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BIENNIAL REPORT



NATIONAL CHEMICAL LABORATORY DR. HOMI BHABHA ROAD PUNE 411008 INDIA

Cover Design (clockwise from top left):

- Space filling molecular model of DNA-containing unnatural 5-amino-deoxy uridine, a view from the major groove.
- 2. Computer-generated structure of ZSM-5 with p-xylene molecule inside the cage.
- 3. Molecular ordering in polymers. Spherulites of large dimensions grown under favourable conditions.
- 4. Somatic embryos of chick pea, an important grain legume in India. Chick pea plants have been successfully regenerated via somatic embryogenesis at NCL.

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	Catalysis & Catalytic Technology Polymer Science & Technology Biochemical Sciences & Biotechnology Organic Synthesis & Technology Materials Chemistry Theoretical Chemistry Chemical Reaction Engineering Energy Conservation Instrument Development Project Planning & Development Library & Documentaion Technical Services NCL Prepares for the Future (special section)

t is a great pleasure to present the Biennial Report (1991–1993) of National Chemical Laboratory(NCL). The report brings out our achievements in both science and technology during this period.

1991 was an important year for India. In July 1991, the new Industrial Policy was announced, which attempted to liberalize the Indian industry from the constraints and took first steps in globalizing. This changes the environment, in which the publicly funded R & D institutes have to operate, since free flow of foreign capital and technology is expected in such a liberalized policy. This, in turn, implies that the processes and products delivered as a result of our R & D effort have to be of international class. NCL welcomes this pressure on its performance under more demanding and competitive conditions and its shift in its efforts to meet this challenge is reflected in this entire Biennial Report.

Apart from a stronger drive for true innovation, globalization has been a key movement in NCL's recent endeavours. No nation is in isolation today. Everyone around the world is looking for complementary skill bases in all corners of the world. The chain of invention to innovation crosses national borders today. NCL has seen this challenge and also the opportunities that it provides. We successfully executed China consultancy project during 1991–92 and won ICMA Award for Export of Engineering Services. We initiated aggressive marketing efforts outside India, and forging linkages with leading companies from Europe and USA has been one of the key features during the last two years. Contract research, joint development, technology licensing, technology services and consultancy services are being provided globally by NCL. Earning dollars is really secondary in this case. What is more important is to upgrade the quality of research that we do, to value time and quality as key determinants of class, to continue work on the cutting edge of science and technology at a competitive level. An increasing number of foreign patents granted to NCL is one indicator of NCL's quality and competitiveness of innovation.

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CATALYSIS & CATALYTIC TECHNOLOGY

In order to take our offerings closer to market place and make our efforts globally competitive we set up a number of facilities. They include major pilot plant facilities in plant tissue culture, a downstream processing facility in biochemical engineering, a class 10,000 clean room facility for synthesizing materials conforming to the stringent purity specifications, a polymer processing centre, and a Kg Lab to take care of initial problems of scale up in organic chemical processes. We have also established a new process engineering unit, which will enable us to do value addition. A major catalyst pilot plant is also coming up with World Bank assistance and this will enhance the already magnificent performance of our catalysis group.

We are taking a lot of new initiatives to create a stimulating environment in which everyone gives his best. Formation of the NCL Research Foundation has helped to create mechanisms by which one can now say Thank you to those who perform in and for NCL. Ideas like kite flying projects are helping to elevate the level of innovations in the laboratory. We do know that in science only those are remembered, who say either the first word or the last word. New initiatives on commercialization are being taken. Formation of a commercial arm of NCL is on the cards. We hope that these and several other such initiatives would create an ambience in which NCL will grow and prosper.

R A Mashelkar

TECHNOLOGIES AT COMMERCIAL SCALE

Albene Technology

NCL's single—step Albene technology for making ethylbenzene (EB) from ethanol was implemented at Hindustan Polymers (HP), Visakhapatnam, and the plant was operated successfully over a long period. United Catalysts India Ltd., Vadodara, manufactured and supplied the new Encilite—2 catalyst on which the technology is based. The Albene process is superior to the conventional process and offers 7–10% reduction in consumption of raw materials and energy. It has a special relevance to India, Brazil, Cuba, Malaysia, and other alcohol—rich countries.

■ Formaldehyde Catalyst

An improved Fe-Mo catalyst with a unique morphology for conversion of methanol to formaldehyde has been developed by NCL. The first commercial charge of the catalyst, loaded in February 1992, is still performing very well at Cibatul, Gujarat. The production of formaldehyde is expected to increase by over 10% by the use of this catalyst. The catalyst was manufactured by International Catalysts Ltd., Pune, by the NCL know-how and with NCL's collaboration.

Para-Diethylbenzene (p-DEB)

A process based on alkylation of ethylbenzene with rectified spirit was demonstrated to Hindustan Polymers (HP), Visakhapatnam. The commercial plant for producing 200 TPA of p-DEB has been erected by HP and commercial trials have begun. p-DEB is a high value solvent used in PAREX process for the adsorption separation of hydrocarbon mixtures. With the NCL technology, the monopoly of the multinationals on the production of this speciality chemical will be broken.

Encilite-3-Based Hydrodewaxing Catalyst

NCL developed a hydrodewaxing catalyst composite based on Encilite-3, and the process for making it has been licensed to a European company. This is the first time that such a sophisticated technology in high-tech materials has been transferred from India to a developed country. UCIL, Bombay, manufactures this catalyst using the NCL know-how.

TECHNOLOGIES AT PILOT PLANT SCALE/ SEMI COMMERCIAL SCALE

Linear Alkyl Benzene (LAB)

LAB is largely used in the manufacture of detergents, foaming agents and surfactants. A new process for the manufacture of LAB using large pore zeolites has been developed. The catalysts used in the conventional processes are highly corrosive, and the use of large quantities of HF, a highly corrosive and toxic chemical, leads to periodical and expensive replacements of the plant parts. This adds to the cost of the product besides creating severe personnel safety and environmental problems. The NCL process does not involve the use of hazardous chemicals. This economically attractive 'green' technology has the potential for replacing the conventional process. The work has been done in collaboration with Reliance Industries Ltd., Patalganga, who are setting up a pilot plant for carrying out trials.

Catalyst for MEK Production

An improved Cu-silica dehydrogenation catalyst has been developed for making methylethyl ketone (MEK) from secondary butyl alcohol. This overcomes the problems in MEK manufacture arising from frequent regeneration of the catalyst (short cycle lengths) and consequent sintering of Cu. The new synthesis procedure developed at NCL stabilizes Cu in a silica matrix far more effectively and thus prolongs the cycle length considerably. The process has undergone successful pilot plant trials at Cetex, Madras, and the catalyst will soon be loaded in commercial plants.

Ethanol Dehydration Catalyst

Samples prepared by International Catalysts Ltd., Pune, were evaluated at NCL under different conditions. Successful pilot plant trials were conducted at Chemplast, Madras.

Acetic Acid and Propionic Acid

Gujarat Alkali & Allied Chemicals (GAAC) Ltd., Ahmedabad, are in the process of setting up a semi-commercial pilot plant for acetic acid based on NCL's Encicarb-1 catalyst. GAAC have nearly completed the design of a 4500-TPA propionic acid plant for installation in Gujarat State.

Hydrogenation of Maleic Anhydride to 1,4-Butanediol

Under sponsorship from Adarsh Chemicals, Surat, NCL has developed a continuous process for the conversion of maleic anhydride [MAN] to 1,4-butanediol [BDO], tetrahydrofuran [THF] and gammabutyrolactone [GBL], which has several advantages over the conventional acetylene-based Reppe process involving handling of the hazardous acetylene and copper acetylide catalyst. Also, acetylene is becoming increasingly scarce and more expensive. Another major advantage in the NCL process is that the reaction conditions can be tailored to obtain the desired product (from amongst GBL, THF and BDO) with high selectivity.

LABORATORY-LEVEL DEVELOPMENTS

Development of Indigenous Catalytic Converter Technology

Under the multi-laboratory phase I programme on the development of catalytic converters for two/four-stroke engines sponsored by DST, NCL has been working on perovskite-based catalysts as probable substitutes for noble metal-based catalysts. NCL has also developed techniques for depositing the catalytic material

on pelleted spheres and cordierite-based ceramic monoliths made available by the Ceramic Technical Institute of BHEL, Bangalore.

Some of these samples have been tested in four-stroke engine exhaust streams at Automotive Research Association of India, Pune, with leaded and unleaded gasolines. The initial results have been encouraging. This work is of great topical importance as auto exhaust emissions account for a large part of the pollution load of the atmosphere; these pollutants include toxic and carcinogenic substances like sulfur, nitrogen, lead, zinc, nickel, NO, CO₂ and CO.

Toluene to Para-Chlorotoluene

Chlorotoluenes are important intermediates in the synthesis of agricultural chemicals, dyes and pharmaceuticals. A zeolite-based catalyst was developed for the selective chlorination of various organic compounds, and its performance evaluated for the chlorination of toluene to para-chlorotoluene. The selectivity of para-chlorotoluene in chlorotoluene mixture, yield of para-chlorotoluene and product ratio of ortho-chlorotoluene to para-chlorotoluene were 78.27%, 69.18% and 0.277, respectively, at 85% conversion of toluene. These are the highest reported values so far for any catalyst used in this process.

Hydrodewaxing

The technical feasibility of using naphthalene-based feedstocks to get value-added speciality oils such as transformer oil and refrigeration-grade oils, using an Encilite-based hydrodewaxing catalyst in the key pour point reduction process scheme, was established. Based on a detailed study on bench scale units, two schemes have been submitted to the Assam Oil Division of Indian Oil Corporation Ltd.

■ Fluid Catalytic Cracking Catalysts (FCCs)

FCC composites based on Encilite-4 were developed in collaboration with Indian Oil Corporation Ltd. (IOC), Faridabad, for hydrocracking under Indian conditions. These match the imported FCCs in quality and performance. Negotiations are in progress with Hindustan Lever Ltd. to produce these composites on a large scale. By the use of these catalysts the octane number of FCC gasoline can be increased.

Hydroquinone and Catechol

Hydroquinone and catechol are widely used precursors and raw materials in the manufacture of fine chemicals, drugs, pharmaceuticals, and polymer composite builders. The technical and economic feasibility of a process for making hydroquinone and catechol from phenol in the presence of a novel Na-zeolite catalyst has been established in collaboration with FICOM Organics, Bombay. A pilot plant is being designed for installation at the site of the factory.

Zeolite Based Catalyst for Pyridine and Picolines

In collaboration with Armour Chemicals Ltd., Bombay, an improved catalyst has been developed for the production of pyridine and picolines from acetaldehyde, formaldehyde and ammonia.

C₃ and C₄ Olefins From Alcohol

Zeolite-based catalyst composites for the transformation of agro-alcohols to olefins, especially C₃ and C₄, have been developed in collaboration with Dhampur Sugar Mills Ltd., Dhampur, U.P. Further investigations at pilot plant level are envisaged.

Acrylic Acid and Esters

NCL has been successful in developing, in collaboration with Dhampur Sugar Mills Ltd., a catalytic system to obtain acrylic acid from methanol and acetic acid, at a per pass conversion of over 60%, with a selectivity of 80% with respect to acetic acid.

Acetonitrile From Acetic Acid and Ammonia

A process and a catalyst were developed for the manufacture of acetonitrile, an important organic chemical and solvent, for the first time in the country. The conversion and efficiency are both above 98%.

■ Removal of Isobutene From C₄ Hydrocarbons

A laboratory-scale process has been developed for the removal of isobutene from C₄ hydrocarbon streams via catalytic oligomerization, using industrial feedstocks. This process is a significant improvement over the conventional process, which has drawbacks like formation of unwanted polymeric products and corrosion of equipment. The NCL process uses an ion-exchange resin catalyst that leads to an isobutene

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removal efficiency greater than 98%, with minimum loss of n-butenes. Another important feature of this process is that 1-butene is substantially converted to 2butene, which is highly desirable for downstream applications. The process can be used with a feedstock with widely-ranging isobutene content and is expected to be more economical than the conventional process. Also, the products of oligomerization - diisobutene and triisobutene - have very important industrial applications.

Phenyl Acetic Acid

In collaboration with Gujarat Alcohol & Allied Chemicals Ltd., Ahmedabad, a laboratory-scale process for phenyl acetic acid has been developed via carbonylation of benzyl chloride under mild conditions using a novel phase transfer catalytic system. It is a significant improvement over the conventional process, in which the hazardous and expensive sodium cyanide is used. The novel feature of the NCL process is that the catalytic complex is prepared in situ using a cheaper precursor. The conversion of benzyl chloride is more than 95%, with a selectivity of 80%.

Oxidative Carbonylation of Allyl Amines

The role of reaction conditions in the selectivity of carbamate formation in oxidative carbonylation of allyl amines was studied. It has been demonstrated that the carbamate selectivity is significantly enhanced by an appropriate choice of catalyst, promoter and substrate concentration. This is important in the synthesis of methyl-N-methyl carbamate (MMC) by a non-phosgene route. This work has led to the development of a laboratory-scale process for MMC, which has been demonstrated to Excel Industries, Bombay.

BASIC RESEARCH

Zeolite Modelling

A computational methodology, developed at NCL, has brought out the structuredirecting and electronic role played by the template molecules in the synthesis of zeolites. The methodology involves a combination of molecular graphics, molecular mechanics and quantum mechanical studies. It can be applied to study guest-host interactions in any chemical system. The methodology provides a way to predict the zeolite phases formed from a specific template and is hence useful in the selection of templates to design zeolites with new structures. The conditions which lead to phase changes in certain molecular sieves have been calculated and this enables one to control the formation of impurity phases. An offshoot of this work was the development of an expert system software package ZEOSYN, for studying physicochemical, structural and catalytic properties. It has a strong potential for use by industrial and academic researchers in the field of zeolites.

Synthesis of a New High Silica Large-Pore Zeolite, NCL-1

High-silica large-pore zeolites are of special interest in catalysis and adsorption. A new aluminosilicate molecular sieve, designated NCL-1, was synthesized using a new organic template. An Al-free silica polymorph (Si-NCL-1), as well as a vanadium silicate analog of NCL-1 (V-NCL-1), was also synthesized. V-NCL-1, the only large pore V-silicate known so far, catalyzes oxidation of bulky organic molecules like naphthalene.

Synthesis of a New Titanium Silicate Analog of ZSM-11 (Ti)-MEL(TS-2)

A new Ti-silicate with MEL structure (TS-2) was synthesized. TS-2 very actively catalyzes the oxidation of phenol and other hydrocarbons.

Shape Selectivity of Medium-Pore Zeolites in Sorption

Studies were carried out on the factors affecting the shape selectivity of high silica zeolites (viz. ZSM-5, ZSM-8, ZSM-11 and mordenite) in sorption at temperatures close to those encountered in catalytic processes. It was found that the shape selectivity is strongly influenced by the channel structure, nature of the cation and its degree of exchange, as also by the presence of the poison molecules in the zeolite channels.

Diffusion in ZSM-5 Zeolites

Diffusion of bulkier sorbates/reaction species in a medium pore zeolite like ZSM-5 has been found to play a very significant role in deciding the shape selectivity of the zeolite and product distribution in the catalytic reactions over the zeolite.

Oxidative Coupling of Methane to C2-hydrocarbons

Extensive studies on the oxidative coupling of methane over metal, mixed-metal and multi-component mixed catalysts have led to a mechanism involving acid-base

pair in the extraction of H from CH₄, and formation of CH₃ radical in presence of free O_2 .

Oxidative Conversion of Methane to Syngas (CO & H₂)

Oxidative conversion of methane to syngas is of great practical importance because of the energy crisis looming ahead. NCL's low temperature exploratory process for selective oxidation of methane to syngas is based on catalysts that have unique features such as operation at low temperatures and atmospheric pressure, high methane conversion, high selectivity, and high productivity for both CO and H₂.

Organometallics as Catalysts

The insertion reaction of alkynes into the metal γ -hydrogen bond is the fundamental step in a number of catalytic processes such as hydrogenation and polymerization of olefinic compounds. Substituted acetylenes were inserted into hexa-coordinated ruthenium (II) hydridocarbonyl chelates to yield stable sigma alkenyl complexes.

Carbonylation of Alcohols

Carbonylation of methanol to acetic acid using highly active and selective Rucomplex catalysts was investigated. H2 was found to promote the reaction. The catalytic species were characterized and a possible reaction mechanism was proposed. This is the first time that an active Ru complex catalyst was developed for methanol-to-acetic acid reaction.

Carbonylation of Alcohols Using Non-Volatile Promoters

Enhanced activity and selectivity of a nickel complex catalyst has been demonstrated by using non-volatile metal iodide promoters. This study is important as volatility leads to complications in the separation and recovery of expensive iodidecontaining promoters in the commercial process for alcohol carbonylation. The proposed catalyst system is a significant improvement. This is the first report on the improvement of the activity and selectivity in Ni(isoq)₄Cl₂ catalyst with nonvolatile metal iodide promoters. In particular, this system reduces the formation of by-products consisting of alkanes and alkenes.

Isolation of Catalytic Intermediates in Carbonylation

A new approach to isolate catalytic intermediates under reaction conditions has been Unusual hydrocarbonyl anions of Rh(III) with the formula developed. [Rh(CO)₂(I)₄] were isolated and characterized as 2,6-diphenyl pyridinium and isoquinolinium salts during the hydrocarbonylation of methyl acetate. The isolated catalytic complex revealed a distorted octahedral environment around rhodium and the existence of trans-[Rh(CO)₂(I)₄] species. The structural features point to the influence of a countercation on the electrochemical characteristics and stabilization of the trans isomer.

Interfacial Catalysis in Carbonylation of Allyl Chloride

A novel catalytic approach for carbonylation reactions involving multiphase catalysis with solid catalyst particles suspended at the liquid-liquid interphase has been developed. This is a unique example of interfacial catalysis which can be extremely useful in achieving higher activity under milder operating conditions. Carbonylation of allyl chloride in a biphasic system has been studied using supported Pd-catalyst at liquid-liquid interphase. The major products were found to be vinyl acetic acid and crotonic acid.

Hydrocarbonylation of Methyl Acetate

Investigations of reactions of CO and CO/H₂ with methyl acetate over Ni as well as Rh complex catalyst, showed that Ni-catalyzed carbonylation of methyl acetate vields acetic anhydride selectively. In Rh-catalyzed hydrocarbonylation, the selectivity of ethylene diacetate was found to be dependent on catalyst concentration and H₂/CO ratio. Greater than 70% selectivity has been achieved in this case. The catalytic species was identified as [Rh(CO)₂I₄] [2,6 diphenyl pyridinium]+.

Hydroformylation of C6-C12 Olefins to Perfumery Chemicals

Hydroformylation of higher olefins such as hexene, octene and dodecene using homogeneous Rh-complex catalyst has been studied with the aim of synthesizing aldehydes for use as perfumery chemicals. High conversions and selectivity were achieved under mild operating conditions. The study indicated that by using optimum values of ligand and olefin concentrations and employing a suitable solvent, the aldehyde yield and selectivity can be improved substantially.

Ruthenium Carbene Catalyst

Investigation of the reaction of terminal alkynes with cyclopentadienyl ruthenium complexes showed that they form air stable, cationic ruthenium carbene complexes in the presence of alcohols. These complexes were also found to react with sodium azide to form the corresponding ruthenium azides. The azides undergo 1,3—dipolarcycloaddition reactions. Further work is in progress on the synthesis and reactions of these and other azidometal complexes.

Modelling of Non-isothermal Multiphase Catalytic Reactors

A mathematical model for the performance of the non-isothermal slurry reactor developed at NCL successfully predicts the runaway conditions and maximum temperature rise in such a reactor. The agreement between the experimental data (for hydrogenation of p-nitrocumene to p-cumidine) and the data predicted by the model was found to be excellent for a wide variety of conditions. This work is directly useful in the design and scale-up of slurry reactors for exothermic reactions.

POLYMER SCIENCE AND TECHNOLOGY

TECHNOLOGIES AT PILOT PLANT SCALE/ SEMI-COMMERCIAL SCALE

Reverse Osmosis Membranes

In collaboration with Thermax, Pune, a cellulose acetate/triacetate membrane with 13 gfd and 96% NaCl rejection at 2000 ppm/420 psi, based on a proprietary formulation, was developed. A polyamide TFC membrane with 5 gfd and 97.5% NaCl rejection at 2000 ppm/2000 psi was also developed. With growing applications in water treatment, waste management and food processing, these membranes hold the promise of indigenous availability at low prices.

LABORATORY-LEVEL DEVELOPMENTS

Science & Technology of Controlled Release

Release-controlling polymeric coating on commercial pesticide granules has the twin advantage of process simplicity and cost effectiveness. A unique technique, developed at NCL under the sponsorship of Ciba-Geigy, Switzerland, uses a room-temperature curing system based on proprietary chemicals/materials for the microencapsulation of commercial pesticides; it is both simple and cost effective, and

also reduces the dermal toxicity. Oxyfluorfen, microencapsulated by this technique, has been found to have low phytotoxicity and to be very effective in weed control; it also improves the yield of paddy. Microencapsulated chlorpyrifos was observed to be very effective in white grub control over a prolonged period (four months). All these formulations have a great market potential.

