In this issue

Molecular charge maps

Successful quantum chemists must possess multifarious skills. First, they must be able to carry out rigorous calculations on systems of direct experimental interest. Sound theoretical knowledge, good programming ability and access to powerful computers are essential pre-requisites. Next, they must translate their findings (usually tables of numerical quantities) to the experimental chemists in an understandable manner. In order to do so, theoreticians must be able to formulate simpler concepts which are preferably amenable to pictorial representation. A thorough understanding of the theoretical basis of the computational models and use of sophisticated graphics are needed at this stage.

An application representative of the modern approach to theoretical chemistry, which combines high-quality computation with visual representations, is presented by S. R. Gadre *et al.* (**page 798**). The problem studied concerns the basicities of the different sites of a large decavanadate cluster $[V_{10}O_{28}]^{6-}$. Using the *ab initio* wave function of this cluster, molecular electrostatic potential (MESP) maps have been generated in different planes. Interestingly, the calculations have been performed with a program developed by the authors incorporating various bounds for simplifying the computation of integrals and implemented on an indigenous parallel computer PARAM. The MESP maps have been visualized on an IRIS workstation, clearly bringing out the various basic sites of the cluster. The authors have pointed out that the results of the present study do not parallel those based on the widely used Mulliken population analysis.

Dissolved uranium

The first major detailed study of the concentration of dissolved uranium and its radio isotopes in the waters of several Indian rivers was reported in 1969 (Bhat and Krishnaswami) in the *Proceedings of the Indian Academy of Sciences* (1969, **70**, 1). It came out of a laboratory which had built up a reputation for the meticulous care with which experiments were done. This paper, which we consider to be a classic, broke new ground and presented many new and unexpected results. Perhaps the most surprising of these was that in the Ganges (Ganga) river system the dissolved uranium (238) concentration was five to six times that of the global average. Further, the contribution of dissolved ^{238}U by the Ganges basin to the oceans was much higher than that of the Amazon system—although the discharge of the latter is almost an order of magnitude larger. Studies were also conducted in some south Indian rivers (Godavari, Krishna and the Cauvery) and west-Indian rivers (Sabarmati, Mutha and Ulhas).

On **page 801** is a paper by M. M. Sarin *et al.* which not only extends the results of earlier 1969 paper, but also reports some brand new and exciting results. Samples were collected at various places from the source rivers of the Ganga—Bhagirathi (right from Gangothri) and Alaknanda (from Devprayag). The uranium weathering rate (the flux of dissolved uranium per unit drainage area) is about 50 to 100 times the corresponding rates for rivers like the Amazon and the Congo! This might also be due to the uranium mineralization in the drainage zone. The Ganga and the Brahmaputra transport annually about 1000 tons of dissolved uranium to the estuaries of the Bay of Bengal. The ^{238}U flux from the Himalayan-Tibetan rivers (Ganga, Brahmaputra, Indus, Chiang, Mekong) is about 3000 tons—much more than that for Amazon and Congo although their water discharge is three times that of the former, i.e. almost 25% of the supply of uranium to the ocean is from the Himalayan rivers. The coral measurements indicate that the uranium accumulation in the ocean is 30% less in the Miocene era. The authors speculate that the present increase might be due to the uranium washed from the newly formed Himalayan system.

Peter Mitchell

In 1978 the Nobel Committee at last honoured itself by awarding the physics prize to Peter Kapitza (1894–1984), who has been described as one of the greatest experimenters of our time. He was then 84 and in his acceptance speech he proudly said, 'I am the oldest person who has received the Nobel prize.' It was in this connection that we read the Nobel Foundation book *Les Prix Nobel 1978* and came across the biographical sketch on Peter Mitchell, the chemistry Nobel prize winner of 1978. It revealed to us a man truly remarkable—a man who belonged to more to fiction than to reality. Like Martin Arrowsmith (of Sinclair Lewis) he completely withdrew from doing scientific research in public institutions and built for himself a small personal laboratory in Glynn Valley in Cornwall. He received little support from grant-giving bodies and had just sufficient funds to employ three or four research workers (including himself). Here he launched on the study of the mechanical relationship between the metabolism of cells and the transport of solutes across cellular membranes.

He did not publish his Nobel prize-winning theory of chemiosmotic reactions in well 'refereed journals' but resorted to a technique that practitioners of pathological sciences are accused of—of using privately published monographs. Not for him the little men who call themselves editors who arrogate themselves to being arbiters of science. His theory was received with great reservation by workers in the field because it was unorthodox, provocative and based on very little experimental evidence. But it slowly gained acceptance first because other hypotheses postulated the occurrence of energy-rich intermediate compounds for which no evidence could be obtained even after intensive search.

He was one who ploughed a very lonely furrow. We would like to quote a part of his speech at the Nobel banquet as it tells us about the bitter process of creation and the travails faced by the innovator:

'... the creative process in science and in art consists of two main activities—an imaginative jumping forward to a new abstraction or simplified representation followed by a critical look back to see how nature appears in the light of the new vision. *The imaginative leap forward is a hazardous unreasonable activity.* Reason can be used only when looking critically back. Moreover in the experimental sciences the scientific fraternity must test the new theory—to destruction, if possible. Meanwhile the originator of the theory may have a very lonely time, especially when his colleagues find his views of nature unfamiliar and difficult to appreciate. The final outcome cannot be known either to the originator of the theory or his colleagues and critics who are bent on falsifying it. Thus the scientific innovator may feel all the more lonely and uncertain. On the other hand, faced with a new theory the members of the scientific establishment are more vulnerable than the lonely innovator. For, if the innovator should happen to be right, the ensuing upheaval of the established order may be very painful and uncongenial to those who have long committed to themselves to develop and serve it.'

Besides his interest in communication between molecules, Peter Mitchell became more and more interested in the problem of communication between higher organisms like human beings in civilized societies, especially in the context of the spread of violence.

Yes, he was truly a remarkable man. He died in April 1992. V. Sitaramam (**page 806**) gives us a personal glimpse of this man.

S&T in India — Editor's note

In our early enthusiasm we invited many directors of science and technology institutes to write articles about their laboratories, highlighting the major research done over the years. The idea was that scientists and readers of *Current Science* should become acquainted with what is happening in science and technology in the country and if possible also learn from the enormous accumulated experience. We even thought such articles may promote cooperation among scientists in different centres and the larger utilization of the pool of scientific instruments collected in India. Unfortunately the experiment has not been much of a success and we have decided to discontinue this presentation after this issue.

A few writers did bring out vividly the philosophy behind the workings of their laboratory and highlighted important pieces of work which made an impact in India and outside. However, many turned out to be routine catalogues of activities over the years not discriminating between good and indifferent work. Invariably these articles have been authored by directors of laboratories, who, for good reasons, shy away from the exercise of critical scientific judgement. We were indeed advised that such a differentiation may produce disquiet amongst the scientists!

What then must be done to bring the significant scientific work done at various centres in India to the attention of interested scientists. One is, of course, through original articles published in learned journals (including *Current Science*). Many laboratories however concentrate in applied science and technology and so do not often publish 'original' communications. One idea that has been suggested to us is to commission knowledgeable scientists (with a flair for writing) to visit laboratories and render critical accounts of the work done in them. One is not too sure whether the idea would be acceptable to many laboratories and whether such writers will be welcome and doors opened to them. Readers are requested to send in their suggestions on this subject.