDE (RDE – Research, Development & Education) award by Shri Labdhinidhan Charitable Trust	Dr. A. A. Natu
Humboldt Fellowship	Dr. A.P. Giri

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- Hindustan Organic Chemicals Ltd., Rasayani

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- Apcotex Industries Ltd., Mumbai
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- NRDC, New Delhi

Dr. (Mrs.) R.D. Wakharkar
- Bakul Finechem Research Centre, Mumbai

EDITOR/ EDITORIAL BOARD MEMBERS OF RESEARCH JOURNALS

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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. (Mrs) Rajani Nadgauda

- Plant Cell Biotechnology & Molecular Biology, Society for Biology and Biotechnology, Salem
- Physiology & Molecular Biology of Plants, Lucknow

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, NewDelhi

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. 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. Murali Sastry

- Associate Editor (Asia), Applied Nanoscience, Open Mind Journals, Auckland, New Zealand
- Bulletin of Materials Science, Indian Academy of Sciences, Bangalore.
- Journal of Biomedical Nanotechnology, American Scientific Publishers, USA
- Journal of Colloid and Interface Science, Elsevier, The Netherlands
- Langmuir, American Chemical Society, USA
- Editor (Nanomaterials), Materials Research Bulletin (MRB), Elsevier, Oxford, UK.

EDITOR/ EDITORIAL BOARD MEMBERS OF RESEARCH JOURNALS

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. Vijayamohanan

- Bulletin of Materials Science, Indian Academy of Sciences, Bangalore

NCL RESEARCH FOUNDATION

NCL RESEARCH FOUNDATION

The National Chemical Laboratory Research Foundation (NCL RF), a non-profit organization, was established in 1991 with a mission to promote excellence in science and technology and build an environment in which everyone in NCL strives to improve their scientific, technical and R&D support skills and reach higher goals in R&D activity. It aims at bringing creative research, knowledgebase and innovative technologies into clear focus that NCL considers important for the furtherance of the goals in science and technology.

NCL RF has the primary aim to motivate and recognize the high level of team and individual efforts of scientists, engineers, technologists, research students and support staff at NCL for their contributions in "advancement of knowledge and in applying chemical science for good of the people" by way of scientific research and innovations.

A corpus fund made up of contributions from private organizations and individuals interested in NCL's progress and welfare has been created and the earnings from the fund are used to further the objectives of the Foundation. The NCL RF recognises the contribution of NCL scientists through institution of various awards such as NCL Foundation Day awards, National Science Day awards and National Technology Day awards to promote excellence in basic science, applied research leading to commercialisation of technology, new initiatives in the R&D support systems, to recognize unusual merit in individuals from the scientific and supporting staff and to promote the safety culture in the laboratory. Besides, it also organises various special lectures in memory/ honour of former NCL Directors.

NCL RF has been registered as a public trust and is managed by a Board of trustees. This Trust has been granted an exemption under U/S 80G of the Income tax act 1961 to enable it to receive donations.

NCL RF is a unique experiment in public – private partnership to encourage all round excellence in all endeavours in the laboratory. It is managed through an independent Board of trustees as a private fund within a public body. It brings to its activities a high level of transparency and accomplishments as well as peer-groups participation in all decision making.

Objectives of the Foundation

- To give awards to the teams of NCL scientists, engineers and technologists for scientific innovations or development of commercial technologies of international class. The work must represent a high level of team effort.
- To give awards, institute fellowships or scholarships, stipends, remuneration and/or other similar payments to NCL scientists and research scholars to facilitate their undertaking a high level of scientific and technological research in the area of interest to NCL.
- To establish and support professions, fellowships, lectureships, scholarships and prizes.
- To award scholarships and fellowships and grants to NCL scientists and research scholars by way of loan and otherwise and on such terms and conditions, as the trustees may think fit for the purpose of undertaking, prosecuting and encouraging research work in chemistry, chemical technology, chemical engineering, biological sciences and other branches of sciences of interest to NCL.
- To encourage and support participation by NCL scientists and research scholars in the conferences and seminars abroad for activities relating to the research areas of interest to NCL.
- To print, publish and exhibit or subsidies the publication of any pamphlets, or posters relating to the research done by NCL scientists and research scholars.
- To provide for, educate and train NCL staff or other institutes in India or abroad to enable them to manage research and other infrastructural groups effectively.