Novel Route to High Molecular Weight Polycarbonate

Polycarbonate is a widely used engineering plastic and the country's present requirements are met through imports. Post polymerization in the solid state is a commonly practised technique to obtain high molecular weight crystalline polymers such as PET or PBT. Poly(arylcarbonates), when made by the conventional melt polymerization method, yield only low molecular weight products. A polycarbonate of a molecular weight of about 80,000, having high melting point ($T_m = 270$ °C) and appreciable crystallinity, has been synthesized using a novel non–phosgene route based on carbonate interchange reaction. Considering the present trend of developing technologies based on non–toxic starting materials, the present research is of strategic importance in the global context.

Surface Modification of Polyethylene (HDPE)

Surface—modified HDPE containers and bottles have a good market potential for use in the automobile industry as fuel tanks, and in the packing industry as bottles to store pesticides, paints and other solvent—containing materials, for which metal containers are used at present. A method for off—line sulphonation of HDPE bottles/containers using gaseous sulphur trioxide was developed to improve their solvent barrier properties, under the sponsorship of Polyolefin Industries Ltd., Bombay.

Photoresists

Negative and positive photoresist formulations comprising polymers, sensitizers, quantum efficiency enhancers, stabilizers, etc., were developed with funding from the Department of Electronics. Photoresists are used extensively in electronics and microelectronics.

Gas Separation by Membranes

Thin film composite membranes for air separation, with a permeability of 2–5 barrers/cm for oxygen, and an oxygen/nitrogen selectivity in the range 3–4, were developed. In a related activity, a novel polyarylate with an intrinsic oxygen permeability of 1–2 barrers and oxygen/nitrogen selectivity of 9 was identified. These membranes offer an economic method for carrying out bulk separations where high purity is not an essential requirement. The oxygen-enriching membrane is being tested in collaboration with KEM Hospital, Pune, where the clinical performance evaluation of the membrane is being carried out.

PTFE Piston and Wear Rings

In a project sponsored by Kirloskar Pneumatic Co. Ltd., Pune, rings were made for reciprocating—type non–lubricated gas compressors using experimentally—optimized conditions, and their wear performance was evaluated. The results showed a significant improvement in the wear resistance as compared to the rings processed indigenously under unoptimized conditions. Also, a non–destructive quality control test method was developed.

Composite Bearing Bush

Prototype bearing bush components used in oil engines were prepared with high performance composite materials, in a project sponsored by Kirloskar Oil Engines Ltd., Pune. These are being subjected to trials by the company.

■ Polyethylene Cable Compounds

Functionally-grafted cable compounds were developed by grafting vinyl trimethoxy-silane on to indigenously-available polyethylene, in a project sponsored by Cable Corporation of India Ltd., Bombay. Laboratory trials have shown them to be capable of meeting the stringent specifications of the cable industry. The process was demonstrated on a 100-kg-scale, and is expected to be commercialized very soon.

Process for Aromatic Polyester

Aromatic polyesters are generally prepared by the transesterification of bisphenol—A diacetate with aromatic dicarboxylic acids. Removal of acetic acid from the reaction medium is a major difficulty in this process. A simple two—stage catalytic process for the transesterification of DMT/DMT with bisphenol—A has been discovered. By

suitable optimization of the process, inherent viscosities as high as 0.5 have been achieved.

BASIC RESEARCH

Living Anionic Polymerization

The first-ever room-temperature polymerization of tertiary butyl acrylate with quantitative yield and a relatively narrow molecular weight distribution was achieved. This opens up new routes for synthesizing new polymers for applications as drag reducers, viscosity index improvers, compatibilizers, etc.

The efficacy of di-t-butyl malonate as a precursor to generate a novel metal-free carbonion that can initiate controlled polymerization of methyl acrylate has been established. Poly(methyl acrylate)s in the molecular weight range 3,000-10,000 were synthesized. Such macromonomers containing a dicarboxyl group have novel structures which could be used for extending chains to produce a variety of graft polycondensates.

Graft Copolymers Through Reactive Processing

Various polyolefin matrix materials were grafted with different co-monomers in the presence of a radical generator (peroxide). Blending them with a catalyst resulted in crosslinked polymers with a higher thermal resistance combined with excellent mechanical and electrical properties, as compared to crosslinked polymers obtained by other routes.

Liquid Crystalline Polymers (LCPs)

LCPs offer a unique combination of thermal, mechanical and chemical properties, unmatched by other high performance polymers. In a project funded by DST, systems with a softening temperature above 210°C were developed by introducing kinks and altering the directional effect of ester-linking groups along rigid-rod polymers like poly(4-oxybenzoate) and poly(1,4-oxyphenylene oxy-1,4carboxyphenylene carboxy). Systems with a softening temperature around 100°C, comprising chemically modified fibre-grade, waste poly(ethylene terephthalate) with (i) 4-acetoxy benzoic acid, and (ii) a combination of terephthalic acid and 1,4diacetoxy benzene, were also developed.

Polymers With Well Defined Architecture

It has been discovered that 2-(1,1,1-tribromomethyl)-1,3-oxazoline (OxzCBr₂), synthesized by the exhaustive bromination of 2-methyl-1,3-oxazoline acts as an efficient trifunctional initiator for the living cationic ROP of MeOxz in acetonitrile. The living nature of the chain ends was demonstrated by their ability to reinitiate fresh polymerization after 100% conversion was achieved. The polymer structure is a three-arm, branched poly(N-acylethylenimine) with a 1,3-oxazoline moiety as the head group. This is the first example of a well-defined, branched polymer of MeOxz obtained by the ROP technique.

Controlled Release (CR) Vaccine Delivery Systems

In a project undertaken with support from DBT, polymeric systems that can release a macromolecular active ingredient over extended periods of time (6-12 months) in a sustained manner were studied. It was shown that carriers based on polyactic acid could release bovine serum albumin over a period of 200 days satisfactorily. The ultimate aim is to design a CR system for the release of a birth control vaccine developed by the National Institute of Immunology, New Delhi.

Water-Soluble Polymers

Pyrene-labelled polyacrylamides and polyacrylic acid (PAA) have been prepared and studied in collaboration with Columbia University (USA) and Tata Research Development and Design Centre, Pune, as part of an Indo-US STI programme on mineral engineering. It was observed that the high eximer content at low values of pH for polyacrylic acid (and hydrolyzed polyacrylamide) is strongly reduced by the addition of polyethylene oxide (PEO) and practically quenched by the addition of polyvinyl pyrrolidone (PVP). The behaviour has been attributed to the cooperative hydrogen bonding of the component polymers (PAA/PEO and PAA/PVP), and the electronegativity of the oxygen in PVP.

Solid State Processing

A study of strength development during sintering of PTFE was carried out. The results are valuable in designing the sintering cycle for PTFE, a critical operation

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in the powder processing. In a study of structure development during melt curing of polyphenylene sulphide, it was observed that the thermal parameters are very sensitive to the structural changes and can be effectively used to monitor the curing process.

BIOCHEMICAL SCIENCES & BIOTECHNOLOGY

TECHNOLOGIES AT COMMERCIAL SCALE

 Technology Transfer, Biotechnological Evaluation and Clonal Multiplication of Eucalyptus, Bamboo and Salvadora

The work on standardization of methods for micropropagation of four forest tree species, namely Eucalyptus tereticornis, E. camaldulensis, Dendrocalamus strictus and Salvadora persica was completed under Phase I of the NABARD Programme.

Two regional laboratories were established for the production of eucalyptus and salvadora plants at Grasim Forest Research Institute (GFRI), Harihar, and Central Salt and Marine Chemicals Research Institute (CSMCRI), Bhavnagar, respectively. GFRI has 30,000 cultures and 2,000 eucalyptus plants, while CSMCRI has 6,000 cultures and 1,000 plants of salvadora in their greenhouses. Successful field trials of these plants are expected to lead to an increase in biomass yield.

Encilium Technology

NCL had developed a process for the continuous fermentation of molasses to ethanol using a special yeast strain called *Encilium*. The unique feature of *Encilium* is that it gets flocculated and hence is retained in the fermenter. The yeast once grown can be used for long periods of time without replenishment, when the prescribed process conditions are maintained. This process can be adopted in the existing batch

distilleries with minor modifications, and can be implemented in new distilleries with economic advantages.

The technology was first implemented by Dhampur Sugar Mills Ltd. in March 1991. The technology has also been licensed to Ugar Sugar Works, Karnataka, and Belganga Sahakari Sakhar Karkhana, Maharashtra, where it is being implemented, and to Co-operative Company Ltd., U.P., and Vasantdada Shetkari Sahakari Sakhar Karkhana Ltd., Maharashtra, where the plants are undergoing commissioning trials.

The Encilium technology is offered by NCL in collaboration with engineering companies on a turn-key basis with guarantees of performance.

TECHNOLOGIES AT PILOT PLANT SCALE/ SEMI COMMERCIAL SCALE

Cellulase-Free Xylanase Technology

An alkalophilic Bacillus strain secreting high activity cellulase-free xylanase has been identified and a process for xylanase production patented. The technology has been scaled up in collaboration with Biocon (India) Ltd., Bangalore, and Biocon (Ireland) Ltd. The enzyme has been evaluated for its potential in biobleaching and biopulping in the paper industry as well as in the preparation of high quality cellulose pulps. The enzyme's stability at high pH values and its cellulase-free nature are positive attributes for paper industry applications. Preliminary evaluation of the enzyme by user industries abroad have shown encouraging results. Further efforts are under way to improve the enzyme activity.

BASIC RESEARCH

Molecular Biological Studies on Xylanase

A genomic library of alkalophilic and thermophilic Bacillus strain, constructed in suitable vectors, was screened to identify six xylanase-positive clones. Xylanase expression by cloned genes in some cases occurred even in the absence of xylan and 70% of the activity was extracellular.

Fungal Xylanase

Under a DBT supported programme, an alkalophilic fungal strain and an actinomycete capable of secreting high levels of xylanase at a pH of 9.0 were discovered. Fungal xylanase strains active at such highly alkaline pH have not been reported so

Fungal Alkaline Protease for Detergent Applications

High-activity alkaline protease secretion from a strain of Conidiobolus and the compatibility of the enzyme with commercial detergents for stability and activity were investigated. The enzyme which remains stable at a pH of 9.7 and a temperature of 60°C has the potential for use in enzyme-based detergents. Interaction with possible user industries and enzyme manufacturers has been initiated and a preliminary evaluation of the product has produced positive results.

Penicillin Acylase

Penicillin acylase of E.coli cells permeabilized by treatment with cetyltrimethyl ammonium salts was studied, and found to be stable after repeated use. Immobilization of the E.coli using a new hydrophobic macroporous polymer resin was also studied. The presence of essential arginine residues on the catalytic sites of the E.coli enzyme was established.

Germplasm Resource Pools for Microbial Biotechnology

Screening for unusual groups of microorganisms from natural ecosystems was continued, and several fungi were isolated and screened for carbohydrases and proteases with unusual properties. Under this programme, supported by DST funding, an alkalophilic actinomycete strain capable of growing at a pH above 9.0 and secreting alkaline protease, and tolerant to high levels of heavy metals like chromium is being investigated for its potential for industrial applications.

Genetic Modification of Higher Plants Through Protoplast Technology

The methods developed at NCL for the regeneration of protoplasts of the important grain legumes, chick pea (Cicer ariefinum) and pigeon pea (Cajanus cajan), up to callus stage, are the first examples reported in the literature. The standardized method has been extended to many genotypes for optimization of the most suitable genotypes for plant regeneration.

Regeneration of complete plants from leaf explants of groundnut has been achieved through organogenesis and embryogenesis. The plants raised via organogenesis are flowering in the field and new lines of groundnut are being isolated from them. The pattern of lipid accumulation in somatic embryos of groundnut at various stages of embryo development shows a characteristic profile.

The above studies on regeneration of protoplasts/explants either through organogenesis or somatic embryogenesis are essential prerequisites in the generation of improved cultivars of grain legumes and oil seed crops bestowed with agronomically desirable traits such as disease and pest resistance and tolerance to abiotic stress. A large number of plants are now being produced through these morphogenic pathways and transferred to the soil in order to assess the frequency of spontaneous variations in the regenerants.

Plant Biochemistry, Molecular Biology & Biotechnology

Genetic diversity analysis, which gives a fairly good idea of the inter-relationships among the various cultivars, has been carried out for eighteen rice cultivars. This has led to the identification of the parental combinations that result in a higher paddy yield. DNA fingerprint patterns of a few indica, japonica and wild rice varieties were developed using oligonucleotide probes.

Genetic Engineering in Crop Improvement

It is often desirable to introduce a specific change in a specific protein in a plant with genetic engineering techniques so as to get an improved crop without altering the original plant architecture. However, for introducing such changes, it is essential to have a complete structural and functional information about the gene coding for the protein. Preliminary studies on the organization of glutelin gene in rice genome indicated that the regulation of this gene is through adenine methylation.

Micropropagation technology was used to develop rice plantlets. Distinct types of variants were noticed among these somaclones, in which the grain yield was enhanced by 30-50%.

Use of RFLP in Rice Genetics and Breeding: Gene Tagging in Rice

In an effort to identify molecular markers linked to the gene resistant to bacterial leaf blight, crossing between resistant and sensitive rice cultivars was carried out. Near isogenic lines were also procured and were grown for multiplication and harvest of leaf tissue. DNAs were isolated from parent cultivars and their restriction enzyme digests were probed with DNA markers from the Pst I genomic library prepared earlier in the laboratory. Nine polymorphic probes were identified for use in the analysis of the F2 progeny.

Cloning and Analysis of Glutelin Storage Protein in Rice

Analysis of glutelin gene from Basmati 370 rice indicated the presence of seven copies of glutelin gene per haploid rice genome. The organization of glutelin gene in rice genome was found to be dispersed or nontandem with two or more subfamilies. Studies also indicated that the regulation of glutelin gene was through adenine methylation.

Development of Plant Tissue Culture Technology for Rice

Shoot base segments of regenerated rice plants of the Indrayani variety were grown in an appropriate liquid medium. Even after subculturing for one year, the rate of multiplication showed no decrease. After acclimatization, these plantlets were grown to maturity in the field. Micropropagation induced by culture of shoot base segments was found to be a very efficient technique for vegetative propagation of elite rice genotypes. Field trials of tissue-culture-raised rice plants were conducted for two years at Agricultural Research Station, Vadgaon Mawal, in Pune District. A wide range of variation with respect to these parameters was noticed. In a few distinct types of these variants, the grain yield is enhanced by 50%.

C₃/C₄ Photosynthetic Gene Regulation

The extent of cytosine residue methylation in the sugarcane genomic DNA was found to have a direct correlation with changes in the transcription levels of phosphoenolpyruvate carboxylase, malic enzyme and pyruvate orthophosphate dikinase genes in the mesophyll and bundle sheath cells. This is the first example in reported literature of c-residue methylation being directly implicated in differential regulation of gene expression in sugarcane. The insight provided by these studies into molecular differentiation of the two cell types and expression of photosynthetic genes can help to increase the photosynthetic efficiency of crop plants.

DBT Tissue Culture Pilot Plant Facility

A plant tissue culture pilot plant facility with computerized controls has been established. Shoot cultures of the forest species Eucalyptus tereticornis, E. camaldulensis, Dendrocalamus strictus and Tectona grandis were grown in polybags and supplied to forest agencies in Andhra Pradesh, Maharashtra, Karnataka and Tamilnadu.

Precocious Flowering in Bamboo

The method of coaxing three species of bamboo plants to flower, reported earlier, has now been extended to *Dendrocalamus hamiltonii*. The plants raised from *in vitro*-developed seeds along with control have been field-planted and constantly monitored for their growth performance. These plants are showing vegetative growth similar to that of controls.

Scale—up studies using bioreactors were initiated, and preliminary data have been collected to initiate investigations aimed at an understanding of the influence of a particular physical/chemical factor on flower induction. These investigations will also reveal the parameters controlling large—scale seed production.

Coconut Plants Through Tissue Culture

A reproducible method was developed for repetitive formation and proliferation of globular structures that regenerate into green protuberance, roots from leaf explants and green leafy (abnormal) structures from rachillae calloid derived from mature coconut trees. This work is of special significance as the coconut tissue is known to be recalcitrant and hence success in culturing mature coconut tissue is rare. Clonal propagation of coconut is very desirable and even preferable to conventional breeding, as there is a significant variation in coconut yield owing to the outbreeding nature of the tree in the latter.

Phenylglycine

D(-)Phenylglycine has key applications in the synthesis of drugs and antibiotics. A microbiological process for the conversion of DL-5-phenylhydantoin to D(-)-N-carbamyl phenyl-glycine or D(-)-phenylglycine has been investigated through extensive strain selection, and a proprietary bacterial strain capable of performing the desired bioconversion under industrial fermentation conditions has been identified. The laboratory scale process has been standardized with 90-95% conversion

efficiency. Conversion of p-hydroxyphenyl hydantoin to N-carbamyl phenylglycine in almost 99% yields has been achieved in laboratory scale experiments.

Marine Natural Products

Three species of red algae capable of secreting valuable products like carageenan were selected for in vitro cultivation studies and protoplast fusion for strain improvement. Species such as Ulva lactuca and Gelidium showed promising potential for in vitro cultivation. Screening unicellular algal strains for polymer production is also under investigation. Thermophilic marine bacteria were investigated for their ability to produce extracellular proteolytic enzymes and amylases, and some promising strains were identified.

Enhancement of Oil Recovery by the Use of Microorganisms

Studies on enhancement of oil recovery through the application of thermophilic serobic/anaerobic microbial cultures capable of producing acid, gas and biosurfactants have been undertaken. Of the five promising strains growing at 65°C, two facultative anaerobes were found to enhance the recovery of oil by as much as 50% when tested for oil release from oil saturated sand.

Chitin Degrading Enzyme

Basic studies on the role of chitin-related enzymes in the expression of dimorphism by the phycomycete strain Benjaminiella poitrasii showed that NADP/NAD glutamate dehydrogenase ratio has a significant role in the yeast mycelial transformation. The potential of using this system as a model for screening compounds for insect biocontrol based on chitinase/chitin synthetase inhibitor is being explored. Chitinase production by a high activity strain of Myrothecium verrucaria and its potential for mycolytic activity, protein production from chitin hydrolysates, and antifungal activity towards root disease fungi are also under investigation.

Production of Taxol, an Anticancer Alkaloid

An extraction and analytical methodology for isolation, identification and estimation of 10-deacetylbaccatin from needles of *Taxus baccata* has been standardized. A fraction containing 80% of taxol, a diterpene alkaloid effective against a number of cancers, has also been identified.

Membrane Bioreactors

Fundamental engineering studies, sponsored by DST, in the analysis of membrane bioreactors and transport processes encountered in them were carried out. Using CGTase production by Bacillus sp. in a two-stage crossflow cell recycle bioreactor as the model, the environmental conditions for initial growth and CGT production by Bacillus macerans were optimized.

■ Improving Yeast Strain in Encilium Technology

Protoplast fusion of the parent strain with a "killer" yeast strain elaborating a toxin to deactivate contaminating yeasts in industrial fermentations has been undertaken. Clones selected with these properties are under evaluation for better ethanol productivity.

ORGANIC SYNTHESIS & TECHNOLOGY

TECHNOLOGIES AT COMMERCIAL SCALE

Prostaglandins

Astra-IDL, Bangalore, has commercialized the prostaglandins process developed by NCL. A modified three-component coupling methodology was developed for the synthesis of PGE₂, carboplast and metanoprost. A process for IR-cis-caranaldehyde, the resolving agent for one of the components, (+) and (-)-4-hydroxycyclopentenone, from an indigenously-available pyrethroid intermediate, was also developed. A similar method for making misoprostol, an antiulcer prostaglandin, was developed on behalf of Standard Organics Ltd., Hyderabad.

A microbial method has been worked out for the selective hydrolysis of meso cyclopentene diacetale to furnish the cyclopentenol with an S-configuration, which is the key synthon for making a variety of prostaglandins.

TECHNOLOGIES AT PILOT PLANT SCALE/ SEMI COMMERCIAL SCALE

Ranitidine

Lasor Drugs Pvt. Ltd., to whom the process for the ranitidine intermediate, methylamino methylthio nitroethane, was released, is planning to conduct pilot-plant studies on the process.

D(-)Phenylglycine and D(-)p-Hydroxyphenylglycine

In addition to the process based on biotransformation (see page 22), NCL has also worked out a synthetic methodology for these compounds, in which the separation of the products of a common reaction sequence is effected by dynamic resolution using the cheaply available L(+)tartaric acid. The process has been released to Lupin Laboratories Ltd.

Mannitol

The NCL process for mannitol was demonstrated and released to Unicorn Organics Ltd., Hyderabad, where production has been started. The process is based on the inversion of cane sugar to glucose and fructose, and hydrogenation of the sugars to mannitol and sorbitol. Mannitol is separated by crystallization. The company plans to produce 220 TPA of mannitol.

Morpholine

Navin Chemical Enterprises, Dewas, has installed a pilot plant for carrying out trials of a process for morpholine from diethylene glycol developed at NCL years ago, as a prelude to the installation of a commercial plant.

Paracetamol

The NCL process for paracetamol, starting from para-nitrochlorobenzene, was released to Shrishma Fine Chemicals and Pharmaceuticals Ltd., Bangalore; it was demonstrated in the pilot plant installed by the company at their Bangalore works. An effluent treatment process forms part of the technology package.

N-Methyl Piperazine & Amino Methyl Piperazine

NCL has developed a novel and highly economical method for the preparation of these valuable pharmaceutical intermediates starting from piperazine. The new process is highly economical and produces only very small quantities of the by-product. The process has been offered at a pilot plant scale to Diamines and Chemicals Ltd., Vadodara. This company has a plant for the production of piperazine, besides a plant for ethylenediamine and polyamines, based on NCL know-how.

