[After organising a discussion meeting and consulting a number of chemists, the Science and Engineering Research Council (SERC) of the Department of Science and Technology has prepared a paper identifying new thrust areas in the field of Chemical Sciences. We are happy to publish this paper which brings out the need for a change in the direction of our research efforts. Chemists should be interested in this paper as the Department of Science and Technology will provide major funding in these areas. It would also be interesting to have our readers' views if there are any major lacunae in the identified areas.—Ed.]

THRUST AREAS IN CHEMICAL SCIENCES

1. Introduction

THE objectives of the science of chemistry from times immemorial have been to study the properties and syntheses of matter. Chemical science today has a part to play in all branches of modern science, from "biophysics to botany and from nucleus to nebula". The dynamic nature of chemical science is manifested by the increasing number of interfaces it forms with other sciences. Chemical science has also much to contribute to national development. Applications of chemical science, whether they be in food, textiles and drugs or in batteries and rockets, are so innumerable and vital that we can truly state that there can be no progress without chemistry. Newer and better processes as well as newer and better materials are being developed continually by chemists. Alternate sources of energy, newer applications and substitutes of raw materials and a better environment to live in, will all eventually be found only with the participation of chemists. While these tasks demand research and development of the highest quality, there is little doubt that chemists with their unlimited abilities in the understanding of structure, dynamics and synthesis are capable of it. This is not to say that chemists have solved or can solve all problems of mankind with their present knowedge. There are many pressing problems glaring at us which require chemical solutions but have not been hitherto solved. For example, chemists are yet to find ways of fixing nitrogen by simple means; chemists are not yet able to say definitively whether the ozone layer is depleted by supersonic flights. Practical ways of converting cellulose to proteins, making hydrogen from water employing solar energy and means of slowing the process of ageing of human beings are yet to be found.

Traditionally speaking, chemical science has been divided into three main branches, physical, organic and inorganic, biochemistry having developed into a discipline in its own right. Although this division of chemical science is not sacrosanct, it is convenient to classify research areas in chemical science under these broad categories. While more unified ways of classifying chemistry have been suggested such as structure, dynamics and synthesis, there are problems in visualising research areas of chemistry under these categories since most chemists tend to think in terms of the traditional areas. We shall therefore briefly examine the status of chemical science employing the traditional classification.

2. The Chemical Scenario

Organic chemistry by and large constitutes the biggest branch of chemical science by virtue of the vast variety of carbon compounds and the large number of practitioners. Organic chemists determine structures of molecules, build structures in the laboratory employing newer and better methods, elucidate step-wise mechanisms of reactions and relate chemical reactivity to structure. Their investigations vary from developing new products to improve the quality of life at one end to carrying out theoretical calculations and computer simulations at the other. In this active branch of chemical science, progress has been unbelievable. Chemists are able to determine structures of increasingly complex molecules with great rapidity employing very small amounts (less than a micromole) of materials. Organic chemists use every conceivable spectroscopic method to the best advantage. The use of X-ray crystallography by organic chemists has now become a matter of routine in the advanced countries wherein structure and stereochemistry are determined as and when compounds are synthesised in the laboratory. Besides such advances in the use of modern physical methods, organic chemists continue to innovate through discovery of newer synthetic metyods, reactions and reagents. Organic chemists today are very much interested in biomimetics and in understanding life processes.

While the above scenario is prevalent in advanced countries, the situation in this country is not altogether encouraging. Although organic chemists in India have flourished more than chemists specialised in other branches, facilities available to them are far from satisfactory. They are unable to compete with their counterparts in the advanced countries. Instrumentation and analytical methods are not readily available to enable them to elucidate structures of compounds rapidly. Special chemicals are not often available. It is also true that in spite of the good contribution made by organic chemists in India, there have been no major reactions or syntheses contributed by Indian organic chemists.

Lewis defined physical chemistry long ago "as anything that is exciting", but a more operational definition would be that this subject deals with physical principles underlying chemical phenomena. In the past few years, physical chemists have explored properties of matter in detail from the molecular and electronic points of view. They have increasingly used various kinds of instruments, particularly spectrometers, with greater and greater sophistication. The instrumentation involved in physical chemistry research is indeed so sophisticated that anyone trained in the old school will find himself completely unfamiliar in a modern laboratory. Computers have become so large and fast that physical chemists are now able to make calculations of great complexity and predict properties of molecules and systems with a fair degree of certainty. Research in many of the traditional areas of physical chemistry seem to be slowly becoming obsolete.