NCL RESEARCH FOUNDATION

- To devise incentive schemes, or reward systems for the supporting staff belonging to administration, finance, purchase, marketing and other related sections, so that they can effectively contribute towards the attainment of laboratory's R&D goals.
- To promote, develop and improve scientific exchange of knowledge as well as technical cooperation between research institutions having objects similar to that of the foundation.
- To do all acts, matters and things as are incidental or conducive to the attainment of the above aims and objects or any one or more of them.
- To takeover or amalgamate with other charitable society or trust with similar objects.

Board of Trustees

The Board of Trustees consists of following members and such other persons as may be appointed from time to time.

- o Director, NCL - Ex-officio member & Chairman
- o Chairman, Research council, NCL - Ex-officio member
- o Director, MUICT - Ex-officio member
- o Two senior most divisional heads, NCL - Ex-officio members
- o Controller of administration / AO, NCL - Ex-officio member.
- o Senior finance & accounts officer / F&AO, NCL - Ex-officio member
- o One Research council member
- o One representative from industry

The Director, NCL is the Ex-officio trustee and the Chairman of the trust. He/ she presides over all meetings of the trustees. In his/her absence, the person whom the Trustees present at the meeting elect as Chairman of the said meeting by a vote of majority acts as the Chairman of the said meeting.

The Ex-officio members are the trustees of the trust by virtue of their post and the person holding the respective post continues as trustee of this trust till he relinquishes the post or another member is nominated in his place by his organization/ department.

As regards the trustees other than ex-officio members, the tenure does not exceed more than three years. However, the Board of trustees have the power to extend the tenure of such trustees.

Board of Trustees

Position	Present board	By virtue of
Chairman	Dr. S. Sivaram	Director, NCL
Member	Prof. M. M. Sharma	Chairman, Research council
Member	Prof. J. B. Joshi	Director, MUICT
Member	Mr. Desh Bandhu Gupta	Representative of donor industry
Member	Dr. B. D. Kulkarni	Deputy Director, NCL
Secretary	Mr. M. S. Vidyanathan	CoA, NCL
Treasurer	Mr. S. Chandrahas	SFAO, NCL
Jt. Secretary	Mr. G. Prabhakaran	In-charge, MIS, NCL

AWARDS

NCL RF gives various awards on NCL Foundation Day and National Science Day.

NCL Foundation Day Awards

Every year, 3rd January is celebrated as NCL Foundation Day. An eminent person is invited to deliver the NCL Foundation Day Lecture. The following awards are given on this occasion:

Scientist(s) of the year award: This award carries a cash prize of Rs. 20,000/- and a citation to the award winner. The award is peer reviewed by an external committee. The two awards in this category are sponsored by **"Shirinbai & Maneckji Neterwala Foundation"** and **"Dr. R.A. Mashelkar Endowment Fund"**.

Technology of the year award: This award is funded by ICICI and carries a cash prize of Rs. 30,000/- and a citation. The award is peer reviewed by an external committee.

CIPLA - Hamied award: This award for the best process development work carries a cash prize of Rs. 15,000/- and a citation.

Highest industrial earning award: This award carries a trophy and a rotating shield to the winner(s) based on the per capita industrial earning of the division.

New initiative taken by the R&D support system: This award carries a cash prize of Rs. 20,000/- and a citation to team members. The award is given for the group activity and not for individual performances.

Individual merit award(s): This award carries a cash prize of Rs. 5000/- each and a certificate of merit. There are total three awards.