LABORATORY-LEVEL DEVELOPMENTS

Alprozolam and Estazolam

Laboratory-scale processes were developed for both these drugs. The process for alprozolam, a very effective antidepressant (less toxic than diazepam), was released to Household Remedies, Bombay.

Non-MIC, Non-CO and Non-Phosgene Route to Carbamates

Methyl N-methylcarbamate (MMC) is an important key intermediate in the synthesis of carbaryl, carbofuran, propoxur and other commercially important carbamate insecticides. A commercially viable process has been developed for the preparation of MMC by two different synthetic routes not involving the use of MIC, phosgene or carbon monoxide. No high pressure reactions need to be carried out in this process. A process for propoxur, starting from MMC, was also standardized. The process for MMC has successfully been demonstrated to Excel Industries, Bombay.

Metalaxyl

A two-step process has been standardized on a bench-scale for this high-cost fungicide, which is at present imported.

D(+) Biotin

D(+) Biotin (vitamin H), a biocatalyst of reversible metabolic reactions of carbon dioxide transport in organisms, is one of the B-complex group of vitamins and has immense commercial importance. A convenient, short and efficient 12-step methodology has been developed for the synthesis of D(+) biotin starting from naturally available and cheap L-cystine.

BASIC RESEARCH

Synthesis of Chiral α -Keto Imide

As part of a project on the synthesis of α -functionalized carboxylic acid derivatives, the preparation of a chiral α -keto imide, with a built-in directing group that would serve as a precursor to enantiomerically pure α -hydroxy acids, was achieved.

Palladium and Cobalt-Assisted Transformations

Palladium- and cobalt-assisted transformation of electron deficient oxa enynes and dienynes derived from propargyl alcohol showed that treatment of oxa enynes with various palladium complexes results in the cleavage of the more stable enal ether functionality in the presence of highly acid-sensitive protected alcohol functionality.

Asymmetric Synthesis of cis-\(\beta\)-Lactams

The enantiospecific synthesis of $cis-\beta$ -lactams was achieved using imines derived from N,O deprotected homochiral aldehyde prepared from easily available (+)-(1S,2S)-2-amino-1-phenyl-propan-1,3-diol. In all the cases only one diastereomer was obtained in good yields.

Organometallic Compounds in Asymmetric Synthesis

It was found that mixed dialkylzinc compounds [MeAnR(Ar)] could be obtained in good yields by reacting MeZnI with RMgX in diethyl ether; during the reaction with benzaldehyde, preferential transfer of alkyl/aryl group takes place from MeZnR(Ar).

New terminally substituted π -allyl complexes of molybdenum were synthesized. Air oxidation of triphenylphosphine catalyzed by molybdenum π -allyl complexes containing pyrazole-derived ligands was observed for the first time.

Pyrolysis of pyrazolines, obtained by Lewis acid mediated conjugate addition of allylsilane and allylstannone to the tetralone benzylidene complexes of chromium tricarbonyl and related acyclic substrates and subsequent dipolar cycloaddition of diazomethane to these complexes, resulted in the formation of tetra-substituted enones. Complete reversal of stereoselectivity was observed in the cyclopropanation of these compounds.

An interesting stereochemical feature of (CO)₅M=C(OR)(Ar) [M=Cr,W] complexes is that the aryl ring is oriented orthogonal to the metal carbene π -plane in the solid state. Such preference may be countered to an extent by the electron releasing (OR) or (NR₂) group in the para position. Clear evidence for the orthogonal orientation of the aryl ring at a low temperature in solution has been obtained from the studies.

Rearrangement Reaction of Chromium Fischer Carbene Complexes

The carbene ligand of aryl arylmethyloxy carbene complexes of chromium was found to undergo a rearrangement and aryl arylmethyl ketones were obtained as their tricarbonylchromium complexes.

Tungsten and Molybdenum Fischer Carbene Complexes

A novel thermal rearrangement of tungsten Fischer carbene complexes was observed. It was a general reaction for a particular group of carbene complexes.

Studies on Molybdenum-Allyl Complexes

In the studies on oxidative dimerization of Mo-allyl complexes it was observed that the complexes containing the bidentate bispyrazolylmethane ligand undergo dimerization when exposed to air and that the Mo(V) species is an intermediate in the overall process. It was also observed that a catalytic amount of the Mo-allyl complex is capable of oxidizing triphenylphosphine to triphenyl phosphinoxide in the presence of atmospheric oxygen.

Asymmetric Dihydroxylation

Asymmetric dihydroxylation (ADH) of unfunctionalized alkenes was carried out with polymer-supported chiral alkaloids. The diols were converted into diamines. aziridines and amino alcohols.

Reactions of Mesylated Pyrimidines With Secondary Amines: Access to New Classes of Potential Antiviral Aminonucleosides

A more efficient inhibition of HIV-1 virus by some modified nucleosides without the free primary hydroxyl group, than by those with it, is reported in literature. The synthesis of 3',5'-dideoxy-3',5'-disubstituted thymidine nucleoside is relevant in this connection. 3',5'-Di-O-mesylthymidine, on reaction with secondary amines, underwent a hitherto unknown 'one-pot-two-steps' transformation to produce 2,3'-0-anhydro-5'-deoxy-5'-alkylamino-thymidines, which could be used as intermediates for the synthesis of a variety of 3',5'-dideoxy-3'-substituted-5'-alkylaminothymidines.

2',3',5'-Tri-O-mesyluridine, under identical conditions, produced a complex mixture. A closely related compound, 2'3'-di-O-mesyl-5'-O-trityluridine, on the other hand, produced 2',3'-O-lyxoepoxide isocytidine derivatives; the amines attacked the C-2 position of 2,2'-O-anhydro-3'-O-mesyl-5'-O-trityluridine.

Synthesis of Natural/Unnatural N-Hydroxy Dipeptides/DKPs and Their Metal

These molecules were synthesized using nitroacetamide as a synthon. The active methylene group in the synthon forms the centre for Pd(o) alkylation, and the attached amino acid acts as a chiral inducer for asymmetric C-C-bond formation. Finally, the nitro group in it was transformed into the hydroxylamine or amine, which enabled the synthesis of natural/unnatural dipeptides. Fe, Cu-hydronamic complexes were made from N-hydroxy DKPs synthesized from nitroacetamide. These N-hydroxy DKPs are a class of sideopheres and metal sequestering agents. A study of the biological applications of these hydroxamic complexes is under way.

Amino Acid Derivatives as Dipeptide Synthons

Use of N-nitroacetyl derivatives of amino acids as dipeptide synthons was demonstrated. Stereoselective Michael addition on L-valine, L-phenylalanine and l-proline derivatives of nitro-acetamides resulted in adducts varying in diastereomeric excess from 0 to 41%. Better results were obtained when L-proline esters were used. A second Michael addition was also performed, thus demonstrating that disubstituted dipeptides could be obtained as well. The absolute configuration at the newly generated chiral centre was established for the first Michael addition.

Chiral Quaternary Carbon

Studies on the generation of chiral quaternary carbon in N-nitroacetyl derivatives of amino acids resulted in a new concept of intramolecular allyl transfer. Michael addition of methyl ester of nitroacetic acid with allyl acrylate resulted in the formation of a mono-alkylated glutamic acid derivative in 88% yield. It was further subjected to Pd(o)-catalyzed intra-molecular allyl transfer to yield an α -allyl glutamic acid derivative. This sequence has been successfully repeated on various substrates (amides and esters of nitro acetic acid).

Photoinduced Electron Transfer (PET) Reactions

The regiospecificity of iminium cation formed in the PET reactions involving unsymmetrically substituted tertiary amines has been explained in terms of the kinetic

acidity of a-CH protons and stereoelectronic factors. It was suggested that the selectivity in radical ion formation in the PET reactions depends upon the AGet values and the concept has been extended to explain the direct carbon-carbon bond formation at α-position of tertiary amines. The utility of tetrahydro 1,3-oxazines, obtained by the cyclization of iminium cation with proximate hydroxyl group in the synthesis of biologically active cis-\alpha, \alpha'-dialkylated piperidines and pyrrolidines by utilizing Barbier reaction was revealed.

Intramolecular cyclization of 2-piperidyl and 2'-pyrridyl radicals, generated by PET desilylation of corresponding radical cation, has been shown to be stereoselective and a general synthetic approach to 1-azabicyclo (m:n:o) alkane systems has been reported. A short synthesis of biologically active alkaloids such as (\pm) heliotridane, (±)-epilupinine and (±)-isoretronecenal has been accomplished from this methodology.

A mild and unprecedented methodology to generate non-stabilized azomethine ylides by PET-mediated sequential double desilylation from corresponding disilylated amines was reported.

Methods for in situ generation and utilization of electrophilic selenium species from the PET reaction of diphenyl diselenide have been developed.

Model Studies in VCR

An extension of heat-induced vinyl cyclopropane rearrangement (VCR) to spirocyclic exo-vinyl VCR leading to a 5,5-ring system has been established. Extension of this method with suitable bicyclic precursors might ultimately yield advanced models of the carbocyclic frame of taxol.

Novel Exo-Selective Diels-Alder Reaction

A highly chemo-selective method was developed for the deprotection of thicketal, based on an innovative approach in which a ketone and an aldehyde could be differentiated. Conditions for an exo-selective Diels-Alder reaction were optimized by applying the novel electrophilic and nucleophilic theory to organic molecules.

Dual Epimerization of Diels-Alder Endo-Cycloadduct

When a solution of endo-adduct of cyclopentadiene in naphthoquinone with 5% triethylamine in ethanol was irradiated at 300 nm, efficient transformation to the exoisomer was observed. The generality of this methodology has been demonstrated

in a variety of models. This study has the potential for altering a variety of selective transformations in organic synthesis. It can also lead to the synthesis of new materials, not possible earlier.

Photochemical β -Cleavage processes

Efficient β -cleavage processes employing electron transfer chemistry has been used to cleave either cyclobutane bonds or cyclopentane bonds. The cleavage of the latter to carbonyl holds the interesting possibility of providing a precursor very close to the carbocyclic frame of taxol. This approach was extended to cyclopropyl β -cleavage as well.

Biologically-Useful Skeletons

The highly useful N-phenyl (triphenylphosphoranylidene) ethenenimine was employed for synthesizing 4H-1-benzothio-pyran-4-one, a possible precursor to deltaiazern and other biologically useful skeletons. The methodology can be extended to the synthesis of quinolone drugs as well.

Bioorganic Chemistry

Chemical cleavage of DNA by Cu(II), Ni(II), Co(III) and Fe desferal complexes

Complexes of Cu(II), Co(III) and Ni(II) with desferrioxamine, currently considered very important, were synthesized and their utility as DNA cleavage agents was studied on plasmid DNA and short oligonucleotides. Co and Ni complexes showed more specificity towards CG-rich sequences. Fe-desferal did not show nucleolytic activity. Hydroxyl radical scavengers (mannitol, glycerol, etc.) and ethidium bromide were shown to inhibit cleavage reactions.

Regiospecific 2'-O-allylation of ribonucleosides

2'-O-Allyl oligoribonucleotides are important antisense probes because of their nuclease resistance, membrane penetration and hybridization properties. Regiose lective synthesis of 2'-O-allyl ribonucleosides thus assumes importance. Dibutyltin oxide-mediated allylation of uridine gave 2'-O-allyl uridine in high yields which was converted quantitatively to 2'-O-allyl cytidine via 4-O-sufonylation/displacement

procedure. The regiospecific 2'-O-allyl pyrimidine ribonucleoside was also obtained by Pd(o)-catalyzed allylation of 4-O-nitrophenyl 3'-5'-O-(tertraisopropyldisiloxane-1,3-diyl) uridine, which could be converted to either 2'-O-allyl uridine or 2'-O-allyl cytidine under different deprotection conditions.

Synthesis of fluorescent oligonucleotide probes

Radioactive labelling of oligonucleotides is a hazardous but the most widely used method of detection in practice today. As an alternative to this practice a number of fluorescent probes were synthesized. This involved the attachment of fluorophore to the 5' end of ribose and incorporation of the label in the backbone. Labelling is achieved by converting the backbone to P=S linkage and labelling the resultant sequence with monobromobimane after deprotecting and hybridizing it. Successful detection could be accomplished with the PCR technique.

More than 100 sequences of lengths varying between 20 and 40 were synthesized and used as primers for PCR, RFLP techniques and in cleavage reactions.

Modified nucleosides & nucleotides

Thymidine was converted to 2,2'-anhydro-5'-morpholino thymidine in high yield. The corresponding piperidino derivative was also synthesized. These compounds are important intermediates for the synthesis of some potent biologically-active modified nucleosides.

5-Amino pyrimidines and 8-substituted purine nucleosides have been synthesized and incorporated into oligonucleotides at well-defined sites. These have important applications like mimicking nuclease active sites and rational design of nucleic acids with altered molecular recognition properties.

Dual Behaviour of Ortho Toluic Acid/Ester

A short and elegant asymmetric synthesis of (+) orthosporin, a phytotoxic metabolite isolated from Rhynchosporium, and semivioxanthin, a fungicide isolated from Penicillium citreovivide, was achieved by a novel exploitation of the dual reactivity profile of orthotoluic acid and orthotoluic ester. Semivioxanthinin was transformed to semixanthomegnin by oxidation with potassium dichromate.

12-Oxocurvularin

Of several curvularins isolated from Penicillium citreoveride-B, 12-oxocurvularin, besides possessing an unusual oxygen function at C-12, exhibits attractive physiological properties. This bioactive molecule in its racemic form has been synthesized for the first time. The synthesis of optically active natural 12-oxocurvularin by a chemo-enzymatic method is in progress.

Brassinolide & Brassinosteroids

Synthesis of brassinolide from 3-hydroxy and rost-5-en-17-one employing resincatalyzed ene reaction on 3-toluenesulfonoxy-(Z)-pregna-5,17 (20)-diene was successfully carried out.

Stereoselective synthesis of the plant growth promoting brassinosteroids, dolicholide, dolichosterone and 28-norbrassinolide was achieved.

Witting olefination of the (22R)-acetoxy-23-aldehyde was worked out to get a stereoselective route to the side chain of brassinolide.

Non-Cysteamine Route to Ranitidine

It was found that the reaction between potassium phthalimide and ethylene dibromide in the presence of TDA catalyst gave high yields of 2-bromoethylphthalimide, under mild conditions in a relatively short time; this compound is an intermediate in the synthesis of ranitidine by the non-cysteamine route.

Drug/Pesticide Intermediates Through Halogenation

By the halogenation of the active methylene site, eight representative substrates were converted into the corresponding halo compounds in high yield. These halo compounds are important intermediates in the manufacture of drugs and pesticides.

Saintopin

The first total synthesis of this new tetracyclic antitumour antibiotic, usually isolated from Paecilomyces species, has been achieved by bringing about a regioselective formation of the tetracyclic framework through decarboxylative coupling.

Diacetyl Obafluorin

A highly stereoselective synthesis of (\pm) diacetyl obafluorin, a broad-spectrum β lactone antibiotic of unprecedented biological activity, was achieved employing a

novel transacylation protocol. The mild reaction conditions prevent the formation of nucleophiles that can destroy susceptible β -lactones.

Novel Transacetalization

A wide variety of thioacetals and oxathioacetals were transformed with ease to the corresponding carbonyl compounds. The key feature is the selectivity. Thus, oxathiolanes and ketones can be selectively deprotected in the presence of thiolanes and aldehydes, respectively. The methodology was successfully used in the synthesis of D (+) biotin (vitamin H).

Macrolides

Macrolides with interesting biological activities, viz. (+) M5032 dimethyl ether, 12-oxacurvularin, R (±)recifeiolide, and R(+) patulolide, were synthesized by employing enzyme-mediated transformation as the key step.

Bostrycordin

Bostrycordin, a 2-azanthraquinone, isolated from Fusarium bostrycoides, has been shown to be active against Mycobacterium tuberculosis. A simple regiospecific synthesis of bostrycordin was realized.

Combretastatin

An efficient synthesis of this novel antitumour antibiotic has been completed employing intramolecular Mitsunobu reaction as the key step. Combretastatins D-1 and D-2, minor constituents of Combretum caffrum and PS cell line inhibitory macrocyclic lactones, have been shown to possess a new oxygen heterocyclic ring. In addition to making the drug available for chemotherapy, the method can also provide substrates for use in studies on shape selectivity and molecular recognition.

Fredericamycin A

Fredericamycin A is an anticancer antibiotic produced by a strain of Streptomyces griseus. The synthetic strategy involves a Diels-Alder approach using spirodione as dienophile and isobenzofuran as the diene. Isobenzofuran and the required spirodione were synthesized by the methodology developed at NCL using cyclic ketals of α-tetralone and 1-indanone.

New and Efficient Photochemical Methodology for the Synthesis of γ-Alkylidene γ-Butyrolactones

 γ -Lactones are known to possess antitumour activity and other biological properties as well. A novel, convenient and efficient route for the synthesis of such compounds has been developed.

Endo to Exo Isomerization of Diels-Alder Cycloadducts

An efficient photochemical method has been developed for the isomerization of the normally obtained endo Diels-Alder products into the corresponding exo isomers.

Evaluation of Oxidation Catalysts

Selective as well as total oxidation of hydrocarbons is industrially important. A simple and rapid test method has been developed to determine the extent of combustion as well as selective oxidation characteristics of a few known catalysts using phenanthrene as the probe. Using this technique, the efficacy of some well-known oxidation catalysts was shown to be in the following order:

 $MnO_2 > MnO_2 + Co > Fe_2O_3 > AgMnO_4$ (t.d.p) $> V_2O_5 > WO_3$, Fe_2O_3 and V_2O_5 .

Ciprofloxacin

This drug belongs to the quinolone group of synthetic broad spectrum antibacterials that hold great promise in medicine. The key intermediates required in its synthesis, viz. 3-chloro-4-fluoro aniline and a bromocyclopropyl derivative, have been prepared and the methods optimized. Efforts are under way to develop a process for the final product.

Captopril

Being one of the best selling and effective antihypertensive drugs, development of an economically viable route to it is important. Under the sponsorship of Amal Rasayan Ltd., Gujarat, two independent routes utilizing chiral reagents were examined. Optimization of a process is in progress.

Synthetic Hormones in Sericulture Development

Introducing synthetic hormones at an appropriate stage in the development of silkworm, or allowing them to be ingested along with the food of the silkworm results in the production of better shaped and sized cocoons from which raw silk of quality may be obtained in high yield. A synthetic programme to develop different analogues of prothoracicotrophic hormone was undertaken under the sponsorship of Department of Biotechnology and a few peptide derivatives have been synthesized.

Laser Dyes

Several new 3-substituted benzoxazolyl/benzimidazolyl-7-diethylamino-2H-1benzopyran-2-one laser dyes were prepared. Some of them may be employed as efficient laser dyes with possibilities of commercial exploitation.

Molecular Sieves/Zeolites in Organic Synthesis

The potential of zeolites in general organic synthesis has not been fully realized. NCL is exploring this area. The catalytic properties of zeolites have been exploited in the following synthetic transformations.

Esterification reaction

Esters of various carboxylic acids were prepared in very good yield (above 90%, based on recovered acids) using alcohols in the presence of zeolite catalysts. This method is a general one and also useful for the preparation of esters of unsaturated acids like acrylic acid, crotonic acid, and cinnamic acid.

H-Y Zeolite, an efficient catalyst for thioacetalization

Carbonyl compounds were thioacetalized by 1,2-ethane-dithiol in presence of H-Y zeolite in almost quantitative yields. A wide range of carbonyl compounds including aromatic and hindered ketones can be thioacetalized by this technique. The catalyst can be recycled for further use after reactivation.

Sulfoxidation of thioethers using titanium silicate

The potential of titanium silicate catalysts in the oxidation of substrate moieties, such as sulphur in thioether, has been demonstrated for the first time. Thus, titanium silicate molecular sieves having MFI (TS-1) or MEL (TS-2) topology have been found to efficiently catalyze the oxidation of various sulphides to their corresponding sulphoxides and sulphones. The generality of the reaction was established in order to utilize this method for the oxidation of penicillin G to penicillin G sulfoxide, a step involved in the process for making 7 ADCA.

A convenient method has been developed for the conversion of acetals to carbonyl compounds, a necessary step in many organic transformations, using commercially available H-mordenite zeolites.

MATERIALS CHEMISTRY

BASIC RESEARCH

Nanoparticles

NCL is developing new materials by dispersing nanoparticles of various elements or their compounds in a suitable matrix. Polyphenylene sulphide and its condensation products have been used for generating nanoparticles of various metal sulphides. Such materials have a large potential for electrochemical applications including electrocatalysis and energy conversion and storage. Preliminary studies have shown that these materials may be used as cathodes and anodes in lithium batteries under nonaqueous conditions. The possibility of their use under aqueous conditions is also being investigated. It was possible to generate nanoparticles of cadmium sulphide, and various transition metals as well as their sulphides. The particle size could be controlled between 50 to 200 Å diameter. An unexpected outcome of an associated study was the finding that it is possible to obtain sintered rods or pellets of the graphitic material in which the nanoparticles are stabilized.

A noteworthy feature of the investigations is that the reactive graphitic matrix-containing sulphur species possess good electrocatalytic properties. Reactions such as hydrogen evolution in alkaline media, and methanol oxidation (for fuel cell application) have been studied. This is the first time that such studies have been carried out by exploring the electrochemistry of these matrix-containing nanopar-

ticles. These materials also have other applications such as high energy density batteries.

