uses of nuclear energy and alleviation of unfounded fear of the public on harmful effects of radiation.
- First response team be created and kept in readiness at various locations, especially in metropolis and big cities. Appropriate 'first action manual' should be prepared for the teams.
- Existing hospitals in different metropolis and big cities may be categorized and equipped for handling various categories of patients and different degrees of emergencies.
- Specialized trauma control hospitals be developed for trauma control.
- Development of biological dosimeters with field applicability to assess the extent of biological damage in the disaster situation.
- Radiomodulatory drugs for post-exposure treatment needs urgent attention. Endogenous or exogenous radioprotections, free radical scavenging drugs of high efficiency and nucleotide modifiers need to be developed and tested.

The recommendations are especially relevant to India due to its vulnerability, large population, geographical spread and largely inadequate medical infrastructure.

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Beyond Gaussian: Theoretical chemistry in India comes of age

India has a reasonably strong theoretical chemistry community that has been growing steadily in the last 2–3 decades. The first formal discussion meeting in theoretical chemistry was organized by B. M. Deb of Panjab University in Chandigarh in October 1986. There were only a handful of theoretical chemists in the country at that time. They were in their prime and were raring to go. They needed a platform to come together and discuss the state of the art. The then President of the Indian Academy of Sciences, Bangalore, S. Ramaseshan came forward to fully support the discussion meeting in theoretical chemistry, so that the theoreticians did not have to run around seeking financial support. The meeting was a grand success and thanks to the continuing support of the Academy, the discussion meetings continued at intervals of 2 years for the next several years. Unfortunately, all good things must come to an end and they did. The Academy decided to stop the support. Fortunately, the theoreticians managed to continue to hold their meetings at regular intervals of 2 years, thanks to the support from DST, CSIR, BRNS and other such funding agencies and also due to the untiring efforts of colleagues in different academic institutions in the country.

The most recent meeting, *Trends in Theoretical Chemistry – 2002*, held at the Indian Association for the Cultivation of Science, Jadavpur, Kolkata, during 17–19 January 2003 was a big success. There were about 100 participants that included seven from outside India, giving the meeting the semblance of an international symposium. There was a total of thirty one half-hour talks, two 45 min evening lectures and about 50 poster presentations. The subjects covered included various topics ranging from formal electronic structure theory and its application to statistical mechanics and chemical dynamics and their applications to a large number of systems including atomic and molecular clusters, proteins and other biomolecules in interfaces.

Not surprisingly, a good number of talks centered around electronic structure theory and its application to chemical and biological systems. While H. F. Schaefer III emphasized the importance of correlation methods, taking the example of silicon dicarbide, M. Nooijen illustrated the use of automatic program generators in implementing multireference coupled cluster theory. A set of lectures dedicated to B. M. Deb (as he has turned 60), understandably focused on density functional theory (DFT) – a subject close to his heart. H. Nakatsuji, highlighted the contributions of Deb and also spoke on SAC-CI theory, while P. Geerlings spoke on conceptual DFT. M. K. Harbola illustrated the use of hydrodynamic variation–perturbation method in calculating van der Waals coefficients and P. K. Chattaraj discussed chemical reactivity dynamics within a quantum fluid density functional framework. G. P. Das presented an overview of spintronics. While A. Perera spoke about the challenges faced by *ab initio* electronic structure theory, Jemmis illustrated its use in understanding planar tetracoordinated carbon and pyramidal tricoordinated boron. Narahari Sastry spoke on its application to Diels–Alder reactions and T. P. Radhakrishnan on modelling molecules in crystals. R. Chaudhuri discussed the use of effective Hamiltonian methods in studying excited electronic states of TiN. S. K. Pati discussed nonlinear absorption in organic molecules and N. Sathyamurthy on the use of *ab initio* methods in studying intramolecular hydrogen atom transfer in ground and excited states of salicylic acid and related systems. S. R. Gadre illustrated the use of electrostatic potential maps in understanding the shape and reactivity of different chemical species. B. P. Das was more concerned with relativistic and correlation effects in atoms.

While one evening lecture by W. H. Miller concerned semiclassical methods, the other by S. Dattagupta focused on coherence versus decoherence. Adhikari spoke on the time-dependent discrete variable representation method. The only talk on quantum chemical dynamics was by V. Aquilanti, who spoke on tunnelling and resonance-enhanced chemical reactivity in (F, H_2) collisions. While M. S. Krishnan was concerned with computing vibration–rotation states accurately, K. Srihari concentrated on intramolecular vibrational relaxation in highly excited states. R. Ramaswamy illustrated the problem of structure optimization in large atomic clusters, and D. Maity discussed the structure of solvated electrons. The talk on blow torch and levitation effects by S. Yashonath was an illustration of how computer simulation could be gainfully employed in industry. S. Bandopadhyaya presented preliminary results from a simulation of surfactant aggregates. B. Bagchi demonstrated how folding of globular proteins could be studied with reasonable computational facility. S. Taraphder was concerned with proton transfer in protein–water systems. G. Gangopadhyaya discussed the use of dendrimers in light-harvesting systems. M. S. Gopinathan showed how

a theorist turned experimentalist can unravel the mysteries of complex systems. K. Bhattacharya on the other hand, was concerned with fractional calculus.