Director's commendation awards: The Chairman NCL RF recognizes an individual or a group of individuals for their exemplary

National Science Day Awards

Every year, 28 February is celebrated as National Science Day. An eminent person is invited to deliver the Science Day Lecture. Award winners of 'Best paper award' in each area of physical & material sciences, chemical sciences, biological sciences and engineering sciences make the presentations of their papers on this occasion.

Keerti Sangoram memorial endowment award for the best research scholars: This award carries a cash prize of Rs. 2500/- each and a certificate of merit for four students in the area of physical & materials sciences, biological sciences, chemical sciences and engineering sciences.

Dr. Rajappa award for the best organic chemistry paper: This award for research students carries a cash prize of Rs. 1000/- and a citation.

Lectures

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

- National Technology Day Lecture: in memory of Prof B.D. Tilak
- 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 has launched a new initiative to provide merit based scholarships for the children of NCL employees in group D (non-tech) and support staff in group I. The scholarship is admissible for children studying in IX to XII Standards. The scholarship amount for the students who stood first is Rs.4000/- and for those who stood second is Rs.3500/- from each class. The scholarship is primarily to facilitate the students to defray the fees, including computer fee, science fee, etc. and will be utilized for providing books and other related materials relevant to their curriculum. Fourteen meritorious children, including nine girls were awarded the scholarships and commendation certificates.

Dr. R. A. Mashelkar, DG-CSIR and Dr. S. Sivaram, Director NCL with recipients of merit based scholarships meant for the children of NCL employees

NCL Foundation Day Annual Awards - 2005

Title of the 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. R. Pedireddi (Organic Chemical Synthesis Division)	For design and synthesis of supramolecular assemblies of exotic architectures of varied geometries and thereby opening a new dimension in the field of Organic Solid State Chemistry & Materials
Highest Industrial Earning Award	Rotating Shield & Trophy	Polymer Science & Engineering	Highest per capita (net) industrial earning during 2004-05
Award for "New Initiative taken by the R&D Support System"	Rs.20,000/- + Certificate of Merit Commendation	Mr. R. P. Purandare Mr. S. R. Wagh Mr. S. M. Mane Mr. M. B. Bhavsar Mr. P. S. Shah Electrical Section Staff : - Mr. S. B. Gaikwad - Mr. K. M. Gaikwad - Mr. V. A. Deshpande - Mr. Y. G. Subhedar - Mr. C. Subramaniyam - Mr. R. Chandekar - Mr. P. H. Chavan - Mr. O. R. Sarkaniya - Mr. Siddarth B. Gaikwad - Mr. M. B. Shete - Mr. A. N. Wachkal - Mr. D. M. Sutar - Mr. K. S. Babra - Mr. C. Mahadevan Mr. S. B. Karanjkar	For introducing a modern electrical system to cope up with the present and future power demands at NCL
Director's Commendation Award	Rs. 5,000/-+ Certificate	Dr. Murali Sastry Ms. Anita Swami Mr. Saikat Mandal Mr.P.R.Selvakannan	For enhancing the prestige of NCL through a paper "New approaches to the synthesis of anisotropic, core-shell and hollow metal nanostructures" which was highlighted in the cover page of "Journal of Materials Chemistry"