Conductimetric Sensors

Conductimetric humidity sensors using magnesium-titanium-chromium oxides have been developed. These sensors are most likely to be active when there is a single spinal phase corresponding roughly to the composition MgTiO₃-MgCr₂O₄. Besides this a novel ceramic material which exhibits the largest resistivity change as a function of relative humidity (20-90%) has been developed. By changing the dopants. this ceramic material can also be made to sense CO, ethanol, etc.; the potential of this application is being studied.

Catalytically Active Materials

Value addition of sensor materials like stabilized zirconia was carried out by incorporating several metal ions of variable valence. These compounds were also found to have catalytic properties with potential applications such as auto-exhaust catalysts (catalytic activity equal to or better than the value reported in literature for non-noble-metal catalysts), oxygenative dehydrogenation catalysts for conversion of ethylbenzene to styrene (more than 90% selectivity at 480°C), and catalysts for oxygenation of cyclohexane to cyclohexanol to cyclohexanone (30% conversion and greater than 70% selectivity at 350°C for products derived from cyclohexanol).

Tubes of these materials for use as potentiostatic and potentiometric catalysts were successfully prepared. Oxygen ion conductivity vs electromotive force relationship was taken advantage of for designing catalysts with specific selectivity.

Langmuir-Blodgett (LB) films

The area of Langmuir-Blodgett films has a recognized potential for applications such as molecular electronics, non-linear optics and sensors. One of the prime requirements for such applications is that the films must have an organized crystallographic structure and be free of pin-holes. Langmuir Blodgett films of different anionic complexes picked up with long chain amines having novel structures have been grown and characterized. This has opened up a new area of inorganic LB films. Ultrathin metal oxide films of excellent quality have been obtained by the decomposition of such LB films. A new structural model has been proposed for metal salts of fatty acids; this replaces a twenty-year-old model. Using LB films as model systems, improved quantitative analysis techniques by x-ray photoemission spectroscopy have been developed.

This model not only explains the "odd-even" intensity oscillation of (001) reflections but is also consistent with well-known chemical principles. It has also been shown that the electron attenuation length is dependent on the nature of the scattering centre and the dielectric properties of the medium. A new model has been proposed for determining attenuation lengths for electrons of different energies in LB films.

An exciting first-ever finding is a configuration change with temperature in lead salts of fatty acids. This observation is consistent with a ferro-electric transition, and is, therefore, likely to be of technological significance.

Deposition of inorganic complexes such as H₂PtCl₆ and titanyl oxalate anions using long chain alkyl amines was investigated in order to examine the possibility of polymerizing inorganic functional groups. Our understanding of the structure of LB films suggests that polymerization involving the organic part of the hydrocarbon chain would lead to distortion, which is not compatible with the stability of the LB films. The decomposition has also resulted in the deposition of nanoparticles of TiO₂, which can be exploited for harvesting solar energy. This work is being carried out in collaboration with Raman Research Institute.

Advanced Ceramics

Rare-earth & zirconia based ceramics

One area of crucial importance in the Indian context is the development of zirconiabased ceramics containing rare earths as dopants. Thus, there are plans for the development and use of yttria-stabilized zirconia which is now considered to belong to the class of wonder ceramics. Single cubic phases of compounds with the general formula, $Zr_{0.76}Y/Ca_{0.16}M_{0.08}O_{2-\delta}$, where M = Cr, Mn, Fe, Ni, Co, Cu, etc., or Al and/orTi, could be prepared by a novel method.

Soft ferrites

Ni-Zn ferrites with a high resistivity (> 106 ohm-cm) and low magnetic losses were prepared for high frequency (MHz range) application. The results indicate that, as a precursor for high-frequency Ni-ZN ferrite, Fe₂O₃ is better than other known materials.

Hard ferrites

A preparation methodology was worked out for obtaining Sr–ferrite in a finely powdered form ($\approx 0.2 \mu m$). Such fine particles possessing high magnetic properties have numerous applications.

High Temperature Superconductors

A new model for the AO₃ close–packing in layered perovskite cuprate superconductors with alternating AO and OO rows in a layer was proposed. In this model the relative orientation of the AO rows to each other are assigned pseudo–spins and the perovskite or rock–salt structures are shown to correspond to the structures found in Cu₃Au and Ni₃Ti, respectively, after the creation of oxygen vacancies.

A model has also been proposed for rationalizing the enhancement of T_c on increasing the number of layers or on replacing the Bi ions by Tl. A crucial element in this rationalization is the low value of the tolerance factor. The study has pointed out for the first time that localization effects are important in the suppression of T_c . It also suggests that in these two-dimensional systems the important parameter is the resistivity.

The main findings of the thermochemical studies on high-temperature superconductors and related systems are that these layered systems seem to require more covalency for metallization to take place compared to three-dimensional systems. The analysis also shows that $H(M)_O$ is an important factor in determining whether a system is metallic or not. Thermochemical measurements indicate that Cu^{+3} , as an isolated ion, is quite stable. It has been found that only 77 KJ of oxygen is incorporated when $YBa_2Cu_3O_6$ gives $YBa_2Cu_3O_7$.

Studies on the normal state properties of high temperature superconductors showed that:

- Some ESR features of LiNiO₂ below 40K, formerly attributed to a quantum spin liquid state, are present at higher temperatures in Li_xNi_{1-x}O. Possibly, holes are created on Ni on its substitution by Li in NiO.
- In compounds in which the metal ions are in triangular lattices, the 90° M–O–M interactions render the ground state ferromagnetic. The suppression of the long range ferromagnetic order in these compounds possibly leads to superparamagnetism.

A new layered system of alternating CuO₂ and CO₃ planes has been developed. Its potential in designing novel chemical systems by reacting the carbonate layer with ammonium salts is being examined. It is also a candidate for potentiometric sensing of CO₂.

Amorphous Silicon Thin Tilms for Photovoltaic Applications

Raman scattering measurements of the disorder in (a–Si:H) alloys used in thin film semiconductor devices, caused by the variation of the short-range-order (SRO) with deposition conditions, were made. They showed that certain undesirable post-deposition effects, caused by an extrinsic stress originating in the thermal expansion of the film and the substrate, can introduce weak bonds in the film that are responsible for the degradation of the electronic properties. This study suggests that the minimization of the spread of the film can improve its electronic properties. Elimination the extrinsic stress effects resulted in a minimum spread of $\Delta\Theta=\pm 6^\circ$, which is necessary to maintain the amorphous state of the film. The project was sponsored by DST.

Organometallic Compounds

Stable hexacoordinated tin (IV) complexes were prepared by reacting ester tin (IV) chlorides with Schiff base ligands derived from aromatic aldehydes. The binding of unsymmetrical alkynes to the Ru-H bond of [RuHCO (PPh₃)₂ (chelate)] resulted in the formation of ruthenium alkenyl complexes.

New dioxomolybdenum (VI) complexes of the type $[(MoO_2)_2L]$ have been prepared using binucleating Schiff bases obtained by the condensation of methyleneor dithio-bis (salicylaldehyde) and primary amines. Studies suggest an oligomeric structure for these binuclear complexes in which each molybdenum atom achieves a pseudo-octahedral structure via $Mo=O \longrightarrow Mo$ bridging. A new precursor $[Mo(NO)_2(acac)_2]$ has been designed to prepare a new class of dinitrosylmolybdenum (O) complexes of the type $[Mo(NO)_2(L)_2]$ (LH is a bidentate ligand). This process is superior to the older ones as this precursor is stable in air.

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Environment-Friendly Materials

Alternatives to CFCs for refrigeration & air conditioning

A modified Joback method with an improved capability of predicting normal boiling point has been developed, with a revised estimate of the group contribution to fluorine and an addition of some groups and corrections for perfluorination, partial fluorination (with or without fluorine) and partial halogenation (without fluorine). The root mean square deviation improved from 26.81% to 6.36%.

A method of predicting properties of organic compounds, like vapour pressure, vapour and liquid specific volumes, liquid and vapour heat capacities, and latent heat of vaporization, was developed. The validity of this method has been assessed by analyzing an ideal Rankine refrigeration cycle. The data for this comparative cycle analysis were derived from thermodynamic data predicted by using the procedure, and also collected from published literature. The agreement was within 5 per cent.

Investigations aimed at identifying suitable alternatives to CFCs have led to the following findings:

HFC-152a (1,1 difluoroethane) is perhaps a better alternative to CFC-12. Among HFCs, from energy considerations, HFC-152a is the best alternative to CFC-12. The performance of HFC-134a, the most popular alternative currently considered, is as good as, and, under certain conditions, even better than CFC-12; the better performance may be attributed to the better heat transfer characteristics of HFC-134a than those of CFC-12. HFC-134 (1,1,2,2 tetrafluoroethane) offers better efficiencies than HFC-134a (1,1,1,2 tetrafluoroethane). Among the fluorinated ethers, tetrafluorodimethylether (CHF₂OCHF₂, HFE-134), appears to be a promising alternative. HCFC-123 is the most promising immediate alternative to CFC-11 in large-size refrigeration and air conditioning systems. HFE-143 (CH₂FOCHF₂) appears to be a potential long term candidate.

THEORETICAL CHEMISTRY

BASIC RESEARCH

Intermolecular Interactions Between Various Proton Donors and Proton Acceptors

Binary systems formed by 1,1,2,2 tetrachloroethane with dimethyl sulphoxide, acetone, acetonitrile and dibutyl ether are of interest because of specific interactions between the molecules in solution. The occurrence of specific interactions between these compounds can be explained as due to the H-bond formation between the H-atom of tetrachloroethane with the O-atom of dimethyl sulphoxide, acetone and dibutyl ether and with the N-atom of the acetonitrile. The values of enthalpy of complex formation suggest that moderately stable complexes are formed with dimethyl sulphoxide, acetone and acetonitrile, whereas weak complexes are formed with dibutyl ether.

Coupled Cluster Methods

Development of a stationary response method for the calculation of static properties was completed using the many-body coupled-cluster method and it was successfully implemented for the nonlinear response property. An important (2n+1) rule in the stationary formulation of response involving computing the 2nth and (2n+1)th

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order property, using the knowledge of derivatives up to nth order, was successfully implemented.

An accurate evaluation of spectroscopic difference energies was made using the coupled cluster model. The first-ever detailed study of the correlation effects in shaping the static exchange potentials in e⁻ molecule scattering was carried out.

A rigorous ab initio test of maximum hardness principle was initiated.

Quantum Mechanical Calculations Using Parallel Computation

The first phase of putting together a package of ab initio programs for computation based on quantum mechanical methods for medium-sized molecules was completed for use in the parallel network of transputers available at C-DAC, Pune. Parallelization of Bender Shavitt's algorithm on transputer clusters to achieve this goal was carried out for the first time at NCL.

Hypermodified Bases in tRNA

Extensive chemical modifications of nucleic acid bases naturally occur at strategic locations in the anticodon loop of tRNA. These modifications may modulate the efficiency of protein biosynthesis besides regulating the cellular metabolism and transport of nutrients. Studies at NCL have led to a better understanding of the effects of crystal packing and intermolecular interactions in terms of the protonation effects.

Nature and Geometry of Ion Binding Sites in Protein Structures

In a DST-funded study to understand the recognition and specificity of metal binding sites in protein structures, it was found that each ligand has a specific orientation for metal coordination. These results have implications in the understanding of protein folding.

X-Ray Crystallography

Some important observations were made in the study of the x-ray structure of the anchored catechol ligand 2,3-dihydroxy benzenemethanimine α -(2-hydroxymethyl) phenyl, which has thermochromic properties. A new hypothesis on thermochromism and photochromism of Schiff bases was proposed, which contradicts the earlier hypothesis advanced by Moustakali-Mavridis and coworkers in 1978. It was shown that for thermochromic compounds, the presence of aliphatic methylene/ ethylene groups between N and five/six membered rings prevents the molecules from being planar and requires that all of them should be photochromic.

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CHEMICAL REACTION ENGINEERING

INDUSTRY-ORIENTED RESEARCH

Monochlorobenzene Plant Design

Hindustan Organic Chemicals (HOC) Ltd. has been operating for several years a 25-TPD plant at Rasayani for manufacturing monochlorobenzene (MCB). NCL has completed the design of a new 50-TPD MCB plant to be put up at HOC incorporating many features in the light of operational experience and knowledge of new developments gained since the 25-TPD plant was originally designed, a couple of decades ago.

Predicting Performance of Distillation Column Train

HOC has been operating a phenol plant at Cochin, under license from UOP, U.S.A. An important part of the process involves separation of the products from the cumene reactor in a train of distillation columns. NCL has been retained by HOC as a consultant for suggesting improvements in the plant. A computer program has been developed for simulating the performance of the multicomponent distillation columns with a vapour-liquid equilibrium option covering the pertinent range of pressure and temperature, for the set of components found at the cumene reactor outlet.

The program has been used to predict the performance of individual columns in the train, and to compare their past and present performance as recorded at the plant. The match between the two has been remarkably good in most instances. The program is also useful in locating specific bottlenecks and assessing the plant performance when the feed composition is changed, which would be the case when a different catalyst is used.

LABORATORY-LEVEL DEVELOPMENTS

Process for Calcium Cyanamide

Calcium cyanamide is an important chemical intermediate for the production of dicyandiamide, guanidine, thiourea, melamine and other substituted triazines. Under the sponsorship of Straw Products Ltd., New Delhi, a novel urea-lime route to calcium cyanamide has been standardized on a 28-kg scale. The process package has been handed over to the sponsors who plan to set up an integrated plant at Ankleshwar for making calcium cyanamide, dicyandiamide and thiourea from calcium cyanamide. The product obtained by the NCL process is of better quality than that obtained by the conventional calcium carbide-based process, used the world over. Also, the NCL process is based on a raw material which is much cheaper than calcium carbide.

Novel Technologies Based on Non-Catalytic Gas-Solid Reactions

- Two gas—solid reactions were studied with a view to reducing industrial pollution and recovering profitable by—products. A method for reducing gypoun, a by—product in phosphoric acid manufacture, with carbon in the presence of cheap catalysts was worked out. Further processing leads to the recovery of sodium sulphide in high yield. Negotiations are in progress with a chemical firm for the joint development of the process into a technology.
- Large quantities of free sulphuric acid that flows into the sea along with the
 waste water from sulphuric acid-based TiO₂ pigment plants can be treated
 using a gas-solid reaction system. Studies at NCL have shown that the sulphuric
 acid content in the wastewater can be reduced by 25% and iron sulphate can
 be recovered economically as a valuable by-product.

BASIC RESEARCH

Model Based on Pattern Recognition Strategies

The mathematical model of a process helps to improve, optimize or control the process. For a number of situations, however, mathematical process models are not available, or experimental limitations restrict the specifications of the complete state of the system. An approach worked out at NCL has made it feasible to carry out fault diagnosis, process modelling, identification and process control protocols. This approach is based on pattern recognition strategies to relate the input—output behaviour in a manner analogous to those in neural networks. Another approach reduces the dimensionality of the available model while retaining the model's prediction abilities in the likelihood of incomplete process state specifications. The applicability of the methods has been tested for chaotic behaviour of systems and newer strategies for servo and regulatory control of the chaotic dynamics of nonlinear processes have been proposed.

Reactor Performance With Periodic Flow Reversal for Complex Reactions

Research into the effects of the periodic feed reversal strategy on conversion and selectivity analysis for complex reactions in packed-bed reactors has shown that it is possible to get better conversions and selectivities than are possible in conventional unidirectional flow operations. More importantly, the improved reactor performance is achieved for lower inlet gas temperatures — a feature that is of considerable practical use. This work was carried out under the auspices of the Indo-Russian Cooperation Programme sponsored by the State Committee of Science and Technology, Russian, and DST.

Controlling Nonlinear Chemical Dynamics

A new method, designated RNCL, for robust nonlinear control of systems has been developed and applied to a non-isothermal continuous stirred tank reactor (CSTR), a system that exhibits dynamic features such as multistationarity and unstable solutions. The simulation reveals the excellent capability of the new method for servo and regulatory control in the presence of deterministic and stochastic process disturbances, and modelling errors.

Situations can arise in which nonlinear systems, due to unforeseen circumstances, go into undesirable chaotic states. Superior system performance may be achieved by eliminating chaos from the system and regulating its dynamics. An algorithm that can accomplish this has been developed. The method has been exemplified by considering a non-isothermal CSTR. The method uses internal modelbased control concepts and can handle process-model mismatches and process load disturbances.

Simulation of Flow in Multiphase Reactors

A general purpose computer code with an easy-to-operate user interface has been developed for simulating turbulent flows in multiphase reactors. This code provides an economical and effective tool for testing various design options (geometrical configuration and operating parameters) for a given process, and it can be used to develop design and selection guidelines for bubble column, gas-lift loop and mechanically agitated gas-liquid reactors.

Reactive Mixing in Agitated Reactors

Mathematical models have been developed to simulate reactive mixing (macro and micro) in agitated reactors. The influence of polymer molecules on turbulence and consequently on mixing has been analyzed. A flow simulation code is being used to optimize the design of the impeller for the liquid phase mixing.

Bubble Column Reactor for Oxidation of Ethylene to Acetaldehyde

Studies on the effect of inlet gas velocity, composition of inlet gases, catalyst concentration and temperature in the liquid-phase oxidation of ethylene to acetaldehyde (Wacker Process) have shown that, for a given set of conditions, a certain critical ratio of oxygen to ethylene in the reactor inlet is required for the overall catalytic cycle to work with maximum efficiency. A mathematical model for a bubble column reactor for this system has been developed. Excellent agreement was observed between the experimental results and the predictions made using the theoretical model. This model is directly useful in the scale up and design of such processes.

ENERGY CONSERVATION

INDUSTRY-ORIENTED RESEARCH

Energy Audit

Under the UNDP-Government of India Energy Audit Project, the Energy Audit Team of Prototype Development & Training Centre, Rajkot, conducted a detailed energy audit at Gokul Dairy, Kolhapur, under NCL's guidance. The identified savings potential is about 14.4% of the overall energy bill.

Absorption Heat Pump

The technical feasibility of an absorption heat pump to provide cooling and heating simultaneously to a plant in Thermax Ltd. was assessed. The optimized use of this absorption system with suitable modifications to the existing utility system was suggested.

INSTRUMENT DEVELOPMENT

TECHNOLOGIES AT COMMERCIAL SCALE

High Performance Liquid Chromatograph

HPLC is a well established and very sophisticated separation technique used in chemical analysis. NCL's know-how for a PC-based HPLC has been licensed to Nucon Engineers, New Delhi.

Infrared Spectrophotometer

NCL's know-how for a PC-based infrared spectrophotometer has been licensed to Electronic Corporation of India Ltd., Hyderabad.

The development of these instruments was funded by the Department of Science and Technology, New Delhi.

PROJECT PLANNING & DEVELOPMENT

Business Development

A meeting of the Centre for Technology Development, Bangalore, with a number of industrial representatives was organized as a part of the strategy to forge a closer link with funding institutions and user industries.

Feasibility Studies and Techno–Market Reports

These included a pre-feasibility report on N-methyl piperidone for Divya Chemicals Ltd., Bombay; a report on business opportunities for membranes in India; a technomarket report on polymer additives for Technology Information Forecasting and Assessment Council (TIFAC), New Delhi; a report on technology scouting studies for Anand Intech Ltd., Pune; a report on engineering plastics for Federation of Indian Chambers of Commerce and Industry (FICCI), New Delhi; and a report on fluoroaromatics for Cadilla Laboratories, Ahmedabad.

Consultancy Services to China

NCL provided consultancy to China under a World Bank-funded project to strengthen the R&D capabilities of two R&D institutions: Nantong Synthetic Materials Research Centre and Suzhou Research Institute of Chemical Industry.

Development of Commercial Database

The first phase of the development of a database on environmental process technology, containing brief descriptions of technologies, their commercial status and sources from which additional information can be obtained, was completed with funding from Technology Information Forecasting & Assessment Council (of DST).

Pre-Research Appraisal

Pre-research appraisal to determine the economic and marketing feasibility of many projects was completed. They included natural gas to middle distillates; carbamate pesticides; dehydration of alcohol to ethylene and its subsequent oxidation to ethylene oxide; hydroquinone and catechol; and drugs and drug intermediates.

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LIBRARY & DOCUMENTATION

The NCL library is functioning as the National Information Centre for Chemistry and Chemical Technology (NICHEM) with financial support from DSIR under the NISSAT scheme. About 75% of the library and information services, such as acquisition, cataloguing, circulation, serials control and information retrieval, has been computerized using a WIPRO 386S system. The various databases developed for this purpose are:

1. Books database	40,000 records
2. Users database	1,350 records
3. Publishers database	1,500 records
4. Periodicals master database	900 records
5. Loose periodicals database	8,000 records
6. Bound periodicals database	9,000 records
7. Indian chemical patents database	4,000 records
8. Union list of periodicals in Pune City libraries	5,000 records

The database on Indian chemical patents is being used for publishing the monthly, *Indian Chemical Patents Abstracts* (annual subscription: Rs. 400.00). NICHEM supplies various types of documents to users on request, and also provides translation, literature search and consultation, and computerized on-line search services. During the period of reporting, 7050 documents of different types were added to the Centre's collection.

NICHEM played an active role in establishing a network of libraries in Pune for resource sharing (PUNENET). A union catalogue of the material available in these libraries is maintained and updated annually by the Centre.