Some of the most significant developments in physical chemistry today are the use of lasers to study state-to-state chemistry and phenomena in the picosecond range. Physical chemists have also contributed significantly to the understanding of liquids. The advent of synchrotron radiation has enhanced the potentiality of many of the structural tools employed by physical chemists. They have also been involved in the study of a number of problems of biological importance where they employ lasers and spectroscopy. Studies of surfaces and solids which hitherto constituted important aspects of physical chemistry are slowly getting recognized as new emerging areas of chemistry.

The above description of physical chemistry provides a glaring contrast to the situation of the subject in this country. There are very few good physical chemists in the country and most of them have not been able to work in areas of thrust and significance at the most opportune time. Physical chemistry laboratories are most ill-equipped and the computer age or the electronics age has not yet started as far as much of Indian physical chemistry is concerned. While part of the reason may be due to the non-availability of sophisticated instruments and computer facilities, part of the blame may go to the practising physical chemists who have not been altogether outgoing. While the status of physical chemistry is highly unsatisfactory, the status of inorganic chemistry in the country is much worse; there are very few good inorganic chemists in the country today. One has indeed to worry about the finite probability that these two branches may soon become extinct.

Inorganic chemistry deals with more than 100 elements. In spite of or because of this vast area of action, the growth of the subject has been rather diffuse. One of the problems has been that many of the areas of inorganic chemistry overlap with those of organic chemistry or physical chemistry. Inorganic chemists are getting increasingly interested in biological problems in recent years. There is indeed a distinct difference between a biologist trying to work on a problem involving inorganic species and an inorganic chemist working on a biological problem. Typical of the problems of interest to inorganic chemists in biological area are, nitrogen fixation, use of shift reagents to study molecular conformations and enzyme models. Other aspects of interest in modern inorganic chemistry are organometallic chemistry and photochemistry. Many inorganic chemists today use spectroscopy in great depth; they also work on many aspects of solid state science. Inorganic chemistry, as practised in this country, however, does not reflect these new directions in the subject. Although significant contributions to inorganic chemistry have been made in India in the past, there are very few good inorganic chemists today in the country and fewer still working in frontier areas.

A number of chemists in India have worked on new analytical reagents and simple wet procedures for analysis, but have not been able to keep pace with the developments in modern analytical chemistry, where instrumentation involving microprocessors is the order of the day. In fact, this is a general problem in all areas of chemistry. There are very few centres in the country where sophisticated instruments are designed and fabricated by research workers. Use of microprocessors with instruments is yet to be initiated in the country.

Of all the sciences, *chemical science has had the biggest information explosion*. It is indeed a nightmare to chemical educators as to how to communicate advances in the subject in a meaningful manner to students. Having a fair proportion of the descriptive component and also a large number of interfaces with other sciences, chemical science does not lend itself easily to a unified treatment of the subject. While this is a global problem, chemical education in most institutions in our country is wrought with many other problems such as ill-equipped laboratories, poor curricula and poorly motivated teachers. Students are not trained properly in theory as well as experimental skills. *One of the major factors responsible for the indifferent quality of chemical research and for the shortage of young talent in chemical science is, undoubtedly, the poor standard of chemical education*. There are many other factors which have contributed to the present state of chemical research in the country. Chief amongst them is our failure to identify crucial areas of research and capable scientists, and providing adequate support for research (particularly instrumentation) at the appropriate time. This has resulted in a tremendous gap beween the status of chemical research in this country and in the advanced countries. It is extremely important to be conscious of the *tremendous rate of change of acceleration in chemical science* in identifying research areas and in supporting them.

3. Thrust Areas

The above description of the chemical scenario in this country and elsewhere clearly brings out the need to support thrust areas of chemical sciences in the country selectively in order to develop and promote these important areas. It is only when adequate funds are provided for research in critical areas that we can expect major advances to be made. It is with this objective that thrust areas have been identified in chemical sciences. It is possible that there are other areas of importance in chemistry which have not been listed, but it is felt that funding of the thrust areas could be a good beginning in bringing about the badly needed change in the quality of chemical research in the country. There should obviously be a *dynamic programme wherein newer areas get identified and supported as time goes on.* There are some areas of chemistry where good work is being carried out at present but have not been listed below for the reason that they may not be thrust areas today. The Science and Engineering Research Council (SERC) will to ensure that *outstanding chemists and good projects are always supported immaterial of the nature of the area or source of funding.*

There are many issues related to the implementation of thrust area programmes which are common to all disciplines and therefore we shall not deal with them here. We would like to, however, stress the need to initiate programmes to attract young talent to research in chemical sciences, to initiate intensive training programmes in chosen areas, to establish properly funded SERC units or centres in chosen areas and to find ways of effectively monitoring the progress of SERC projects. SERC will also identify those areas of chemical science which will be of immense benefit to industry and national development if long-term research in the areas is supported.