NCL Foundation Day Annual Awards - 2005

Title of the Award	Award	Award winner	Awarded for
	Rs. 5,000/-+ Certificate of Commendation	Dr. V. R. Pedireddi Mr. Sunil Varughese	For enhancing the prestige of NCL through a paper "Hydrogen bond mediated open-frame networks in coordination polymers: supramolecular assemblies of Pr(III) and 3,5-dinitro-4-methylbenzoic acid with aza-donor compounds"which was highlighted in the cover page of "Chemical Communications".
Individual Merit Award	Rs.5,000/-+ Certificate of Merit	Mr. V. V. Borkar (CEPD Division)	For the complete design and development of a process control and unique data acquisition system for super critical reaction assembly.
	Rs.5,000/- each+ Certificate of Merit	(SHARED) Mr. B. K. Ghodke (Engineering Service Unit) & Mr. P. B. Kokney (Engineering Service Unit)	For their dedicated efforts and skill for the installation, commissioning and tiding over teething problems for the changeover to the new telephone exchange in a limited time without a break in the services.
	Rs.5,000/- each+ Certificate of Merit	(SHARED) Mr. S. S. Deo(CMC) & Mr. R. S. Gholap(CMC)	For their services for the smooth operations of the central facilities like LC-MS, MALDI-TOF & Mass-Spectrometer, and for offering committed support to various aspects of instrumentation required during installation & further maintenance.

National Science Day Awards

Keerthi Sangoram Memorial Endowment Award for best research fellows for the calendar year - 2005

Area	Best Research Scholar of the year	Guide	Award
Chemical Sciences (Sharing)	Mr. J. Prakasha Reddy Mr. Vasudeva Naidu Sagi	Dr. V.R. Pedireddi Dr. Pradeep Kumar	Rs.1,250/- +Citation Rs. 1,250/- +Citation
Physical & Material Sciences (Sharing)	Mr. C. Rajsankar Mr. Niranjan Suryakant Ramgir	Dr. P.A. Joy Dr. K. Vijayamohanan	Rs.1,250/- + Citation Rs.1,250/- + Citation
Biological Sciences	Mr. Vipul Bansal	Dr. (Mrs.) A. Prabhune	Rs. 2,500/- +Citation

Dr. Rajappa Prize Award for the Research Student (2005)

Area	Title and Journal	Author (s)	Guide	Award
Dr. Rajappa Prize for the research paper in Organic Chemistry (S) Division	Nucleobases in molecular recognition : Molecular adducts of adenine and cytosine with –COOH functional groups Angew Chem	Mr. P. Sathyanarayana Reddy and E. Suresh	Dr. V.R. Pedireddi	Rs. 1,000/- + Citation

DATELINE NCL

DATELINE NCL

April 7: Dr. Vijay Nair, Emeritus Scientist, Regional Research Laboratory, Trivandrum delivered the ninth Prof. Sukh Dev Endowment Lecture on "Engaging zwitterions in carbon-carbon bond forming reactions: a promising synthetic strategy".

May 2-13: Training programme on plant tissue culture to encourage educated unemployed people to take up tissue culture as a viable enterprise and also to train manpower for tissue culture industries. The training programme was mainly targeted at entrepreneurs, extension workers, farmers, teachers, etc.

May 7-8: A symposium on science education "Emerging trends in teaching and learning was organised by The Maharashtra science teachers association. Prof. D.V. Prabhu, Wilson College, Mumbai and Prof. S.P. Kamat, Goa University delivered keynote address on "New perspectives in science education in teaching and laboratory experiment".

May 16: Prof. Colin D. Bain, Department of Chemistry, Oxford University delivered the fifth Prof. J.W. McBain Memorial lecture on "Marangoni effects: where surface chemistry and fluid dynamics meet".

June 7: Dr. Nitya Anand, Former Director, Central Drug Research Institute, Lucknow delivered the forth Prof. K. Venkataraman Memorial Lecture on "My life in drug research: and lessons learnt".

July 11-12: Orientation programme for newly joined research students and staff members was organised in four modules as: systems and procedures, good laboratory practices, information and communication and student academic affairs.

July 18-21: Indo-French workshop on "New solid state NMR methods and materials characterization".

July 25: Shri. Sanjit 'Bunker' Roy, Founder Director, Barefoot College, Tilonia, Rajasthan delivered the third Prof. B.D. Tilak Memorial Lecture - on "Demystifying technology to meet basic needs: the barefoot approach".

Aug. 12-14: Workshop on "Termite and mosquito management". Dr. Y.L. Nene, Former Deputy Director, ICRISAT delivered the keynote address.