The NISSAT Access Centre for International Databases (NACID), established at NCL with financial assistance from DSIR, provides on-line information services to users from the western region comprising Maharashtra, Gujarat, Madhya Pradesh, Goa, Diu and Daman. International databases, such as CA Files, CAB, BIOSIS, COMPENDEX, MEDLARS, Belstein, SCI, and PREDICAST, are regularly accessed through telex/PSTN/GPSS/PAD modes. During the period in question on-line searches on about 900 topics were made — about 425 for NCL scientists and the rest for other users.

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TECHNICAL SERVICES

■ Planning, Monitoring and Research Co-Ordination

Annual research programmes, annual plans, and Five-Year Plan documents were prepared in consultation with project leaders and divisional heads.

Industrial Liaison, Technology Transfer, Etc.

Assistance was rendered in formulating grant-in-aid, sponsored, collaborative, and consultancy proposals and getting them approved from the appropriate authority.

Services were rendered to potential clients about NCL processes, new contracts, research proposals, etc.

Monitoring of funds due to NCL in respect of consultancy / sponsorship / collaborative charges was carried out, and where necessary, appropriate action was taken to recover the amounts from the concerned parties.

Publicity, Public Relations

DTS played a major role in the organization of the CSIR Golden Jubilee Year (1991) celebration, which culminated in the CSIR Foundation Day on 26 September 1991. A lecture by Prof. Jayant Narlikar, Director, Inter-University Centre for Astronomy and Astrophysics, Pune, was arranged. DTS helped in the interaction between NCL and visiting delegations from Germany, Iran, Thailand, Australia, China, Poland, Syria, the Netherlands, Korea, Vietnam and France. A distinguished visitor to NCL during this period was the Minister of State, Mr.P.R. Kumaramangalam.

Biennial Report 1991-93

A write-up was prepared on "Catalysts and Related Products" for submission to the Chairman, Indigenous Technology Evaluation on Catalysts.

Four issues of the quarterly house journal, NCL Bulletin, were brought out.

Workshops, Exhibitions, Etc.

DTS organized NCL's representation in a number of exhibitions and trade fairs including, IITF-91 at New Delhi, Tech-Trans at Aurangabad and Faridabad, PLASTO '93 at Pune, IETF '93 Exhibition at New Delhi, and TRANSTECH-93 at Bombay.

International Collaboration

DTS coordinated the deputation of scientists under CSIR bilateral exchange programmes, and the INSA, DBT, DST, and TOKTEN exchange programmes.

Reports, Etc.

Technical services were rendered for the preparation of a number of technoeconomic reports on products like aniline and anthraquinone, EVA-based and silicone-based adhesives, naphthalene, epoxy resins, and phenolic resins. A prefeasibility report on citric acid was also prepared.

Technology status studies on the following products were prepared:

- 1. Vitamin C and Sorbitol, for Department of Scientific and Industrial Research (DSIR);
- 2. Carbon tetrachloride, for DSIR;
- 3. Polyacetal resins, for DSIR; and
- 4. H acid and G salt industry in India, for Central Pollution Control Board (CPCB).

Project profiles for marketing a number of NCL's technologies were prepared.

Patents

The division processed 90 patent applications by interacting with the applicants on the one hand, and the CSIR Patent Unit on the other. (A list of patents granted during 1991-93 is given on page 155).

Extramural Activities

Bibliometric analysis of the publications of NCL scientists was carried out for the years 1988-90 and 1989-91. The results of the analysis were published in the NCL Bulletin.

Databases were created on external cash flow, externally funded projects and consultancy projects, and on chemical manufacturers, market data, prices of chemicals and equipment.

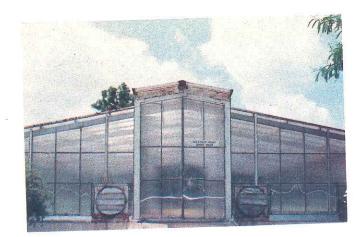
DTS staff participated in the UNDP-supported international symposium on INRIST-TOKTEN Interaction with Industry held at New Delhi as also in MCCI-CMET-Industry Meet held at Pune.

A students-scientists meet was arranged at NCL in association with NCERT, New Delhi.

NCL PREPARES FOR THE FUTURE

N keeping with the new course that the country is taking with respect to globalization, NCL is getting ready to meet the new challenges that future is expected to bring. As part of this enterprise, some state—of—the—art facilities have been added, or are being added, to its research infrastructure, with the aim of adding value to the technologies developed in the laboratory to make them readily acceptable and competitive within and outside the country. This section gives a few glimpses of these facilities.

NCL'S CONTRIBUTION TO THE GREENING OF INDIA

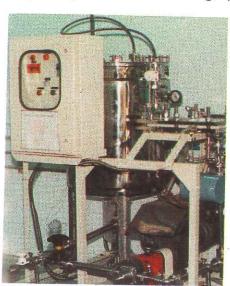




A pilot-plant facility, for producing tissue-cultureraised plantlets of forest and other tree species in large numbers has been set up at NCL with funding from Department of Biotechnology, Government of India. This facility comprises a semiautomated air-conditioned laboratory and greenhouse, with a computerized monitoring system. The aim is to demonstrate the feasibility of using tissue-culture technologies for producing plantlets useful in the afforestation programmes in the country. A brainchild of a DBT task force on production of biomass, the facility fulfills a long-felt need to initiate a coordinated plan in this direction involving research institutions on the one hand and silviculturists on the other.

FACILITY FOR APPRAISAL OF BIOLOGICAL PROCESSES

A downstream processing facility, with support from Department of Biotechnology, has been created by the biochemical engineering group for separation and recovery of proteins and other bioactive molecules. This facility consists of equipment for solid-liquid separation, membrane filtration, low pressure chromatography and bulk-freeze drying. It can be



used for pre-pilot plant appraisal and scale-up of promising laboratory processes to a level typically up to 100 litres of biological fluids, such as fermentation broths and plant/tissue extracts. Up to 5 kg of the desired product could be made in this facility. NCL's effectiveness in offering biotechnological processes to industry has been enhanced considerably by the establishment of this facility.

CLEAN FACILITY FOR SYNTHESIZING SPECIALITY POLYMERS

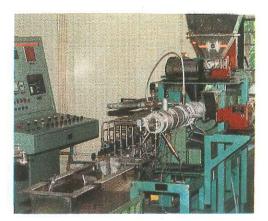
THE polymer science and engineering group now has a Class 10000 clean facility for synthesizing photochemically—active chemicals and polymers used in microelectronics, conforming to the stringent purity specifications. This is the only such synthesis facility in India, set up with a generous support from Department of Electronics. The particulate matter in the air in the clean space is reduced to 0.1 micron size using a series of microfilters, and a sodium vapour lamp is used as the source of illumination to

prevent photochemical damage. Synthesis of the chemicals is carried out on three Class 100 tables. The design of the facility is such that the air passing over the synthesis tables is vented out to prevent a build—up of solvent vapours.



POLYMER PROCESSING FACILITIES GET A BOOST

New polymer processing facilities such as a pultrusion unit and a reactive extruder have been added by the polymer science and engineering group to augment the processing capabilities that are already among the best in this part of the world. The new facilities include a ultra-modern capillary-



flow rheometer, a sonic modulus tester and a hot—stage polarizing microscope. With these additions NCL will now be able to take up high—quality research work on short—fibre composites, polymer blends, cable extrusions, and on advanced thermoplastics and thermosets, and also complement the know—how developed with a better know—why.

FROM GRAMMES TO KILOGRAMMES

A new facility, called Kg Lab, comprising reactors of different sizes and made of different materials of construction, extractors, evaporators, etc. is now an integral part of the infrastructure in the area of organic synthesis and technology at NCL. The aim is twofold. Firstly, the facility will be used to make products on a kilogramme—scale. This is necessary because the organic chemists developing synthetic routes usually make only a few milligrammes or grammes of the products, and considerable additional efforts are required to make them in sizeable amounts for scale—up trials and tests. Also, by producing the materials on an enlarged scale, one can get the real 'feel' of the entire process. Secondly, the facility will provide the data required for designing the pilot/semi—commercial plant in which a process would be scaled up to make it commercially viable.

PROCESS ENGINEERING UNIT FOR VALUE ADDITION



A modern and fully equipped process engineering unit was recently inaugurated at NCL. The new facility will enable the scientists and engineers to add value to the processes and technologies developed in the laboratory, and to prepare basic engineering packages

which is an essential step in the commercialization of the processes. The process engineering unit will act as a bridge between the scientists involved in R&D and the key persons from industry. Thus the process engineering unit will be involved in the entire range of innovation steps from the initiation of a project to the commissioning of the commercial plant based on the project.

APPENDICES

HONOURS & AWARDS

1991 - 92

Institutional Awards

The first CSIR Technology Prize for 1990 for Chemical Technology was awarded jointly to IIP, Dehradun, and NCL. The NCL group comprising Dr.P. Ratnasamy, Dr.B.S. Rao, Dr.I. Balakrishnan, Dr.V.P. Shiralkar and Dr.A.N. Kotasthane received the prize for their outstanding contributions to the development of zeolite catalysts and associated application technologies.

NCL was chosen for ICMA award for the year 1991 for export of engineering services in view of its successful completion of the world bank-funded R & D management consultancy assignment in China during 1991.

Group & Individual Awards

Dr.R.A. Mashelkar, Director, NCL, was elected President of the Maharashtra Academy of Sciences for a three-year term.

Dr.A.F. Mascarenhas, Dr.S.S. Khuspe, Dr.R.R. Hendre, Dr.(Ms.)R.S. Nadgauda, and Ms.V.A. Parasharami of the Plant Tissue Culture Division received the CSIR Technology Award for the development of new techniques of plant tissue culture for the propagation of high-yielding and disease-resistant varieties of sugarcane, cardamom, turmeric, ginger, pomegranate, cotton, etc.

Dr.S. Rajappa, Head, Organic Chemistry: Synthesis Division, was awarded the Dr.K.G. Naik Gold Medal of the Maharaja Sayajirao University of Baroda for the year 1989.

Dr. V.M. Nadkarni, Head, Chemical Engineering Division, was awarded the Special Rubplas '91 Award by the Rubber & Plastics Institute, Bombay, for his important contributions to the Indian plastics industry.

Dr. V.S. Patwardhan, Scientist, Chemical Engineering Division was elected Fellow of the Indian National Academy of Engineering, New Delhi. He was also awarded the Herdillia Award for 1991 by the Indian Institute of Chemical Engineers for excellence in basic research in chemical engineering.

1992 - 93

Group & Individual Awards

Dr.R.A. Mashelkar was awarded the Om Prakash Bhasin Award for Science and Technology, instituted by Shri Om Prakash Bhasin Foundation, New Delhi, for the year 1990. The award came to Dr. Mashelkar for his outstanding contributions in the field of engineering and technology.

Dr. Mashelkar was elected President of the Physical Sciences Section of National Academy of Sciences, in its 61st Annual Session.

Dr. Mashelkar was awarded an honorary doctorate degree in science by the University of Salford, U.K., in recognition of his outstanding contributions to science.

Dr. Mashelkar has been invited by Pergamon Press, U.K., to deliver the 1994 Danckwerts Memorial Lecture in U.K. This lecture series has been jointly founded by Pergamon Press and the Institution of Chemical Engineers, U.K.

Dr. Mashelkar was conferred the Pandit Jawaharlal Nehru National Award for 1991 for technology by the Madhya Pradesh Government, which he shared with Dr.S.S. Datta Roy of IIT, New Delhi.

Dr.S. Rajappa was awarded the Prof.K. Venkataraman Lectureship by the University Department of Chemical Technology, Bombay. He delivered this lecture on 16 and 17 November 92.

Dr. Rajappa was invited to deliver the 13th Dr.G.P. Kane Trust Lecture at the Indian Chemical Manufacturers' Association, Bombay.

Dr.T. Ravindranathan, Head, Organic Chemistry: Technology Division, was selected by the Ranbaxy Research Foundation, New Delhi, for the Ranbaxy Research Award for 1991 in the field of pharmaceutical sciences.

Dr. Sivaram was elected Fellow of the Indian Academy of Sciences, Bangalore, from 1991. The honour comes to Dr. Sivaram in recognition of his outstanding contributions in the field of polymer chemistry.

Dr.V.M. Nadkarni, Head, Chemical Engineering Division, Dr.V.R. Choudhary, Scientist, Chemical Engineering Division, Dr.K.N. Ganesh and Dr.G. Pandey, both scientists, Organic Chemistry: Synthesis Division, were elected Fellows of the Indian Academy of Sciences, Bangalore, from 1992.

Dr.M.C. Srinivasan, Head, Biochemical Sciences Division, was elected President of the Mycological Society of India for the year 1991 at the Society's 17th Annual Meeting.

Dr.A.V. Ramaswamy, Scientist, Catalysis Division, (along with others in the team at IIP, Dehradun) was awarded the 1992 CSIR Prize for Chemical Technology for the development of the Pt-Re bimetallic catalytic reforming catalyst.

Dr.V.R. Choudhary was invited to be a member of the International Scientific Advisory Committee for the International Symposium on Natural Gas Conversion, to be held in Sydney, Australia, in July 1993.

Dr.R.V. Chaudhari, Scientist, Chemical Engineering Division, was elected Fellow of the Indian Academy of Sciences from 1992, in recognition of his contributions in the area of industrial homogeneous catalysis and multiphase catalytic reactor engineering.

Dr.S.K. Date, Scientist, Physical Chemistry Division, was awarded the MRSI Medal for 1993.

Dr.K.N. Ganesh was awarded the 1990 B.M. Birla National Science Award for Young Scientists in Chemistry. The award, given to scientists under 40 years, was in recognition of Dr. Ganesh's important contributions in the field of basic chemistry.

Dr. Ganesh received the Bruker NMR Award for Young Scientist for the Year 1989, in recognition of his outstanding work in the field of NMR and its applications.

Dr.P. Chakrabarty, Scientist, Physical Chemistry Division, received the International Union of Crystallography Young Scientist Award instituted by the European Science Foundation Network of the European Association of Crystallography of Biological Macromolecules, Italy.

Dr.(Ms.)M.V. Rele, Scientist, Biochemical Sciences Division, was awarded the Raman Research Fellowship for 1992 by the CSIR.

Dr. Rajiv Kumar, Scientist, Catalysis Division, received the Alexander von Humboldt Research Award/Fellowship.

Dr.M. Islam Khan, Scientist, Biochemical Sciences Division, and Dr.V.V. Ranade, Scientist, Chemical Engineering Division, were chosen for the 1992 Young Scientist Award of the CSIR.

Dr.R.H. Naik, Scientist, Organic Chemistry: Synthesis Division, was awarded the Raman Research Fellowship for 1993.

Dr.S. Sivaram, Dr.M.C. Srinivasan, Dr.K.N. Ganesh, Dr.V.R. Choudhary, Dr.R.V. Chaudhari, Dr.V.S. Patwardhan, and Dr. Ganesh Pandey were elected Fellows of the Maharashtra Academy of Sciences from 1992.

MAJOR TECHNOLOGY TRANSFERS

■ 1991 - 92

- 1. Process for can sealing composition based on natural rubber was released to Pawan Rubber Products Kasarwadi, Pune, through NRDC.
- 2. Radiosonde thermistor technology was released to Pawan Rubber Products, Pune, through NRDC.
- 3. Encilium technology was licensed to Dhampur Sugar Mills, Dhampur, U.P., and Ugar Sugar Works, Sangli, Maharashtra.
- 4. Process for 1-methylamino-1-methylthio-2-nitroethane, an intermediate for antiulcer drugs, was transferred to Globe Organics Ltd., Hyderabad.
- 5. Technology for alprazolam was released to Household Remedies, Bombay.

■ 1992 - 93

- 1. Encilium technology was released to Co-operative Co-Ltd., Saharanpur, U.P., through Resource Projects India (P) Ltd., and to Vasantdada Shetkari Sahakari Sakhar Karkhana Ltd., Sangli.
- 2. Technology for a catalyst for conversion of methanol to formaldehyde was released to International Catalysts Ltd., Pune.
- 3. Technology for a catalyst for conversion of C₄ feedstocks to methyl ethyl ketone was released to International Catalysts Ltd., Pune.
- 4. Process for the manufacture of special grades of PTFE was licensed to Hindustan Fluorocarbons Ltd., Medak.
- 5. Process for making PTFE piston and wear rings for compressors was transferred to Kirloskar Pneumatics Ltd., Pune.

- 6. Process for the manufacture of polyurethane water proofing coatings, developed jointly with CBRI under CSIR mission on low cost building materials, was released to Dr. Beck & Co., Pune.
- 7. Process for the manufacture of vincristine and vinblastine sulphate was licensed to Aditya Alkaloids Ltd., Madras.
- 8. Process for polyethylene—based cable compounds was transferred to Cable Corporation of India, Bombay.
- 9. Design package for a 50-TPD monochlorobenzene plant was handed over to Hindustan Organic Chemicals Ltd., Rasayani.

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PAPERS PUBLISHED DURING 1991-93

BIOCHEMICAL SCIENCES DIVISION

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CHEMICAL ENGINEERING DIVISION

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DEPUTATIONS

1991 - 92

A nine-member team of NCL scientists visited China for 17 days from 12 May 1991 to provide consultancy services for strengthening the R&D capabilities of two chemical institutions there. The team consisted of:

Dr.R.A. Mashelkar

Dr.S.H. Iqbal

Dr.V.M. Nadkarni

Dr.S. Sivaram

Dr.S. Rajappa

Dr.T. Ravindranathan

Dr.S.P. Vernekar

Dr.S.S. Kulkarni

Mr.R.R. Hirwani

Dr. Mashelkar also visited Germany as part of a six-member delegation in June 1991 for discussions on Indo-German Cooperation in Science & Technology, and to identify specific proposals for further collaboration, at the invitation of the President of DAAD.

Dr. Mashelkar visited Karlsruhe to give a Plenary Lecture on "Chemical Engineering Contributions to Development by the Year 2000 – The Indian Scenario" at the Fourth World Congress on Chemical Engineering in June 1991.

Dr. Mashelkar visited USA to give an invited talk at the Gordon Research Conference and visit various laboratories, institutes and universities in August 1991.

Dr. Mashelkar visited U.K. in October 1991 to visit various universities and R&D centres in London under the British Council Visitorship Scheme.

Dr.P. Ratnasamy, Deputy Director, NCL, visited Germany to deliver a plenary lecture at the 4th World Congress on Chemical Engineering in Karlsruhe held in June 1991.

Dr.S. Sivaram, Head, Polymer Chemistry Division, spent a period of eight weeks in 1991 visiting France, Italy, Germany, Belgium and the United Kingdom. In France he held discussions at the University of Blaise Pascal on the joint collaborative research programme between the University and NCL. He also visited the following academic centres for discussions and lectures: University of Paris, Institut Charles Sadron, Strassbourg, Centre for Research in Organic Materials, Lyon, University of Catania, Italy, Universities of Mainz and Dusseldorf, Max Planck Institute for Polymer Research, Mainz, University of Liege, Belgium, and University of Strathclyde, Glasgow.

Dr.V.M. Nadkarni, Head, Chemical Engineering Division, visited Canada to attend the PPS-7 Meeting at Hamilton in April 1991.

Dr.S. Sivasanker, Scientist, Catalysis Division, went to USA in November 1991 for inspecting four units of BTRS being purchased from Autoclave Engineers, USA, for the project on development of novel shape selective zeolite catalysts under the on–going UNDP programme at NCL.

Dr.A.V. Ramaswamy, Scientist, Catalysis Division, visited France, USA and Japan in 1991 under the UNDP project on, "Development of Novel Shape Selective Zeolite Catalysts":

Dr.C. Gopinathan, Scientist, Inorganic Chemistry Division, went to USA for three months from April 1991 to receive training in catalysis under the UNDP project, "Development of Novel Shape Selective Zeolite Catalysts" at various institutes.

Dr.S. Devotta, Scientist, Chemical Engineering Division, went to USA for attending the TERI Workshop on, "CFC-free energy efficient refrigerators" in Washington in September 1991. Dr. Devotta went to Thailand in November 1991 to attend a workshop on the implementation of the Montreal protocol for protection of the ozone layer.

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Dr.(Ms.)R:S. Nadgauda, Scientist, Plant Tissue Culture Division, was deputed to Australia to attend the International Centenary Conference on Bio-Resources at Sydney in July 1991.

Dr.S. Ponrathnam, Scientist, Chemical Engineering Division, visited France for six weeks in March 1992 under the CSIR-CNRS Exchange Programme.

Mr.R.S. Singh, Scientist, Library, visited China in 1991 to attend a regional seminar on, "Chemistry Information" and the China Steering Committee Meeting at Beijing.

Dr.B.S. Rao, Scientist, Catalysis Division, went to Czechoslovakia in September 1991 to visit institutes in the area of his interest and to participate in "The International Symposium on Zeolite Chemistry and Catalysis" under the CSIR-CSAV Exchange Programme.

Dr.S. Pal, Scientist, Physical Chemistry Division, visited Theoretische Chemie of Physikalisch Chemisches Institut, University of Heidelberg, Germany, for three months from in 1991 as Alexander von Humboldt Fellow.

Mr.P.M. Suryawanshi, Scientist, Physical Chemistry Division, was deputed to USA under "Raman Research Fellowship" for six months from March 1991, to work on "High-Field FT-NMR Instrumentation" at the School of Chemical Science, University of Illinois,

Dr.D.C. Agarwal, Scientist, Plant Tissue Culture Division, was deputed to U.K. in 1991 under the ACIS-CNRS Exchange Programme.