We list below thrust areas in chemical sciences with a brief description of each area.

I. *Molecular Structure and Dynamics*

(*a*) Recent developments in spectroscopy such as two-dimensional FTNMR, multi-nuclear solid state HRNMR, FTIR spectroscopy and photoacoustic spectroscopy.

(*b*) Laser chemistry and laser spectroscopy.

(*c*) Fast (nano- and pico-second) kinetics involving relaxation and other methods.

(*d*) Gas phase kinetics including molecular beams and plasma chemistry.

New techniques have enhanced the ability of chemists to probe in detail, chemical structures of complex systems and to follow dynamic changes in chemical reactions with ultra-short time resolution. Some of these have been identified as relevant to the growth of chemical sciences in our country and listed below are areas in which research should be initiated and funded.

Structure : Recent developments in magnetic resonance such as fast fourier transform methods, magic angle spinning and 2-D FTNMR have led to high resolution possibility even in the condensed state. It has now become possible to elucidate detailed structures of large bio-molecules, polymers, solid materials, etc. and there is an upsurge in the utilisation of these techniques in many areas of chemical sciences. FT-IR spectroscopy has revolutionized the sensitivity and resolution of IR spectroscopy with considerable reduction in time and the sample size required for the analysis of large molecules. The recently developed area of photoacoustic spectroscopy allows chemists to study energy transfer through non-radiative mechanisms and enables surface analysis. It is felt that these are some of the new branches of spectroscopy which are bound to change, qualitatively by orders of magnitude, our investigative ability in the study of large molecules and the condensed state.

Dynamics : The aim of any chemist is to elucidate the dynamics of each individual step and identify the intermediates especially of primary reactions and recent developments have provided a time resolution of the order of nano and pico seconds. Also of great interest is the follow-up of the reaction path between well-defined states.

(a) Relaxation studies such as T-jump and magnetic relaxation studies provide information between milliseconds and nano-seconds.

(b) The short pulse width of lasers allow nano- and pico-second dynamical studies. High monochromaticity allows state-to-state chemistry leading to understanding of finer details of chemistry. High intensity and coherence have opened up the new field of infrared photochemistry and non-linear spectroscopy (CARS, HORSE). Laser chemistry apart from basic study has already found many applications such as isotope separation, new synthetic routes, environmental studies and atom-atom purification and many more are in the horizon.

(c) Gas kinetics using molecular beams are important from the fundamental point of view while plasma chemistry is closely related to high temperature chemistry and upper atmosphere chemistry.

II. *Solids, Surfaces and Catalysis*

(a) Ultra-micro structure of solids.

(b) Solid state organic chemistry.

(c) Solid state electrochemistry, energy conversion and storage.

(d) Synthesis and properties of novel materials.

(e) Newer techniques of surface characterization such as electron energy loss spectroscopy, photoelectron spectroscopy, SIMS, Auger spectroscopy, LEED, etc.

(f) Heterogeneous and homogeneous catalysis including catalyst development and characterization, and phase-transfer catalysis.

(g) Micelles, membranes, reverse osmosis.

Solid state chemistry is an important and essential component of modern materials science. (a) An important aspect of this area is the study of solids under atomic resolution employing lattice imaging techniques. (b) Highly specific organic reactions occur in solid state due to constraints of the crystal packing and this forms an important aspect of solid state chemistry. (c) Solid state electrochemistry is an emerging area with implications in energy research. (d) Synthesis of tailor-made complex materials with desired properties becomes possible only because of the ability of chemists who understand the relation between structure, bonding and properties. (e) Surface characterization : Research in modern surface science wherein one can examine the first few atomic layers of solids (approx. 25 Å) depends entirely on emerging, techniques of electron spectroscopy (ESCA, Auger, etc.) and cognate techniques (like LEED, etc.). Research in this area is at present being carried out by very few chemists in the country and needs to be supported in a major way. (f) Catalysts : More than 90% of our chemical industry is based on the use of catalysts. Whatever be the raw material its conversion into useful products invariably involves catalysis. To improve upon the existing catalysts as well as to develop newer ones to meet the needs of modern society, a major effort in catalysis research is required. The development and demonstrated viability of a catalyst require the application of modern instrumental techniques and use of extensive testing facilities involving an interplay of several disciplines. A conscious effort to foster this interdisciplinary collaboration and the provision for adequate facilities is necessary to generate indigenous capability in this area. (g) Other surface and interfacial phenomena : The supramolecular organisation of amphiphilic molecules in aqueous and in organic media has been, and will be, receiving intensive attention in the light of their applications in catalysis, ability for organizing molecules at the molecular level, penetration of water through membranes, photophysical phenomena, tertiary oil recovery and fluid immobilization of enzymes and polymeric catalysts.