DATELINE NCL

Aug. 29-31: Workshop on CSIR e-journals consortium – user interface.

Sept. 8-14: Hindi week was celebrated. Prof Ashok Kamat, Head, Sant Namdev Adhyasan Peeth, Pune University released the NCL Hindi bulletin, "Alok".

Sept. 19-20: Interactive programme for finance & accounts officers.

Sept. 22: Interactive meet with seed industry to understand current R & D requirements of seed industry. Dr. P.S. Rao, Director, Dept. of Biotechnology, PES Institute of Technology delivered the keynote address. Representatives of about thirty seed industries from all over India attended the meet.

Sept. 26: CSIR Foundation Day - Dr. G. Thyagarajan, Former Director, RRL, Jorhat, RRL, Hyderabad and CLRI, Chennai delivered a lecture on "The CSIR in India's life and part of it - glimpses of events, people and places" under the series "Builders of CSIR".

Sept. 27: Visit of the Parliamentary Standing Committee on Science & Technology, Environment & Forests.

Sept. 30: Visit of members of organization of plastics processors of India.

Oct. 3-4: Orientation programme for newly joined research students and staff members.

Oct. 20: NCL Research foundation award of merit based scholarship to the children of NCL employees were distributed by Dr. R. A. Mashelkar, DG CSIR.

Oct. 23-28: The International Union of Pure and Applied Chemistry (IUPAC) sponsored "International symposium on ionic polymerization" was organised.
Nov. 7-11: Vigilance Awareness Week.

Nov. 8: Prof. Arup K. Chakraborty delivered the seventh Dr. L. K. Doraiswamy Endowment Lecture.

Nov. 10: Prof. Joseph P. Kennedy, Distinguished Professor of polymer science and chemistry, Institute of Polymer Research, The University of Akron, USA delivered the second Dr. R. A. Mashelkar Endowment Lecture on "A career in polymers".

Nov. 25-26: Symposium on Royal Society of Chemistry-West India Section.

Dec. 8: Dr. Charles Kresge Vice President, Basic Plastic and Chemicals R & D, Hydrocarbons and Energy R & D, The Dow Chemical Company, Midland, Michigan delivered the second Dr. Paul Ratnasamy Endowment Lecture on "Novel porous materials".

Dec. 15-16: CSIR Programme on "Youth for Leadership in Science" (CPYLS).

Jan. 3: Prof. Robert H. Grubbs, Noble Laureate, Victor Elizabeth Atkins Professor of Chemistry California Institute of Technology, USA delivered NCL Foundation Day Lecture on "Chemistry develops drugs, bugs and bats".

Jan. 5-6: Workshop on "Design and scale-up of catalytic multiphase reactors".

Jan. 7-9: ACS and CSIR sponsored Joint international conference on "Building bridges, forging bonds for 21st century organic chemistry and chemical biology".
Jan. 30- Feb. 2: Symposium on "National biodiversity and ecosystem information infrastructure: challenges and potentials". Dr. Haanu Saarenmaa, Deputy Director, global biodiversity information facility (GBIF), Denmark delivered the keynote address.

Feb. 21: Workshop on Rocks: Rotary cement kiln simulator.

Feb. 27- 28: National Science day - Prof. Partha Majumder, Head, Anthropology and Human Genetics Unit, Indian Statistical Institute, Kolkata delivered lecture on "Where do we come from? A statistical - genetic traceback".

March 6: National safety Day – Shri R. Veeraraghavan former Head, Fire and Safety Department, HPCL, Mumbai delivered the special lecture on "Safety and its management in the laboratory".