Dr.M.V. Badiger, Scientist, Chemical Engineering Division, went to UK in December 1991 to do research at the Department of Pure and Applied Chemistry, University of Strothclyde, Glasgow, under the Post Doctoral Fellowship of the European Community.

Dr. Rajiv Kumar, Scientist, Inorganic Chemistry Division, spent one year at the University of Stuttgart to work in the area of zeolite synthesis and catalysis under the Alexander von Humboldt Fellowship.

Dr.R.P. Singh, Scientist, Polymer Chemistry Division, was deputed to France for six months from January 1992 to carry out research work in the collaborative project, "Thermal and PhotoChemical Degradation and Stabilization of Polymer Blends and Alloys" under the aegis of Indo-French Center for Promotion of Advanced Research.

■ 1992 – 93

Dr.R.A. Mashelkar, Director, NCL, went to China in April 1992 to attend the meeting of the Asia-Pacific Society for Advanced Materials, at Shanghai.

Dr. Mashelkar went to Germany in June 1992 under the CSIR-DAAD Collaborative Programme; to Italy for attending the Editorial Board Meeting of Chemical Engineering Science in Turin; and to U.K. to visit Unilever Laboratories.

He visited USA in July 1992 to attend the Indo-US Joint Council Meeting on the Programme for Advancement of Commercial Technology (PACT) at Meridian Corporation, Alexandria, and to visit Exxon Research & Engineering Company, Annandale; Hoechst Celanese, Short Hills, New Jersey; Hercules Incorporated, Wilmington; Himont Research & Development, Wilmington; Monsanto Chemical Company, Springfield; Cargil Incorporated, Minneapolis; and General Electric Company, Schenectady for exploring possible collaborations with NCL.

Dr.P. Ratnasamy, Deputy Director, NCL, visited France in May 1992 to give lectures on oxidation reactions over zeolite catalysts, under the auspices of the Indo-French Centre for the Promotion of Advanced Research.

Dr. Ratnasamy also went to Canada in July 1992 to attend the 9th International Zeolite Conference in Montreal, and to Hungary to attend the 10th International Congress in Catalysis in Budapest.

Dr.P. Ganguly, Head, Physical Chemistry Division, visited Italy to participate in a meeting on superconductivity at Spring College, Trieste; France to visit University de Bordeaux, and attend the International Conference on Electronic Materials; and Germany to visit Universital at 24 Koln.

Dr. Ganguly went to Argentina to take part (and deliver lectures) in an experimental workshop on, "High Temperature Superconductors and Related Materials" at the Centro Atomico Bariloche, San Carlos de Bariloche, held in January 1993.

Dr.T. Ravindranathan, Head, Organic Chemistry: Technology Division, visited U.K. in October 1992 under the CSIR-British Council Visitorship Programme.

Dr.S. Siyasanker, Scientist, Catalysis Division, visited Hungary for three weeks in July 1992 under the INSA-Hungarian Academy of Sciences Exchange Programme.

Dr.K.N. Ganesh and Dr.G.Pandey, Scientists, Organic Chemistry: Synthesis Division, visited Korea in November 1992 to attend the INSA-KOSEF Joint Seminar on Natural Product Chemistry held at Seoul.

Dr. Ganesh also went to USA in December 1992 to work in the University of Pittsburgh, under the Indo-US S&T Fellowship offered by the DST.

Dr.P.K. Ranjekar and Dr.(Ms.)V. Gupta, Biochemical Sciences Division, went to Thailand in February 1993 to attend the annual meeting of the "International Programme on Rice Biotechnology" sponsored by the Rockefeller Foundation.

Dr.V.R. Choudhary, Scientist, Chemical Engineering Division, went to France for three months from April 92 under the IFCPAR collaborative project on, "Deactivation due to coking and regeneration of zeolite catalysts."

Dr.R.V. Chaudhari, Scientist, Chemical Engineering Division, visited Germany for six weeks in 1992 to review the progress made on the CSIR-KFA collaborative project and to work on joint publications.

Mr.R.R. Hirwani, Head, Project Planning and Development Group, went to the UK, France and the Netherlands in May 1992 under the CSIR-British Council Programme for discussions with consultants identified by NCL for the World Bankaided project on management system upgradation.

Dr.(Ms.)R.S. Nadgauda, Scientist, Plant Tissue Culture Division, went to U.K. in November 1992 to visit Wye College under the ALIS-Link Programme of the British Council on Coconut Tissue Culture.

Dr.B.B. Lohray, Scientist, Organic Chemistry: Synthesis Division, went to Germany in 1993 to take up the Alexander von Humboldt Fellowship.

1991 - 93

- Dr.R.A. Mashelkar,
 - * Some Recent Findings in the Science and Applications of Super Absorbers DuPont Experimental Research Centre, USA.
 - * Separation of Macromolecules Through Swelling, Superswelling and Shrinking Polymers Gordon Research Conference, USA.
 - * Diffusional Limitations in Polymerising Systems Eastman Kodak, USA.
 - * Some Recent Findings in the Science and Applications of Super Absorbers Texaco Inc., R&D, USA.
 - * Diffusional Limitations in Polymerising Systems University of Maryland, USA.
 - * Modelling of Industrial Processes Some Personal Experiences Exxon Research & Engineering Co., New Jersey (USA).
 - * Diffusion in Polymers Problems of Swelling Dissolution & Reversible Bilayer Membranes Hoechst Celanese Corporation, New Jersey, (USA).
 - * Superabsorbers: Science & Applications Hercules Incorporated, Research, Wilmington (USA).
 - * Dynamics of Diffusion and Mobilization in Swelling/Dissolving Polymers Himmont R&D Centre, Wilmington, DE (USA) Monsanto Chemical Co., Springfield (USA) Cargil Incorp. Central Research, Minneapolis (USA) General Electric Corporate Research & Development, Schenectady (USA).

- * Materials Research & Development: The Indian Perspective Asia Pacific Society for Advanced Materials (APSAM) Shanghai, China.
- * Some Recent Advances in the Science & Applications of Superabsorbing Polymeric Materials Asia Pacific Society for Advanced Materials (APSAM) Shanghai, China.
- * Indian Chemical Engineering 2000: New Vistas, Opportunities and Chal-Presidential Address at the 61st Annual Session of the National Academy of Sciences India in Meerut.
- * Fascination of Non-Newtonian Fluids (The second Morris Travers Memorial Lecture) Indian Institute of Science, Bangalore.
- * On Some New Explorations in the Hydrodynamics and Diffusion in Macromolecular Systems Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.
- * Emerging Challenges and Opportunities for Indian Engineering Scientists: The Post-Liberalisation Scenario Institution of Engineers (India), Bangalore, Eighth Acharya P.C.Ray Memorial Lecture.
- * Science & Technology in India in the Post-Liberalisation Era: Challenges & Opportunities American Alumni Association, Bombay.
- * R&D at NCL: The Present & the Future 'Top-20'Institutions in Pune Meet.
- * Towards Greener and Safer Chemical Technologies Seminar on Thermal Hazards of Chemical Reactions, CLRI, Madras, Keynote address.
- * India 2000 Technological Challenges College of Engineering, Pune.
- * Emerging Technological Perspectives for India in Year 2000 Shri Laxminarayan Institute of Technology, Nagpur.

- * Role of Technology in Indian Industrial Development: Perspectives for the Coming Decades Turf Club, Pune.
- ★ India 2000: The S&T Perspectives Nowrosjee Wadia College, Pune, Diamond Jubilee Celebration.
- * Environmental Pollution: New Approaches and Challenges Institution of Engineers (India), Ahmednagar Local Centre & Maharashtra pollution Control Board, Ahmednagar.
- * Changing Frontiers in Chemical Engineering CSIR Golden Jubilee celebrations at IICB, Calcutta.
- * Chemical Engineering 2000: The Indian Scenario 2nd Navnitlal Memorial Lecture at ATMA Hall, Ahmedabad.
- * Inaugural address at the Executive Meet of R&D Chiefs on at Hotel Klassic, Ahmedabad.
- * New Frontiers in R&D on Sugar By-Products held under the auspices of Mauritius Sugar Authority.

Dr.S. Rajappa

- * Nitroacetyl Group as a Novel Peptide Synthon, RRL, Trivandrum.
- * Nitroenamines SPIC Pharmaceutical Research Centre, Marai Malai Nagar, Madras.
- * Nitroacetyl Group as a Novel Peptide Synthon Indo-US Peptide Symposium at CCMB, Hyderabad.
- ★ Innovation for Industry

Recent Developments in Synthetic Organic Chemistry at Ruia College, Bombay, M.S.University, Baroda, (K.G.Naik Gold Medal Lecture) Malti-Chem Research Centre, Baroda.

Dr.P. Ganguly

- * Current Status and Future Trends in Condensed Matter Physics University of Poona, conducted by TIFR, Bombay.
- * Chemical Aspects of High-temperature Superconductors Inter-University Consortium on Neutron Spectrometer at BARC, Bombay.
- * Preparation of Nanoparticles of Inorganic Salts and Exotic Carbon Compounds Through Reaction with High-temperature Thermosetting Polymers Indian Institute of Science, Bangalore.

Dr.S. Sivaram

- * Chaired the inaugural session of the National Conference on Synthetic Membranes and their Applications, CSMCRI, Bhavnagar.
- * New Horizons in Polymer Synthesis Shivaji University Post-graduate Centre, Solapur.
- * Synthesis and Applications of Chiral Macromolecules National Symposium on Chiral Synthesis at IICT, Hyderabad as part of the CSIR Golden Jubilee celebrations.

Dr.V.M. Nadkarni

- $\star \ \textit{Processing-Structure Property Relationship in Engineering Polymers}$ at IIT, Kanpur.
- * A series of lectures on polymeric materials, characterization and processing, At UDCT, Bombay, as part of the Chemical Weekly/Raghavan Visiting Professorship in polymer science and technology.

Dr.M.C. Srinivasan

- * Biology of Actinomycetes DST-organised "Brain-storming session in the area of Microbiology" at MACS, Pune.
- * Biotechnology of Fungal Enzymes Mycological Society of India at N.I.N., Hyderabad.

■ Dr.K.V. Krishnamurthy

- * Lectures on plant tissue culture and its applications The orientation course/workshop for Academic Staff Colleges at University of Poona.
- \star Plant Tissue Culture, Theory and Practice Academic Staff College, University of Poona.
- * Gene Transfer Through Innovative Biotechnological Approaches Botany Dept., University of Poona.

Dr.S.K. Date Chemical Processing of Magnetic Ceramics, at NPL, New Delhi.

Dr.K.N. Ganesh

- * Design of Chemical Nucleases Indo-US Peptide Symposium held at CCMB, Hyderabad.
- * Artzymes: Approaches to Chemical Nucleases Indian Institute of Science, Bangalore.
- * Non-Fluorescent Detection of Nucleic Acids Workshop on PCR reaction organized by Perkin-Elmer/Labindia, in Bombay.

Dr.R.N. Sharma

- * The Utilization of Essential Oils and Some Common/Allelo-Chemic Constituents for Non-Insecticidal Pest Management Strategies The International Symposium on Newer Trends in Essential Oils and Flavours, Jammu-Tawi, 1991.
- * Biorational Prophylaxis of Guineaworm Disease by a New Natural Cyclopcide, 'GWINCIL' Workshop on Rural Drinking Water in Developing Countries, held at NGRI, Hyderabad.
- Dr.P.K. Ranjekar Characterization of Glutelin Storage Protein and Gene in an Indica Rice,

Role of Plant Biochemistry and Biotechnology in Improving Crop Productivity at IARI, New Delhi.

- Dr.A.V. Ramaswamy Catalysts in the Petroleum/Petrochemical Sector - Recent Advances Research and Consultancy Directorate of ACC, Thane.
- Dr.H.R. Sonawane Asymmetric Synthesis of Sesquiterpenes with Rhodium-Carbenoids IICT, Hyderabad.
- Dr.V.S. Patwardhan Mathematical Modelling in Petrochemical Industry Pan Commonwealth Awareness Workshop on Mathematical Modelling CLRI, Madras.
- Dr.V.R. Choudhary
 - * Design and Development of Catalyst for Oxidative Coupling of Methane to C2-Hydrocarbons International Workshop on Catalyst Design, ICS, Trieste, Italy,
 - * Oxidative Conversion of Natural Gas to Value-Added Products The International Seminar on Natural Gas Utilization, New Delhi.
 - * Compressed Natural Gas as Transportation Fuel R&D Establishment (Engineers), Dighi, Pune
- Dr.S. Devotta Energy Conservation in Chemical Industries Energy Management for Energy Conservation, at Hotel Blue Diamond, Pune.
- Dr.S.T. Kshirsagar Raman Scattering in Amorphous Silicon and Related Alloys Indo-USA Bilateral Workshop on Physical Processes in Amorphous Silicon and Related Alloys, University of Poona.
- Mr.N. Rajagopalan Some Recent Developments in Controlled Release Science and Technology "Advances in Agrochemicals" held in Madras

- Dr.(Ms.)R.S. Nadgauda Bamboo Flowering University of Poona.
- Dr.V. Shankar
 - * Fungal Nucleases DST-organized "Brain-storming session in the area of Microbiology" at MACS, Pune.
 - * Enzyme/Whole Cell Immobilization Yashwantrao Chavan Institute of Science, Satara.
- Dr.R. Tewari
 - * The Significance of the Partial and the Complete Modification of Nucleic Acid Bases in the tRNA anticodon CDRI, Lucknow
 - * Synthesis of Advanced Ceramics Nanophase Route Shivaji University, Kolhapur
- Dr.D.V. Gokhale
 - * Isolation of Yeast Strains Exhibiting Higher Ethanol Productivities and Lipolytic Activities Conference of AMI at Madurai Kamaraj University.
 - * Protoplast Technology Yashwantrao Chavan Institute of Science, Satara.
- Dr.P. Chakrabarti What do Metal Binding Sites in Proteins Tell us About Folding, Recognition and Catalysis TIFR, Bombay
- Dr.M.V. Deshpande
 - * Chitin Synthesis/Degradation and Fungal Morphogenesis DST-organized "Brain-storming session in the area of Microbiology" at MACS, Pune.

- * Industrially Important Enzymes Yashwantrao Chavan Institute of Science, Satara.
- Dr.A.H. Lachke Cellulases from Trichoderma sp. and Sclerotium rolfsii IIT, New Delhi
- Dr.V.K. Jayaraman A series of lectures on Unit Operations in Chemical Engineering, as a Visiting Scientist at the Polymer Chemistry Dept., University of Madras.
- Dr.B.M. Khan Recent Trends in Genetic Transformation of Plants University of Poona.
- Dr.S. Pal Predictive Theoretical Chemistry TIFR, Bombay.
- Dr.B.B. Lohray
 - * Synthesis and Selective Transformations of Ketosilanes IICT, Hyderabad.
 - * Catalytic Asymmetric Dihydroxylation of Alkenes and the Chemistry of Cyclic Sulfites and Sulfates N.V.Subba Rao Memorial Lecture at Osmania University.
- Dr.V.V. Ranade Turbulent Mixing in Dilute Polymer Solutions IIT, Bombay.
- Dr.P. Ghosh Biomimetic Chemistry of Copper Proteins and Enzymes Indian Institute of Science, Bangalore.
- Dr.I.I. Sutar Culture Collection: Its Function and Use in Biotechnology Yashwantrao Chavan Institute of Science, Satara.

- Mr.P.K. Chitnis Technique of RFLP for Germplasm Characterization At DBT sponsored workshop on "Techniques of in vitro conservation and cryopreservation of plant germplasm" at NBPGR,
- Mr.N.B. Dahibhate, Use of Computers in Libraries New Arts, Commerce and Science College, Ahmednagar.

PAPERS PRESENTED AT SYMPOSIA / SEMINARS / WORKSHOPS

1991 - 92

• K.V. Krishnamurthy, R.B. Naidu, A.P. Sagare, D.D. Kulkarni and D.A. Godbole, Plant protoplast technology for grain legumes, XV Annual Conference of Plant Tissue Culture Association (India) held at Bangalore, Feb.19-21, 1992.

• R.S. Singh

- * Chemical information system, 10th Annual Convention and Conference of the Society for Information Science, at RRL, Trivandrum, from 17th to 19th January 1991.
- * Chemical reactions information system, The Regional Seminar on Chemical Information at Beijing, China, on 30.8.91.
- * 36th All-India Library Conference held at the University of Jodhpur 26 -29 December 1991.
- * Role of NICHEM/NISSAT in networking of libraries and information centres, one day seminar on "Networking of Libraries and Information Centres", at MACS, Pune, on 12th November 1991.
- . M.B. Patil. Development of bibliographic database on Indian chemical patents at NCL, Pune: A Case Study, by M.B.Patil and R.S.Singh. at Dr.I.N.Sengupta National Festschrift Seminar on, "Bibliometrics and Information Handling" at Indian In-

Technology Meeting at Calcutta on 4-6 Sept.1991.

stitute of Chemical Biology, Calcutta, 29 - 30 April 1991. • A.V. Ramaswamy and S. Sivasanker, Catalytic dewaxing for production of lubes and speciality oils, 6th Refinery

- · S. Devotta, Alternatives to CFC-12 for refrigeration - Needs of the developing countries, International workshop on, "Technology Transfer to Eliminate Ozone Depleting Chemicals" at the US National Academy of Engineers, Irvine, California, from 22nd to 25th April 1991.
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- · G.T. Panse.
 - * Stereoselective microbial conversion of isobutyric acid (IBA) to D- and Lhydroxybutyric acid (β-HIBA), International Symposium 1992 (IUPAC-NOST) on, "Enzymes in Organic Synthesis", 6-9 Jan.1992.
 - * Selected medicinal plants for cultivation and drug development: Swadeshi approach, National Workshop on, "Promotion of Non-wood Forest Produce through Social Forestry", Vaikunth Mehta National Institute of Cooperative Management, Pune, 8-11 March 1992. (Organised by BAIF, Pune.)
- T.P. Prakash, R. Krishna Kumar and K.N. Ganesh,
 - * Low temperature catalytic oxidative conversion of methane, Discussion Meeting on, "From Heterogeneous to Homogeneous Catalysis", IISc., Bangalore, Jan.27-29, 1992.
 - * Molecular recognition in aqueous media: Nucleosidyl phosphate complexation by amines, 4th National Symposium on Bio-organic Chemistry, at BARC, Bombay, 27-29 Jan. 1992.
- A.Y. Houde, B.B. Idage, S.S. Kulkarni and M.G. Kulkarni, Effect of ester and ether linkages on sorption and transport properties of polysulfones, Eighth Polymer Processing Society Annual Meeting, New Delhi, March 24-27 1992.

- A. Raj, K.R. Reddy and R. Kumar, Catalytic properties of some ferrisilicate medium-pore zeolites in toluene methylation and m-xylene isomerization, 10th Int. Cong. on Catal., Budapest, Hungary, July 1992.
- V.M. Chauthaiwale and V.V. Deshpande, Molecular cloning and expression of Chainia DNA sequences involved in transcription initiation in E. coli, DAE Symposium on, "Molecular Biology of Microorganisms", NCL, Pune, 28–30 Jan.1992.
- M.S. Ghatge and V.V. Deshpande,
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- A. Shendye and M. Rao,

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 Biology of Microorganisms", NCL, Pune, 28–30 Jan.1992.
- J. Chauthaiwale and M. Rao, Extracellular production of xylose (glucose) isomerase by alkalophilic and thermophilic Bacillus, DAE Symposium on, "Molecular Biology of Microorganisms", NCL, Pune, 28–30 Jan.1992.
- S. Gite, G. Reddy and V. Shankar,
 - * Active site characterization of Si nuclease: I. Affinity purification and influence of Amino group modification, DAE symposium on, "Molecular Biology of Microorganisms", NCL, Pune, Jan. 28 30, 1992.
 - * Nuclease from Rhizopus stolonifer: Medium optimization and properties of partially purified enzyme, DAE symposium on molecular biology of Microorganisms, NCL, Pune, Jan. 28 30, 1992.
- V. Gupta, Characterization of seed storage protein genes in rice with special reference to glutelin, CSIR – TAB sponsored brain storming session on Molecular Biology and genetic engineering, New Delhi, Mar.11–13, 1992.

· A.N. Kotasthane

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- D.S. Hebbalkar and R.N. Sharma,
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- R. Tewari,
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- P. Chakrabarti,
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- S. Hazra, Somatic embryogenesis in groundnut, XV Annual Conference of Plant Tissue Culture Association (India) held at Bangalore, Feb.19–21, 1992.
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- K.B. Bastawde, S.G. Patil and D.V. Gokhale, Production of xylan degrading enzymes by a novel yeast strain, National Symposium on Yeast Biology, Hissar, Feb.20-21, 1992.
- S. Radhakrishnan and Roy Joseph, Structure development in fluoropolymer composites processed by powder metallurgical technique, Polymer Processing Society Conference, PPS-8, New Delhi, 1992.