III. *Frontiers of Organic Chemistry*

(*a*) New synthetic strategies : Synthesis of organic molecules utilsing new and innovative synthetic schemes and techniques, including photochemical and electrochemical methods and phase transfer reactions; new synthetic strategy for bulk organic chemicals with a view to achieving material, energy and environmental conservation, computer aided design and simulation.

(*b*) Newer reactions and reagents : Development of efficient reagents for carrying out regio- and stereo-specific reactions with chiral selection is an extremely important aspect of organic chemistry which needs strengthening.

(*c*) Mechanism of organic reactions : Studies directed towards better understanding of novel bond making and breaking processes, with emphasis on reactive intermediates. and stereochemical aspects have to be supported.

(*d*) Polymer synthesis and mechanism of polymerization : Some of the important aspects of polymer chemistry that should be supported are : synthesis of novel polymers or newer methods of synthesis of known polymers; heteropolymers based on elements other than C, H and O ; study of the mechanism of polymerization especially under unusual conditions such as high pressures, high and low temperatures, heterogeneous, homogeneous and vapour phases; application of modern instrumental methods for delineating the bulk and micro structures of polymers and use of polymers as reaction matrices and enzyme mimics.

(*e*) Total synthesis of complex natural products and other exotic molecules including bioactive molecules having intricate carbon frameworks and posing stereochemical challenges as well as synthesis of novel and theoretically interesting organic molecules form an important areas of organic chemistry.

(*f*) Efforts towards the isolation and structural elucidation of bioactive principles from marine, insect and other unexplored sources have to be promoted.

IV. *Coordination Chmistry and Organometallic Chemistry*

(*a*) Electron transfer reactions and mechanistic coordination chemistry.

(*b*) Structure, spectroscopy and photochemistry.

(*c*) Activation of molecules and catalytic synthesis including reactions of carbon monoxide.

(*d*) Novel organometallics and their applications in organic synthesis.

In this general area of thrust, considerable interfacing will occur among inorganic and organic chemistry, spectroscopy and theory. Electron-transfer reactions pervade chemistry and a study of such reactions is an important component of this area as is the elucidation of the conformations and dynamics of molecules of mononuclear and cluster types.

Carbon monoxide is readily made from coal and the possible conversion of carbon monoxide into useful organic chemicals is a necessity of the day in view of the abundance of coal in India. Catalytic synthesis using carbon monoxide and through activation of other molecules is thus a relevant and important thrust area. Also, generation and utilsation of novel organometallics (for example, in the synthesis of organic molecules) is an area full of exciting possibilities.

V. *New Interfaces of Chemical Sciences with Biology*

(*a*) Biomimetic Chemistry : Areas of particular importance include the synthesis and study of chemical models mimicking functional biological systems.

(*b*) Membranes and Model Systems : Ion transport, energy transduction, liposomes and surfactant assemblies, membrane dynamics.
(*c*) Metal Ion Interactions with Biomolecules: Metalloproteins, fixation and transport, trace elements in biology.
(*d*) Chemistry of biopolymers and their constituents.

4. Other Important Aspects

Theoretical Chemistry

Theoretical chemistry is not practised or taught widely in the country. Teaching and promotion of theoretical chemistry should be encouraged at all levels; for this purpose, summer institutes and other training programmes should be organised on a regular basis. Although major funding may not be required for this area, research on newer techniques of theoretical chemistry, applications of many body theories, statistical mechanics, molecular dynamics, reaction theory, computer simulation and such areas should be supported.

Computer charges and puchase of micro computers should also be supported while granting projects.

Instrumentation

Very few chemists design and fabricate instruments. It is important that projects involving design and fabrication of sophisticated instruments are supported. Use of micro-processors with instruments should be encouragted.

Alternate Energy Sources

There are many aspects of energy research where chemists have much to contribute. Typical of these are photoelectrolysis of water, photodecomposition of water, fuel cells, new batteries, restructuring of biomass and chemical storage of solar energy. Projects involving these should be adequately supported.