राजभाषा का कार्यान्वयन

केन्द्र सरकार का प्रतिष्ठान होने के फलस्वरूप संघ सरकार की राजभाषा नीति राष्ट्रीय रासायनिक प्रयोगशाला पर भी लागू है । अतः इस प्रयोगशाला के मुख्य कार्यकलापों के साथ-साथ राजभाषा के कार्यान्वयन हेतु भी अनेक प्रकार से हर स्तर पर प्रयास किए जाते हैं।

राष्ट्रीय रासायनिक प्रयोगशाला रसायनविज्ञान एवं रासायनिक अभियांत्रिकी के अंतर्राष्ट्रीय शोध केन्द्र के रूप में विख्यात है । 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 अँग्रेजी 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 । प्रयोगशाला स्टाफ के सभी संवर्गों के पदों के रोस्टर द्विभाषी बनाए गए हैं । इसी प्रकार वैज्ञानिकों के तथा अन्य सभी पदों से सम्बन्धित नियुक्ति पत्र द्विभाषी रूप में जारी किए जाते हैं। सभी साइनबोर्ड 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 अँग्रेजी शब्द का हिन्दी पर्याय तथा एक सुविचार लिखा जाता है। इससे कर्मचारियों के हिन्दी के ज्ञान में वृद्धि होती है और वे अपना दैनंदिन 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 पुस्तके प्रतिवर्ष खरीदी जाती हैं । निदेशक महोदय का स्टाफ को सम्बोधित पत्र प्रत्येक तिमाही में अँग्रेजी के साथ-साथ हिन्दी तथा मराठी में भी जारी किया जाता है । प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानों एवं आयोजनों की रिपोर्टें "सीएसआईआर न्यूज" एवं "सीएसआईआर समाचार" में प्रकाशनार्थ हिन्दी और अँग्रेजी 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 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 अधिकाशं 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 (डॉक्युमेंटरी फिल्म) का भी निर्माण किया है ।

प्रयोगशाला में प्रतिवर्ष हिन्दी दिवस/हिन्दी सप्ताह मनाया जाता है । इस उपलक्ष्य में विभिन्न प्रतियोगिताओं एवं सांस्कृतिक कार्यक्रमों का आयोजन किया जाता है । इसके अलावा सी.एस.आई.आर. मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन य़ोजना, वैज्ञानिक कार्यो में हिन्दी पुरस्कार योजना तथा विज्ञान चिन्तन लेखमाला आदि योजनाओं में भी 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 ।

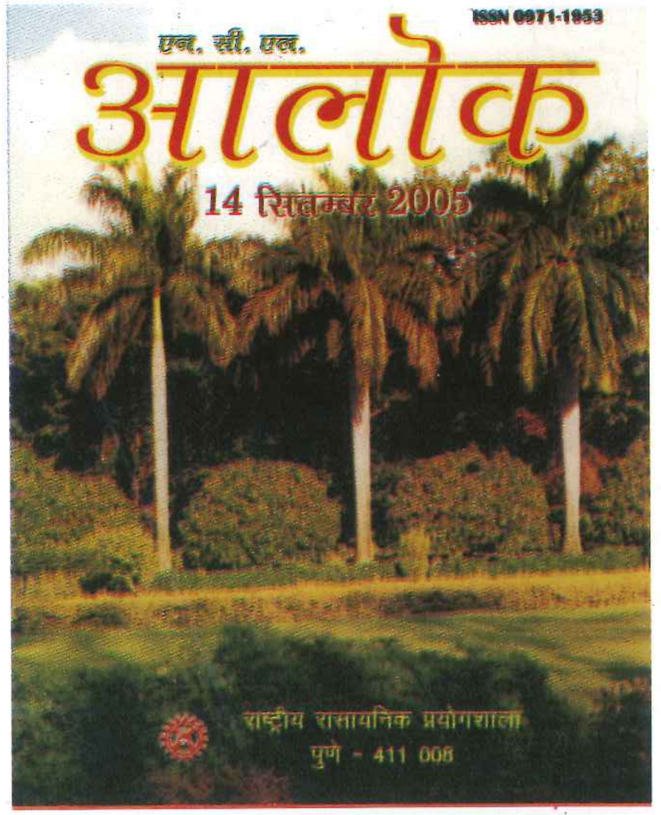
यह प्रयोगशाला वैज्ञानिक अनुसंधान के क्षेत्र में राजभाषा के प्रगामी प्रयोग की दिशा में पूर्ण रूप से सजग है । यहाँ के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाले राष्ट्रीय विज्ञान सम्मेलनों/संगोष्ठियों में भाग लेकर हिन्दी में अपना शोधपत्र प्रस्तुत करते हैं । प्रयोगशाला में भी राजभाषा के प्रयोग को बढ़ावा देने के लिए समय-समय पर हिन्दी माध्यम से विज्ञान संगोष्ठियों एवं कार्यशालाओं का आयोजन किया जाता है । वैज्ञानिक कार्यकलापों में हिन्दी का प्रयोग और अधिक बढ़ाने के लिए सतत प्रयास जारी हैं ।