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- · S. Siyaram and G. Satyanarayana, Novel soluble magnesium-titanium catalysts for ethylene polymerization, American Chemical Society Meeting, Washington D.C., U.S.A., Aug.21-24, 1992,
- S. Sivasanker, A. Thangaraj, R.A. Abdulla and P. Ratnasamy, Shape selective alkylation of benzene with long chain alkenes over zeolites, 10th International Congress on Catalysis, Budapest, Hungary, July 19-24, 1992.
- · P.K. Ranjekar,
 - * Architecture of an eukaryotic genome, DBT sponsored training workshop on Development and use of RFLPs in plant biotechnology, NCL, Pune, Dec. 2 - 23,1992.
 - * Genetic Engineering: Cloning of genes, DBT sponsored training workshop on Development and use of RFLPs in plant biotechnology, NCL, Pune, Dec. 2 - 23,1992.
- S. Ernst, R. Kumar and J. Weitkamp, Hydrothermal transformation of zeolite ZSM-39 into ZSM-23, 9th Intl. Zeolite Conf., Montreal, Canada, FP-43, 1992.

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- R. Kumar, K.R. Reddy, A. Raj and P. Ratnasamy, Synthesis and characterization of a new high silica molecular sieve, NCL-1, 9th Intl. Zeolite Conf., Montreal, Canada P.A-6, 1992.
- M.C. Srinivasan and M.V. Rele, Screening for cellulase-free xylanases from naturally occurring microbial strains from Indian soils for paper industry applications, Fifth International Conference on Biotechnology in Pulp and Paper Industry, Kyoto, Japan, 27-30 May 1992.
- · V.R. Choudhary,
 - * Conversion of natural gas into liquid fuels, Intl. Symposium on Oil and Gas Refining, Transportation and Utilization, Bombay, Oct.17, 1992.
 - * Design and development of catalyst for oxidative coupling of methane to C2-hydrocarbons, Intl. workshop on Catalyst Design, ICS, Trieste, Italy, Nov.10-14, 1992.
- S.D. Prasad, Information theory approach to site energy distribution with adsorbate interactions, International Symposium on Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids, Kazimiers Dolny, Poland, July 12-19, 1992.
- A. Raj, J.S. Reddy and R. Kumar, Catalytic properties of Al-, Ga- and Fe-silicate with MEL structure in C₇ and C₈ aromatic reactions, 9th Intl. Zeolite Conf. Montreal, Canada, 1992.
- V.S. Gupta, R.R. Hendre, P.K. Ranjekar, Use of tissue culture and RFLP technology in selective rice breeding, 2nd Annual meeting on Rice Biotechnology, Hyderabad, November, 18-19, 1992.
- S. Gite and V. Shankar, Characterization of S1 nucleases: Involvement of carboxylate groups in metal binding, 61 Annual General Body Meeting of the Society of Biological Chemists, Hyderabad, December 1992.

- J.M. Kher, M. Gujar, and M.I. Khan, Isolation and screening of thermophilic microorganisms for use in MEOR, 61 Annual General Body Meeting of Society of Biological Chemists, Hyderabad, India, December 1992.
- V.V. Ranade, Numerical simulation of flow in bubble column reactors, AIChE Conference, Miami, Nov. 1992.
- · V. Gupta, Introduction to RFLP technology in plant breeding, DBT sponsored training workshop on Development and Use of RFLPs in Plant Biotechnology, NCL, Pune, Dec. 2 - 23,1992.
- R.R. Hendre, Nutrition and plant tissue culture, DBT sponsored training workshop on Development and use of RFLPs in plant biotechnology, NCL, Pune, Dec. 2 -23,1992.
- · Nirmala Sahasrabudhe, The GUS reporter system as a tool to study plant gene expression, DBT sponsored training workshop on Development and Use of RFLPs in Plant Biotechnology, NCL, Pune, Dec. 2 - 23,1992.
- M.B. Sabne, Role of PVC in construction industry, National Seminar on Use of Polymers in Construction, Pune, Dec.5-6 1992.

MEMBERSHIP OF COMMITTEES

1991 - 93

- 1. Dr.R.A. Mashelkar
- Chairman Scientific Advisory Committee for Petrochemicals in Department of Chemicals & Petrochemicals (Ministry of Petroleum & Chemicals).
- Chairman Committee to look at reforms in higher education appointed by the Governor of Maharashtra.
- Chairman Expert Committee on Downstream Processing, Department of Biotechnology.
- Chairman Plasto '93.
- Chairman Awards Committee on Parallel Processing, Centre for Development of Advanced Computing (C-DAC), Pune.
- Chairman Grasim Industries Award for Applied Research & Development (BATRA).
- President Maharashtra Academy of Sciences.
- Member Research Advisory Council - Rajiv Gandhi Institute for Contemporary Studies under the Rajiv Gandhi Foundation.
- Member Advisory Committee constituted by the Director General -Technical Development for planning a suitable strategy in the area of technology evaluation.

- J.M. Kher, M. Gujar, and M.I. Khan, Isolation and screening of thermophilic microorganisms for use in MEOR, 61 Annual General Body Meeting of Society of Biological Chemists, Hyderabad, India, December 1992.
- V.V. Ranade, Numerical simulation of flow in bubble column reactors, AIChE Conference, Miami, Nov. 1992.
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- R.R. Hendre, Nutrition and plant tissue culture, DBT sponsored training workshop on Development and use of RFLPs in plant biotechnology, NCL, Pune, Dec. 2 -23,1992.
- Nirmala Sahasrabudhe, The GUS reporter system as a tool to study plant gene expression, DBT sponsored training workshop on Development and Use of RFLPs in Plant Biotechnology, NCL, Pune, Dec. 2 – 23,1992.
- · M.B. Sabne. Role of PVC in construction industry, National Seminar on Use of Polymers in Construction, Pune, Dec.5-6 1992.

MEMBERSHIP OF COMMITTEES

■ 1991 - 93

1. Dr.R.A. Mashelkar

- Chairman Scientific Advisory Committee for Petrochemicals in Department of Chemicals & Petrochemicals (Ministry of Petroleum & Chemicals).
- Chairman Committee to look at reforms in higher education appointed by the Governor of Maharashtra.
- Chairman Expert Committee on Downstream Processing, Department of Biotechnology.
- Chairman Plasto '93.
- Chairman Awards Committee on Parallel Processing, Centre for Development of Advanced Computing (C-DAC), Pune.
- Chairman Grasim Industries Award for Applied Research & Development (BATRA).
- President Maharashtra Academy of Sciences.
- Member Research Advisory Council - Rajiv Gandhi Institute for Contemporary Studies under the Rajiv Gandhi Foundation.
- Member Advisory Committee constituted by the Director General -Technical Development for planning a suitable strategy in the area of technology evaluation.

- Member
 Scientific Advisory Committee to the Department of Biotechnology.
- Member
 Programme for the Advancement of Commercial Technology (PACT): Indo-US
 Joint Council.
- Member
 Irdia-China Sub-Committee on S&T Cooperation, Government of India.
- Member
 Indo-German Consultative Group, Government of India.
- Member
 Board of Governors, Birla Research Institute for Applied Sciences, Nagda.
- Member
 Governing Body-Agharkar Research Institute, Pune.
- Member Governing Council of C-DAC, Pune.
- Member Governing Council-Dr.Reddy's Research Foundation (Standard Research Centre).
- Member
 Academic Council, University of Poona (Chancellor's Nominee).
- Member Academic Council of Goa University.
- Member
 Board of Management, Yashwantrao Chavan Maharashtra Open University,
 Nashik.
- Member
 Advisory Committee, Bharatiya Vidya Bhavan.
- Member Governing Body of Chemical Park (Jawaharlal Nehru Entrepreneurs' Chemical Park).

Member

Programme Advisory Committee on Chemical Engineering Science, DST.

- Member
 Science & Engineering Research Council, DST.
- Member
 Board of Awards for Import Substitution & Technology Development (DGTD).
- Member
 Standing Committee for Emeritus Scientist Scheme, CSIR.
- Member
 Physical & Chemical Sciences Research Committee for Sponsored Projects, CSIR.
- Member
 Sectional Committee for Engineering & Technology Indian Academy of Sciences.
- Senior Associate
 National Institute of Advanced Studies (IISc, Bangalore).
- Member ICMA Awards Selection Committee.
- Member Indian council as member of the Programme for the Advancement of Commercial Technology (PACT) managed by Industrial Credit and Investment Corporation of India (ICICI) Ltd.
- Member
 Steering Committee on Micro-level Planning for Pune District (BAIF).
- Honorary Professor
 Jawaharlal Nehru Centre for Advanced Scientific Research Bangalore.
- Editor Chemical Engineering Science.
- Editor
 Chemical Engineering Communications.

Editor

Journal of Non-Newtonian Fluid Mechanics.

- Editor Rheologica Acta.
- Member Editorial Advisory Board, Chemical Industry News.
- Member Editorial Board for the Proceedings of INSA, Part A, Physical Sciences, New Delhi.
- Member Editorial Board, Defence Science Journal.
- Member Working Committee of the Current Science Association Bangalore.
- 2. Dr. Paul Ratnasamy
- Member Scientific Advisory Committee, Ministry of Petroleum and Natural Gas, Government of India, New Delhi.
- Member Advisory Committee, BSC-I (BRNS), BARC, Bombay.
- Member Research Advisory Committee, Associated Cement Companies Ltd., Bombay.
- Research Council, Indian Institute of Petroleum Dehra Dun.
- Council Member International Zeolite Association Germany.
- Member Editorial Board, ZEOLITES, Butterworths, USA.
- Member Editorial Board, Zeitschrift fur Physikalische Chemie, Leipzig, Germany.

3. Dr.J. Barnabas

- Member Reconstituted SERC (1991-94).
- 4. Dr.S. Rajappa
- Member Sectional Committee-III, INSA, New Delhi.
- Member Sectional Committee-III, IAS, Bangalore.
- Member Programme Advisory Committee (Organic Chemistry), DST, New Delhi.
- Member Evaluation Committee: National Awards for R&D Efforts, DST, New Delhi.
- Member Editorial Board, Indian Journal of Chemistry, Section B.
- 5. Dr.S. Sivaram
- Member Research Council of CLRI, Madras.
- Member Technology Advisory Board of the CSIR.
- Member Programme Advisory Committee in Organic Chemistry, SERC, DST, New Delhi.
- Member Editorial Board of the Indian Journal of Fibre and Textile Research.
- 6. Dr.G.R. Venkitakrishnan
- Member Research Advisory Council, Guiarat State Fertilizer Corporation, Vadodara.

- Member By-Products Committee, Deccan Sugar Technologists Association, Pune.
- 7. Dr.V.M. Nadkarni
- Member Editorial Board of Indian Journal of Technology.
- Member Editorial Board of Popular Plastics & Packaging.
- 8. Dr.S.K. Date
- Member Editorial Board of Indian Journal of Chemistry, Section A.
- 9. Dr.S. Sivasanker
- Member Indigenous Technology Evaluation Group on Catalysis and Related Products constituted by DGTD, New Delhi.
- 10. Dr.V.R. Choudhary
 - Member Research Advisory Committee for R&D (Catalysis), of Projects & Development India Ltd., Sindri.
- 11. Dr. Sourav Pal
 - National Representative World Association of Theoretical Organic Chemists (WATOC).
 - Life member The Society for Scientific Values, New Delhi.
- 12. Dr.R. Tewari
- Member World Association of Theoretical Organic Chemists.

13. Mr.R.S. Chaudhari

- Member Institution of Electronics and Telecommunication Engineers, New Delhi.
- 14. Dr.(Ms)A. Pant
 - Member JGOFS (India) Steering Committee, CSIR Antarctic Research Steering Committee.
- 15. Dr.P.P. Moghe
- Adviser/Consultant For the investigation of cattle mortality and human morbidity in some villages in Thane District and in Dahanu Taluka District.
- 16. Dr.B.B. Idage
- Co-opted Member Board of Studies in Chemistry, Marathwada University, Aurangabad.

STAFF MEMBERS, RESEARCH RELLOWS, AND GUEST WORKERS WHO RECEIVED Ph.D DEGREES

(The names of the research guides are given in the brackets)

1991 - 92

- 1. Ms. Ahuja, J.R. University of Poona Synthesis of some optically active sesquiterpenes and α -arylpropanoic acid (Dr.H.R. Sonawane)
- 2. Bahulekar, R.V. University of Poona Studies in polyethyleneimine: Matrix polymerization and enzyme immobilization (Dr.N.R. Ayyangar, Dr.S. Ponratnam)
- 3. Ms. Belhekar, A.A. Shivaji University Coformational and hydrogen bonding behaviour of complex molecules (Dr.C.I. Jose)
- 4. Bhide, S.R. University of Poona Studies in application of high-performance liquid chromatography (Dr.N.R. Ayyangar)
- 5. Chaudhari, S.K. Shivaji University Thermodynamic properties of binary liquid mixtures (Dr.S.S. Katti)
- 6. Daniel, T. Shivaji University Novel organic intermediate and reactions (Dr.N.R. Ayyangar)
- 7. Ms. Gopalakrishnan, V. University of Poona Chemical synthesis and structural studies of 3'-5' and 2'-5' oligoribonucleotides (Dr.K.N. Ganesh)
- 8. Houde, A.Y. University of Poona Sorption and transport in polymers (Dr.M.G. Kulkarni)

- 9. Jagtap, S.B. University of Poona Studies in fluid solid reactions (Dr.A.N. Gokarn)
- 10. Ms.Kamble, K.R. University of Poona Synthesis, characterization and catalytic reactions over metal phosphate molecular sieves (Dr.Paul Ratnasamy)
- 11. Kaulgud, R.A. University of Poona Sucrose esters as surfactants form renewable resources (Dr.H.R. Sonawane)
- 12. Keskar, S.S. University of Poona Studies on actinomycete xylanase (Dr.M.C. Srinivasan)
- 13. Ms.Khale, A. University of Poona Dimorphism in fungi (Dr.M.C. Srinivasan)
- 14. Ms. Mayadevi, S. University of Poona Adsorption and mass transfer in solid catalysts and adsorbents (Dr. V.R. Choudhary)
- 15. Muralidharan, E.M. University of Poona Biochemical studies in plant tissue culture (Dr.A.F. Mascarenhas)
- 16. Ms.Pore, V.S. University of Poona Studies directed towards the synthesis of brassinosteroids and chloramphenicol (Dr.B.G. Hazra)
- 17. Ms. Sanas, C.A. University of Poona Study of biologically active compounds by HPLC (Dr. V.H. Deshpande)
- 18. Sunil Madhav Kher University of Poona Synthetic studies in biologically active compounds (Dr.G.H. Kulkarni)
- 19. Ms. Sunita Sanjay Sawant University of Poona Studies in terpenoids (Dr.N.R. Ayyangar)
- 20. Thangaraj, A. University of Poona Synthesis, characterization and catalytic properties of titanium silicate molecular sieves (Dr. Paul Ratnasamy)

- 21. Waghamare, K.J. University of Poona Studies on petroleum refining catalysts containing pentasil zeolite (*Dr. Paul Ratnasamy*)
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- 1. Ms.Archana Sharma University of Poona Modelling biological systems: A fractal approach (Dr.B.D. Kulkarni)
- 2. Avadhani, C.V. University of Poona
 Synthesis of diisocyanates, polyurethanes and thermally stable polymers
 (Dr.S.P. Vernekar)
- 3. Ms.Biswas, S.S. Shivaji University
 Studies in chromatography: GLC and TLC FID (Dr.N.R. Ayyangar)
- 4. Chauthaiwale, V.M. University of Poona Molecular aspects of Chainia (Dr.(Ms). V.V. Deshpande)
- 5. Deshpande, S.R. University of Poona
 Synthetic studies in bioactive nitrogen, oxygen and sulphur hetrocycles
 (Dr.R.B. Mitra)
- Idage, S.B. University of Poona
 Synthesis and characterization of polymers containing (I) arylene sulfone and (II) aromatic azomethine linkages (Dr.S.P. Vernekar)
- 7. Kelkar, H.S. University of Poona Studies on pullulan hydrolyzing activity from Sclerotium rolfsii (Dr.M.V. Deshpande)
- Malshe, A.P. University of Poona
 Pulsed laser induced surface synthesis and deposition of some special coatings (Dr.S.T. Kshirsagar)
- Ms.Maybhate, S.P. University of Poona Studies on synthesis and reactivity of carbonimidodithioc acid esters (Dr.S. Rajappa)

- 10. Mukherjee, S.N. Shivaji University
 Studies on some biological effects of Azadirachtin on Tribolium castaneum, Achaea janata and Spodoptera litura (Dr.R.N. Sharma)
- Palnitkar, S.S. University of Poona Microbiology and biochemistry of D-xylose fermentation by Candida shehatae (Dr.A.H. Lachke)
- Ms.Prabhune, A.A. University of Poona
 Microbial enzymes: Studies on penicillin acylase from Escherichia coli (Dr.(Ms)
 H. Sivaraman)
- 13. Rane, V.H. University of Poona
 Preparation, characterization and evaluation of basic solid catalysts for direct
 conversion of methane to higher hydrocarbons (Dr. V.R. Choudhary)
- Rode, C.V. University of Poona Studies in multiphase reactors (Dr.R.V. Chaudhari)
- 15. Shukla, P.G. University of Poona Studies on encapsulation with starch derivatives (*Dr.S. Sivaram*)
- 16. Ms. Tambe, A.S. Shivaji University Studies in chromatography (*Dr.N.R. Ayyangar*)
- 17. Vyas, P.R. University of Poona Studies on chitinolytic enzymes (*Dr.M.V. Deshpande*)

SEMINARS, WORKSHOPS, SPECIAL TRAINING COURSES, ETC. ORGANISED BY/AT NCL

The XI Annual Convention and Conference, organized by the Society for Information Science, was held at NCL on 21-22 January 1992. The valedictory address was delivered by Mr.N.Vittal, Secretary, Department of Electronics, Government of India.

A symposium on, "Molecular Biology of Microorganisms", jointly organized by Basic Sciences Committee-II and the Department of Atomic Energy, was held at NCL on 28-30 January 1992.

Dr.S. Sivaram, Head, Polymer Chemistry Division, conducted a seminar-cumdiscussion programme for senior executives of TELCO on, "Emerging trends in polymer materials and their applications" at the Tata Management Training Centre, Pune, on 16.4.92.

SPECIAL EVENTS

CSIR GOLDEN JUBILEE AND FOUNDATION DAY AT NCL

NCL celebrated the CSIR Foundation Day on 26 September 1991. Mementoes were given to members of staff who had retired during the past year and to those who had completed 30 years of service in CSIR. The most important feature of the celebrations was the popular science lecture by Dr.J.V. Narlikar, Director, Inter-University Centre for Astronomy and Astrophysics (IUCAA), Pune, on the latest findings in astronomy.

NCL celebrated the concluding session of CSIR Golden Jubilee and Foundation Day on 25 and 26 September 1992. Open days were organized on both the days to highlight NCL's achievements and current activities. The open days on both days drew an overwhelming response from the general public. On 26 October 1992, Hon'ble C. Subramaniam, Governor of Maharashtra, was the Chief Guest.

A cover of special philatelic value to stamp collectors, commemorating the CSIR Golden Jubilee, released in New Delhi on same day by the President of India, was formally presented to the Chief Guest by Shri K.R. Rambhad the Postmaster General, Pune Circle.

NCL celebrated the National Science Day on 28 February 1991 and 28 February 1992. On 28 February 1991, the guest speaker was Prof. Govind Swarup, Director, GMRT Project, Pune, who spoke on "The Radio Universe." The highlight of the celebration on 28 February 1992 was a lecture on, "The Present Crisis and Policy Options" by Prof.V.M. Dandekar, President of the Council of the Indian School of Political Economy.

A one-day National Seminar on, "Plant Growth Regulators in Indian Agriculture and Horticulture - Present Status and Prospects" was held at the NCL on 27.11.91. The participants included chemists, agriculturists, horticulturists, botanists and scientists of related disciplines from all over India. A monograph highlighting NCL's achievements in plant chemistry from 1967 to 1987 was released during the inauguration.

Dr. Mashelkar inaugurated the Hindi Day on 16 September 1991. Dr. Sridhar Sohoni, Vice Chancellor, Tilak Maharashtra Vidyapeeth and noted Sanskrit scholar, was the Chief Guest. Dr. Sohoni released the "NCL Alok", the Hindi journal published for the first time by the laboratory.

Two CSIR-UGC Eligibility Tests were conducted during 1991 (30.6.91 and 29.12.91) at NCL for the award of Junior Research Fellowships and recruitment as lecturers in science, engineering and mathematics. The examinations were organized and conducted by Mr.S. Chidambaram, Scientist, Process Development Division and his team.

The National Safety Day was celebrated at NCL on 4 March 1993. Mr.J.N. Sharma, Sr. Safety Manager, IPCL, Baroda, was the Chief Guest. Prizes were distributed for the Best Slogan, Best Cartoons and the Best Suggestions on Safety.

NCL FOUNDATION DAY 1992, 1993

1992

NCL celebrated its Foundation Day-1992 on 3 January 1992. This was the first celebration of the Foundation Day at the laboratory, which was founded on this day in 1950. Dr.R.A. Mashelkar, Director, welcomed the Chief Guest and the Foundation Day Speaker, and announced the formation of NCL Research Foundation. He said that its central aim was to foster excellence in research at NCL, and recognize unusual initiatives taken by its researchers and supporting staff to take NCL to new heights of achievement. He added that, in the light of new economic, industrial and fiscal policies announced by the Government, recognition of meritorious performance with awards had become very important.

Mr.K. Ramakrishnan of the Catalysis Division, was the only winner of the award, for designing a single-tube reactor and operating it within a record time of two weeks. This enabled the loading of NCL's catalyst for testing in the industrial reactor of the client, Cibatul.

Prof.M.M. Sharma FRS, Director, University Department of Chemical Technology, Bombay, was the Chief Guest. He hoped that the awards instituted under the NCL Research Foundation would act as a spur for the scientists to develop globally-competitive technologies.