It was clear from the presentations that theoretical chemistry in India has come of age and that the work is of international standard. Although there were several posters on the use of GAUSSIAN packages for a variety of chemical systems, it was clear that a lot of effort has gone into the development of home-built software, be it for mapping electrostatic potential or time evolution of wave packets or molecular dynamics and Monte Carlo simulation of large atomic and molecular systems. Indian theoretical chemists are no longer limited by the availability of computers. Many of them seem to manage with Pentiums and Pentium clusters. Some of them in well-endowed institutions are lucky to have workstations, though many of them are still unfortunately handicapped because of the lack of access to international journals. The 'never-say-die' spirit seems to keep them going by following the dictum, 'Beg, borrow or steal' and carrying out work of international standard. Many universities in the country have several faculty positions vacant. If only they would appoint theoretical chemists of quality to their chemistry departments, India will be able to take a leap forward in consolidating its strength and the theoretical chemists will surely do India proud.

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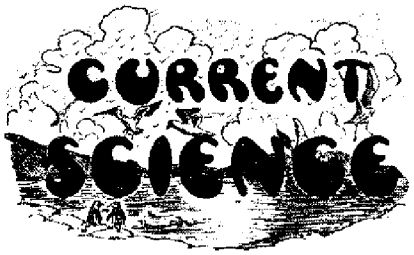
FROM THE ARCHIVES



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Cinchona cultivation in India

The production of quinine and the associated cinchona alkaloids in India has been the subject of repeated discussions during the last decade both in the legislatures and in the press. In a country, where malaria is the dominant problem in public health and a major cause of low economic efficiency, the question of an adequate supply of cheap quinine, along with that of preventive measures, is one of perennial interest.

The present position of quinine supplies in India is, without doubt, unsatisfactory. The minimum requirements of quinine in the country, as estimated by the public health authorities, are 600,000 lbs per annum. The actual average consumption in the pre-War years has been estimated at 21,000 lbs. This enormous gap between the real or clinical demand and the effective or economic demand may be ascribed largely to the high price of quinine relative to the purchasing power of the country as a whole. The problem of a reduction of price is complicated by the fact that only a third of the present effective demand is met by production within the country. The foreign manufacturers, who supply the bulk of the Indian demand, are not particularly interested in a reduction of price, as this demand has not appreciably increased over a long period and continues to form only a small portion of the total world demand. There is a large market for quinine in Russia, the United States of America and the South American countries which can afford high prices. The Royal Commission on Agriculture in India, reported in 1925, that for India to embark on any large campaign for fighting malaria, it would first be necessary to reduce the price of quinine within the country, and this could be effected only if India were self-supporting in cinchona products.

One of the causes which may have delayed the expansion of cinchona cultivation in India is the fear of competition from Java which has great natural advantages in the growing of this exotic species. The risk of competition is not however as great as may appear. In the first place, the present standard of production in India with reference to yields and costs is certainly capable of improvement and, in the second place, there are still large tracts of land that should prove naturally suitable for cinchona. Java, moreover, is not likely to be greatly concerned about the Indian market until it expands very considerably to bear comparison with the world market.

Apart from purely commercial considerations, the quinine industry has a special interest in India. In spite of the many synthetic antimalarials put on the market in recent years, quinine (together with other cinchona alkaloids) still holds the first place in the treatment of malaria. It is the one antimalarial which, having no pronounced toxic effects, may be administered under very simple instructions and without qualified medical supervision. It is also likely to be the cheapest remedy for a long time to come. Both these are important considerations in a country like India and quinine may well be regarded as an industry of national importance in which self-sufficiency should be the aim. The more so as, under present conditions, not only the price of quinine but also the regularity of its supply is affected by every world event which disturbs the normal courses of trade and commerce.

A rational long-period policy for India as a whole can only be based on a complete knowledge of our ultimate resources, though the rate at which such resources could be developed would depend on circumstances. Even for individual production schemes of any appreciable size the preparation of efficient working plans requires the collection of data in greater detail than available at present. A broad co-ordination of regionally separate and economically independent schemes is not a mere counsel of perfection. If the distressing conditions that have overtaken many of the plantation industries in recent years are to be avoided in the case of cinchona, there is no doubt that production should be developed, from the earliest possible stage, on an all-India basis instead of through a multiplicity of competitive schemes. This is more important in view of the fact that cinchona is a long period crop and any appreciable maladjustment of short period supply and demand would take time to correct itself resulting in considerable hardship to the producer or the consumer as the case may be.

India's need for adequate supplies of quinine is urgent. The times are favourable for the development of an indigenous industry. What would appear to be necessary is the formulation of a coordinated scheme of work and the pooling of all resources in its execution.