राष्ट्रीय रासायनिक प्रयोगशाला में हिन्दी सप्ताह समारोह का आयोजन

राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में दि. 8 सितम्बर से 14 सितम्बर, 2005 की अवधि में हिन्दी सप्ताह समारोह का आयोजन किया गया । इस दौरान प्रयोगशाला के स्टाफ हेतु चार प्रतियोगताएँ आयोजित की गईं । समारोह के पहले दिन 08.09.2005 को शब्दज्ञान प्रतियोगिता का आयोजन किया गया जिसमें लगभग 25 कर्मचारियों ने भाग लिया । दिनांक 09.09.2005 को हिन्दी निबन्ध प्रतियोगिता आयोजित की गई । इस प्रतियोगिता में स्टाफ के 12 सदस्यों ने भाग लिया । तत्पश्चात दिनांक 12.09.2005 को हिन्दी वाक् प्रतियोगिता का आयोजन किया गया जिसमें लगभग 10 कर्मचारियों ने भाग लिया । अन्त में दि. 13.09.2005 को सामान्य ज्ञान प्रतियोगिता आयोजित की गई जिसमें कुल 22 कर्मचारियों ने भाग लिया । उसी दिन अर्थात दि. 13.09.2005 को अपराह्न 3.00 बजे प्रयोगाला की राजभाषा कार्यान्वयन समिति की तिमाही बैठक सम्पन्न हुई ।

हिन्दी दिवस के अवसर पर दि. 14.09.2005 को अपराह्न 3.00 बजे **हिन्दी सप्ताह समापन समारोह** का आयोजन किया गया । समारोह का प्रारंभ सरस्वती वन्दना से हुआ । इस अवसर पर बहुभाषाविद् एवं मूर्धन्य विद्वान तथा पुणे विश्वविद्यालय में संत नामदेव अध्यासन पीठ के संस्थापक एवं विभागाध्यक्ष प्रो. अशोक कामत मुख्य अतिथि के रूप में उपस्थित थे । उन्होंने प्रयोगशाला की वार्षिक राजभाषा पत्रिका, **'एनसीएल आलोक'** का लोकार्पण किया । अपने सम्बोधन में प्रो. कामत ने हिन्दी भाषा को बहुत ही सहज एवं सरल बताते हुए उसकी वैज्ञानिकता पर प्रकाश डाला । उन्होंने कहा कि हमारी भाषाएँ हमारे सर्वांगीण विकास में सहायक होती हैं । भाषा के माध्यम से ही हम अपनी संस्कृति, सभ्यता और संस्कारों को अक्षुण्ण रख सकते हैं । उन्होंने इस सन्दर्भ में फादर कामिल बुल्के का भी दृष्टान्त दिया कि किस तरह उन्होंने तुलसीदास जी की केवल दो पंक्तियों को पढ़कर अपने जीवन की दिशा बदल दी । प्रो. कामत ने कर्मचारियों विशेष रूप से वैज्ञानिकों का आह्वान किया कि वे अपने दैनंदिन कामकाज के अलावा शोधकार्यों में राजभाषा हिन्दी का प्रयोग करना शुरू करें ताकि आम जनता के साथ उन्हीं की भाषा में संवाद या सम्पर्क स्थापित किया जा सके ।