Prof.Brian A. Thrush, Head, Department of Chemistry, University of Cambridge, UK, was the Foundation Day Speaker. In his lecture he dealt with the depletion of the tenuous ozone layer in stratosphere that protects the Earth from harmful ultraviolet radiation, caused by chlorofluorocarbons and other chemicals produced by human activity. The concentrations of ozone in the column of air over Antarctica have sharply declined in recent years. This led to Montreal Protocol of 1987 aimed at a global understanding to limit the release of halocarbons. The increased awareness of the problem and the concern over its solution have already generated a very useful pool of scientific knowledge, he added.

1993

NCL celebrated the Foundation Day-1993 on 3 January 1993. Dr.A.S. Ganguly, Director, Unilever, UK, delivered the Foundation Day Lecture. Dr.R.A. Mashelkar, Director, NCL, welcomed the guests.

In his lecture Dr. Ganguly said that nothing short of a revolution can raise R&D in India to international standards. Acceptance of the fact that a sound understanding of basic science is critical for the success of the industry is vital to make this dream come true. He suggested the formation of a think-tank for evolving the country's S&T policy for the 21st century, a policy that should blend in itself not only the needs of science and industry, but also the country's economic plans.

Referring to the need for globalization, he said that it can be achieved only by forming alliances with agencies in the country and with international ones. In doing so, international covenants must be respected and adhered to. Touching upon the ever-shrinking federal support to science, he said that R&D institutions should work out a strategy for finding alternative sources of funds within and outside the country. He paid rich tributes to Pune's hoary int llectual tradition.

He gave away awards to individuals and groups of NCL for new initiatives taken, and for offbeat and original contributions.

Dr.S.H. Iqbal, Head, Division of Technical Services, proposed a vote of thanks. The following were the Foundation Day award winners:

- Scientist of the Year Award 1992 Dr.B.D. Kulkarni
- Technology of the Year Award 1992 (Encilium Technology) Dr.G.R. Venkitakrishnan, Mr.S. Nene, Mr.V.V. Jogdand, Mr.G.M. Chaphekar, Mr.B.A. Baliga, Mr.H.S. Jagtap, Mr.S.H. Vaidya, Mr.K.R. Bhinge, Mr.B.G. Gaikawd, and Mr.M.L. Kaul
- Highest Industrial Earning Award Division of Organic Chemistry:Synthesis, headed by Dr.S. Rajappa
- Individual Merit Award Mr.P. Venugopal, Mr.G. Prabhakaran, Mr.K. Radhakrishnan Mr.K.B. Kadam Mr.G. Mathew, Mr.S.M. Joshi, Mrs.M.M. Kenkre Mr.N.N. Palnitkar Mr.R.M. Pawar Mr.P. Joseph

LECTURES DELIVERED BY SCIENTISTS VISITING THE LABORATORY

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• Composite sample techniques for the classification of samples as to presence or absence of pollution (Trait)

Prof.M.T. Bosswell

Dept. of Statistics Pennsylvania state University, USA.

■ Genesis and maintenance of transbilayer phospholipid asymmetry in biological membranes

Liposomes as vehicles in drug targeting

Dr.C.M. Gupta

Head, Division of Membrane Biology

Central Drug Research Institute, Lucknow.

• Interface stability in semiconductor structures

Prof. Krishna Rajan

Materials Engineering Dept.,

Rensselaer Polytechnic Institute, USA.

• Influence of field gradients on the selectivity in cracking reactions over zeolites Basicity of zeolites and new selectivity

Prof.Denise Barthomeuf

Universite Pierre et Marie Curie, France.

■ Contemporary chiral chromatography (HPLC)

Dr. John Lough

School of Pharmaceutical and Chemical Sciences,

Sunderland Polytechnic, U.K.

■ The 3D structure of dehalogenase: An enzyme that degrades 1,2 dichloroethane Dr.B.W. Dijkstra

Lab. of. Chem. Physics, University of Groningen Netherlands.

- Research on pollution prevention and hazardous wastes treatment Dr. Subhas K. Sikdar Director, Water & Hazardous Wastes Treatment Research Division, United States Environment Protection Agency, U.S.A.
- Ion beam effects on oxide films Dr.S. Mohan Instrumentation and Servicing Unit, I,I,Sc., Bangalore.
- Carbohydrate transport to microorganisms Prof. John Villadsen Dept. of Biotechnology Institutet for Bioteknologi, Denmark.
- Alkylbenzenes ammoxidation over alumina-supported V-Sb-Bi-oxide catalyst : Reaction mechanism and control of catalytic activity Oxidative coupling of methane over Bi₂O₃-M_xO_y catalysts Prof. Eduard Mamedov Head, Lab. for Studies of Catalytic Reaction Mechanisms Azerbaijan Republic.
- Phosphatidyl inositol analogues: Synthesis and application Dr.M.S. Shashidar Dept. of Org. Chem., IISC, Bangalore.
- Thyroid disorders and Cu, Zn metabolism Prof.G.B.V. Subramanian Dept. of Chemistry, University of Delhi.
- Studies on intact EYE lens and its proteins-crystallins Prof.D. Balasubramanian CCMB, Hyderabad.

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CSIR Distinguished Lecture 1992

- Prof. Charles Townes, Nobel Laureate, delivered the CSIR Distinguished Lecture at NCL on 13 February 1992. He spoke on, "What is happening at the centre of our galaxy".
- Prof. Townes's lecture dealt with the latest findings made by cosmologists with new instruments like satellite-borne telescopes. The findings about our galaxy, the Milky Way, pointed to the strong possibility of the existence of a black hole at the centre.
- Globalization of science: A perspective from the south Mr. Subbiah Arunachalam Science writer and information analyst.
- Radial flow chromatography Mr. Shirish Joshi Sepragen Corp., USA.
- A general concept of catalysts in air pollution control Dr.S. Bhargava Royal Melbourne Institute of Technology, Australia.
- Preparative chromatography in downstream bioprocessing Dr. Guhan Jayaraman.
- Non-equilibrium thermodynamics in biological processes Separation of proteins by preparative electrophoresis Dr. Sunil Nath, Indian Institute of Technology.
- Potential of zeolites in the synthesis of fine and intermediate chemicals Prof. Wolfgang Holderich Institute for Chemical Engineering and Heterogeneous Catalysis, Aachen, Germany.

 Hydrogenation of adiponitrile catalyzed by Raney nickel in slurry reactors Selectivity and conversion in industrial processes using homogeneous transition metal catalysts

Dr. Jean F. Jenck Head, UMR 45, Rhone Poulenc Industrialization, Devines, France.

■ The design and synthesis of novel trypnocidal and leishmanicidal drugs Prof. Malcolm Hooper Director, Tropical Diseases Chemotherapy Research Unit, Sunderland University, U.K.

 Palladium based catalytic membranes Basicity in alkali exchanged zeolites: an IR and XPS study of chemisorbed pyrrole

A multitechnique study of the environment of Ti in TS-2

Prof.S. Kaliaguine

Dept. of Chemical Engineering, University of Laval, Canada.

■ Molecular recognition: Directed hydrogen bonding in the design of catalytic and self-assembling structures

Prof. Andrew Hamilton Dept. of Chemistry,

University of Pittsburgh, Pittsburgh.

■ Ultrafiltration - Technical consideration Mr. David Chainav International Sales Manager, AMICON Inc., USA

SERVICES RENDERED TO INDUSTRY, RESEARCH INSTITUTES, UNIVERSITIES ETC.

The laboratory has been extending its assistance, whenever possible, to industry, R&D units, educational institutes and project engineering organizations. This is briefly described below.

CONTRACT RESEARCH

The laboratory welcomes contract research work if it fits into the following general criteria.

The proposed work is within the scope of the present areas of activity of the NCL and the laboratory has the necessary facilities and expertise to carry out the work, subject to consideration of internal workload.

There is an innovative R&D content in the proposed work. The technology to be developed/application of R&D results will have sufficient socioeconomic impact after completion.

The technology to be developed is not repetitive and is not already established indigenously.

The project is of a kind that only a few parties can implement.

Technologies of wider interest and having possibilities of multi-client sale are developed by the laboratory on its own.

The contract research covers following type of projects:

SPONSORED PROJECTS

Projects having specified R&D objectives, and well defined expected project output/results, generally culminating in generation of intellectual property and completely executed at laboratory, are taken up as sponsored projects.

COLLABORATIVE PROJECTS

Whenever possible and desirable, the laboratory collaborates with industry on industrially important projects that are engineering intensive and involve development of complex technologies with high investment risk. In such cases, laboratory looks for complementary facilities and expertise with the industrial partners. As in sponsored projects, the expected project output/results are well defined.

The sponsored and collaborative projects are full funded by the clients.

■ GRANT-IN-AID PROJECTS

The laboratory seeks or requests for grant—in—aid assistance/facility from scientific departments/agencies or international bodies for supporting basic or exploratory research, or for establishing and maintaining major R&D and infrastructural facilities. These projects are undertaken with a view to supplementing the laboratory's efforts in ongoing or new R&D projects or for creating new capabilities.

■ CONSULTANCY SERVICES

Over the years, NCL has built a rich reservoir of expertise in the different branches of chemistry, chemical technology and chemical engineering. About a decade ago, the laboratory decided to offer this expertise to industry on consultancy basis. This service to industry has worked out so well in practice that industry now places a high value on NCL's ability to offer expert advice on many critical problems confronted by it. NCL offers, all under one roof, advisory consultancy in the following areas:

- O Process simulation, optimization and energy conservation
- Process improvements and modernization studies
- Process design and engineering
- Research and technology management planning, development application and market development
- Technology search, evaluation and selection
- Analytical and other technical services

NCL has been offering consultancy services to agencies within and outside India. NCL's clientele abroad includes Du Pont, Eastman Kodak, Rohm and Haas, Toyobo, Toray, Occidental, etc. Among the Indian companies to which NCL has acted as a consultant are: Indian Petrochemicals Corporation Ltd., Macneil & Magore Ltd., Hindustan Lever Ltd., Century Enka Ltd., Hindustan Development Corporation Ltd., Kores (India) Ltd., Diamines & Chemicals Ltd., Hico Products Ltd., Hindustan Antibiotics Ltd., and others.

■ TECHNICAL SERVICES

Technical services comprising of testing and analysis, training, technical assistance of an advisory nature, fabrication/production of special products, repair and maintenance, supply of information etc. are offered to industry on ad-hoc basis on payment of fees.

CONSULTANCIES DURING THE PERIOD FROM 1991 TO 1993

CLIENT		TITLE
A Plus Projects & Technology	-	Design & commissioning of nitration reactor
Adarsh Chemicals & Fertilizers Limited, Surat	-	Application of maleic anhydride in down stream products Improvement of DL-malic acid process
Alchemie Research Centre, Thana	_	Use of computer for quantum mechanical calculations
Alkyl Amines Chemicals Ltd., New Bombay	-	Characterization and optimization and use of catalysts
Armour Chemicals Ltd.,	=	Manufacturing operations
Arochem Silvassa Ltd., Silvassa	_	Energy audit of LAB sulphonation plant
Bajaj Auto Ltd., Akurdi	_	Two / three wheelers

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Bakul Chemicals Pvt. Ltd., Bombay	-	Diversification programme and research and development activities of the firm
Balmer Lawrie and Co. Ltd., Madras	-	Product recovery in the manufacture of DBPC and PTBP.
Bangalore Pharmaceutical and Research Laboratory Pvt.Ltd., Bangalore.	-	Setting up a general research laboratory.
Bharat Heavy Electricals Ltd., Hyderabad	785	Design of a wash cooler Transformer oil analyzer
Bharat Petroleum Corporation Ltd., Bombay		Testing of catalyst samples for suitability in the cracking units Testing of catalysts and related technical matters
Biocon India, Bangalore	-	Services in the field of mycology
Cadila Lab. Ltd., Ahmedabad	-	Preparation of pre-research appraisal report on fluoro-aromatics
Central Pollution Control Board, New Delhi	_	Preparation of status report of H/G acid
Chemstar Organics (India) Pvt.Ltd., Bombay		Diversification of company's product range based on their present activities and R&D strengths
China National Chemical Construction Corp.Ltd., Nanjing, China	i de	- Strengthening of R&D institutions
DCL Polyesters Ltd., Nagpur		Diversification / expansion of synthetic fibre plant
DCW Ltd., Bombay		- Commissioning of isopropyl bromide plant

DSIR, New Delhi	9-22	Technology status study on carbon tetra- chloride Technology status study on vitamin C and sorbitol
DST, New Delhi	_	Technology status report on polyacetal resin
Dhanani, K.R., Bombay	_	Prefeasibility study on methyl piperidinone
Director of Animal Husbandry Disease Investigation Station, Pune	* <u>-</u>	Prevention of industrial pollution
Excel Industries Ltd., Bombay	-	Manufacturing process for pharmaceuticals /agrochemicals Technical advice & assistance in selecting manufacturing processes for pharmaceuticals & agrochemicals
Gas Authority of India Ltd., New Delhi		Approach / scope for R&D efforts to be made by GAIL on effective utilization of natural gas
Gharda Chemicals Ltd., Bombay	-	Evaluation of activated carbon
Gujchem Distilleries India Ltd.	-	Diversification and project selection based on alcohol
Gujchem Distilleries India Ltd.	70 <u>-11</u>	Designing of gas-liquid reactors
Gujrat Alcohol and Allied Chemicals Ltd., Ahmedabad	-	Implementation of acetic acid, propionic acid projects
Gujrat State Fertilizers Corp. Ltd., Fertilizernagar, Dist:Vadodara	-	TFC membranes
Hindustan Antibiotics Ltd., Pune	-	Reactor agitator design for bioconversion of penicillin G to 6 APA and 7

		ADCA/new methodologies for bioconversion
Hindustan Lever Ltd., Bombay	_	Interpreting data on chemical characterization of catalysts and raw materials
Hindustan Organic Chemicals Ltd., Rasayani		Implementation of monochlorobenzene process Preparation of simulation package for the distillation train in the cumene section of the phenol plant: First phase General guidance for technical operations Simulation of distillation train in the cumene section of phenol plant of HOC: Second phase
ICICI, Bombay	-	Setting up of an online search facility
IPCL, Vadodara	Remarks	Improvement of chlorine, ethylene dichloride, vinyl chloride monomers and polyvinyl chloride
Indian Gum Industries Ltd., Bombay	-	Useful products from guar gum
J.K. Synthetics Ltd., Kota	-	Modelling and simulation of PET reactors
Kaushal Aromatics (P) Ltd., Nag- pur	-	Acrylamides
Kerala Salicylates & Chemicals Ltd., Thiruvananthapuram	-	Technical audit of salicylic acid and aspirin plant
Kirloskar Pneumatic Co. Ltd., Pune	- <u>- i</u>	PTFE piston and wear rings
Kirloskar Consultants Ltd., Pune	\$ 555	Preparation of technoeconomic reports on naphthalene, epoxy resins, phenolic resins, etc.

Lasor Drugs Pvt. Ltd. Pune	- Ranitidine intermediate (MMV)
Lona Industries Ltd., Bombay	 Optimizing laboratory process for 4A-type zeolite
Lupin Chemicals Ltd., Bombay	- Prefeasibility study on citric acid
Mahanagar Telephone Nigam Ltd., New Delhi	 Selection of polymeric material and testing for PCO booths
Morris Electronics, Pune	- Rubber bonded magnets
Niphad S.S.Karkhana, Niphad, Dist. Nasik	 Reduction of fermentation period for lactic acid
Ordnance Factory, Pune	 Development of indigenous substitute for acrylic polymer
Orion Photosensitive Systems, Karad	- Improvement in photosensitive systems
Polychem Ltd., Bombay	 Technical audit of polychem plant opera- tions at Nina and Baroda
Pudumjee Pulp & Paper Mills Ltd., Pune	 Structural characterization 'punec' bagasse lignin
Ring Gears India Ltd., Bombay	 Setting up of tissue culture/ green house facility
Satya Enterprises, Tanaku	- Bleaching & dyeing of human hair
Shriram Fibres Ltd., Madras	- Polyphenylene sulphide
Shrishma Fine Chemicals Pharmaceuticals (Karnataka) Ltd., Bangalore	- Effluent treatment in the salicyclic acid and analgin plant
Shwetadri Speciality Papers Pvt. Ltd. Mysore	- Solvent recovery and recycling of toluene

TIFAC, DST, New Delhi	 Techno-market survey report on business opportunities in membrane separation Techno-market survey report on additives for thermoplastics
Thermax Ltd., Pune	 Prediction of performance of absorption heat pumps
Voltas Ltd., Bombay	 Optimization of process, development of formulation & generation of bioefficacy, toxicity data on pest control agent from karanja / neem oil cakes

PATENTS

PATENTS GRANTED - INDIAN

1. 169546

An improved process for the preparation of chloramphenicol-2,2-dichloro-N-[2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl] acetamide.

2. 169687

An improved process for the preparation of 1,1,1-trichloro-4-methyl-pent-3ene-2-YL diazoacetate.

3. 169688

Preparation of γ -lactone of 2,2-dimethyl-3-(2,2,2-trichloro-1-hydroxyethyl)cyclopropane carboxylic acid.

4. 169746

A facile enzymatic resolution process for the preparation of R-(-)-1,1,1-trichlo- ${\it ro-2-hydroxy-4-methyl-3-pentene}.$

PATENTS GRANTED - FOREIGN

1. US Patent No. 5118654

A process for the preparation of an improved Li–promoted MgO catalyst useful for oxidative coupling of methane to ethane and ethylene.

- 2. Australian Patent No. 625926 Reforming of pyrolysis naphtha.
- 3. US Patent No. 5141908 Reforming of pyrolysis naphtha.
- 4. Australian Patent No. 621640 Conversion of natural gas to middle distillates.
- 5. European Patent No. 0268710 Codeine from morphine.

- 6. US Patent No. 5066819 Aryl N-alkyl carbamates.
- 7. US Patent No. 5080121 Polymer for drag reduction in hydrocarbon fluids.
- 8. US Patent No. 5118654 A process for the preparation of an improved Li-promoted MgO catalyst useful for oxidative coupling of methane to ethane and ethylene.

PATENTS APPLIED - FOREIGN

1991 - 92

1. (841/DEL/90)

An improved process for the preparation of cumene European patent application No. 91309531.

2. (1233/DEL/89)

An improved process for the production of cumene European patent application no. 91309530.3 US patent application No. 07/780,860.

3. (766/DEL/91)

A process for the preparation of novel crystalline molecular sieves US patent application No. 07/816/211 European patent application No. 92300166.3.

4. (957/DEL/89) and (958/DEL/89)

A process for the preparation of catalyst composite material and for reforming of pyrolysis naphtha.

US patent application No. 07/788,222.

5. (841/DEL/90)

An improved process for the preparation of cumene US patent application No. 07/780858.

6. (283/DEL/89)

An improved process for the preparation of alkyl carbamates US patent application No. 07/812753.

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1. (1236/DEL/91)

An improved process for preparation of high molecular wt. poly (arylcarbonate)s

US patent application No. 07/878932

European patent application No. 92304098.4.

2. (23/DEL/92)

A process for the production of linear alkylbenzenes US patent application No. 07/863590 European patent application no. 92303028.2.

3. (1239/DEL/89)

A process for the preparation of novel bioxyanion catalysts useful for the preparation of polycarbonates and a process for the preparation of polycarbonates using the said catalysts

US patent application No. 865951 European patent application no. 92303078.7.

4. (66/DEL/92)

An improved process for the synthesis of D(+) Biotin US patent application No. 07/863794 European patent application No. 92303027.4.

5. (222/DEL/90)

A process for the preparation of new reactive anionic initiators useful for polymerisation of vinyl monomers US patent application No. 07/876563.

6. (1113/DEL/91) and (1114/DEL/91)

Composite catalyst useful for oxidative conversion of methane (or natural gas) to synthesis gas and an improved process for production of synthesis gas by oxidative conversion of methane (or natural gas) using composite catalysts US patent application No. 07/930007 European patent application No. 92306906.6.

7. (714/DEL/90)

A two step process for production of liquid hydrocarbons from natural gas US patent application No. 07/911448.

8. (1081/DEL/90)

An improved integrated two step process for conversion of methane to liquid hydrocarbons of gasoline range US patent application No. 912969.

9. (652/DEL/91)

Novel composite catalysis containing transitional and alkaline earth metal oxides useful for oxidative conversion of methane (or natural gas) to carbon monoxide & hydrogen(or synthesis gas) US patent application No. 07/943,183.

10. (653/DEL/91)

An improved process for the production of synthesis gas by oxidative conversion of methane using composite catalyst containing transitional & alkaline earth metal oxides US patent application No. 07/943,181.

- 11. (1318/DEL/90), (1319/DEL/90) and (1320/DEL/90) An improved process for the preparation of arylysubstituted aryl/alkyl substituted alkyl easter of n-alkyl/aryl carbamic acid US patent application No. 07/962774.
- 12. (1113/DEL/91) and (1114/DEL/91), Divisional application Methane to natural gas conversion US patent application No. 08/033106.
- 13. (1124/DEL/90), (1125/DEL/90) and (1126/DEL/90) Triterpene derivatives US patent application No. 07/977,618.

NATIONAL CHEMICAL LABORATORY, PUNE

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5. Dr.K.H. Gharda Managing Director, Gharda Chemicals Pvt. Ltd. Bandra Bombay 400 050.

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