इस अवसर पर प्रयोगशाला के उपनिदशेक, डॉ. भास्कर कुलकर्णी ने अपने अध्यक्षीय भाषण में हिन्दी के प्रति गहन समर्पण भाव प्रदर्शित करते हुए कहा कि हिन्दी एक अतीव वैज्ञानिक भाषा है । इसके शब्दों के अर्थ और उनकी व्युत्पत्ति में भी वैज्ञानिकता के दर्शन होते हैं । "सम" शब्द के अर्थ का निरूपण करते हुए उन्होंने कहा कि यह जीवन के प्रत्येक क्षेत्र और प्रत्येक स्थिति में संतुलन बनाए रखने का प्रतीक है । डॉ. कुलकर्णी ने हिन्दी के उत्तरोत्तर प्रयोग पर बल दिया और कहा कि हमें अपने दैनंदिन कामकाज में राजभाषा को अपनाकर राष्ट्रीय अस्मिता की रक्षा करनी होगी । इस समारोह में हिन्दी सप्ताह के उपलक्ष्य में आयोजित विभिन्न प्रतियोगिताओं के विजेताओं को मुख्य अतिथि ने पुरस्कार प्रदान किए । प्रयोगशाला के प्रशासन नियंत्रक, श्री एम.एस. वैद्यनाथन ने धन्यवाद ज्ञापन किया । इसके पूर्व प्रयोगशाला के वरिष्ठ हिन्दी अधिकारी, डॉ. रमाशंकर व्यास ने सभी का स्वागत करते हुए हिन्दी सप्ताह समारोह की भूमिका को रेखांकित किया तथा हिन्दी सहित सभी भारतीय भाषाओं की अपरिहार्यता एवं महत्त्व पर प्रकाश डाला । समारोह का संचालन हिन्दी अधिकारी, श्री उमेश गुप्ता ने किया।



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.

Statutory Committees	Chairperson
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
Medical Services Committee	Dr.(Mrs.) Vidya Gupta
Colony Affairs Committee	Dr. M.K. Gurjar
Confirmation and Probation Committee	Dr. R.V. Chaudhari
Patents Committee	Dr. R.V. Chaudhari
Staff Quarter Allotment Committee	Dr. B.D. Kulkarni
Information and Library Committee	Dr. M.G. Kulkarni
Standing Disposal Committee	Dr. R.V. Chaudhari
Normalisation Committee for APAR gradings (for Tech. Officers in Gr.III)	Dr. B.D. Kulkarni
Standing Purchase Committee II	Dr. A.J. Verma
Sub-committees of Standing Purchase Committee-II	Dr. Anil Kumar
Standing Purchase Committee – I	Shri M.S. Vidyanathan
Building and Construction Committee	Dr. P.V. Rao
Grievance Redressal Committee	Dr. K.N. Ganesh
Compassionate Appointment Committee	Dr. B.D. Kulkarni
Standing Committee on Lab. Safety	Dr. S. Sivaram

Institutional/Ad-hoc Committees	Chairperson
Committee to examine comprehensively future communications and conferencing needs of NCL	Ms. Neelima Iyer
Committee to prioritise major equipment purchase from CSIR/Lab. Reserve funds	Dr. K.N. Ganesh
Coordinating Committee for Central NMR facility	Dr. K.N. Ganesh
Human resource development and management committee	Dr. S. Sivaram
Monitoring Committee on Stores Management	Dr. M.G. Kulkarni
Students Academic Committee	Dr. Sourav Pal
Support Grant to Student to participate in International Conference	Dr. Sourav Pal

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Chairman

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