delivered little of what was expected from them and the very existence of PSUs needed serious review, he added. In fact, as one participant pointed out, there was no attempt to analyse causative reasons for failure of PSUs and perhaps, this would have to be left for another INAE seminar!

Then came the deliberations of where the manufacturing industry was heading. Manufacturing industries are vital to a country as they minimize imports and help growth of other sectors such as agriculture. But due to resource conservation and delaying investment in technology and R&D, India had lost the opportunity to becoming a global manufacturing hub, felt Prakash M. Telang, Tata Engineering. He spoke of the lessons we could learn from China by adopting staged innovation strategies, hiring people with advanced degrees and providing intense in-house technical training with a focus on process R&D. He suggested how this industry could meet challenges, for example, by changing product mix rapidly, making marketable products based on our own R&D with a focus on Third World consumers, bringing down costs by process innovation, better coordination along the supply cycle and tuning to client needs. Tata Engineering had introduced knowledge-based engineering system tools for optimizing design, process and product performance supported by a variety of conventional CAD tools, for example, in converting a 2D drawing to a 3D model in a die casting or a cutter body modelling for crankshaft milling, or surface modelling of a vehicular body. The Indian manufacturing industry needed a review of its mode of operation for creating an environment that was globally compatible and enabled by a cross-functional team. This had to be amply supported in equal measure by reforms for this sector from the government in areas such as indirect taxes, labour laws, import duties, power sector reforms, etc. he added. More exports from this sector would, it was felt, change attitudes and establish international benchmarks much quicker. The plus points for the Indian industry would be taking advantage of outsourcing contracts and industry loans for frontline areas of research such as nanomaterial-based catalysts, fuel cells, carbohydrate or alkane-based feedstocks, etc.

There were presentations from two young and successful Web entrepreneurs from Hungama.com and Herald Logic. So, while there is reorientation of business models for keeping afloat in industry circles, there was also a plea for an urgent drive for streamlining IPR issues in various select areas such as biotechnology, etc. for dispelling the mistrust prevailing among pharmaceutical manufacturers, well in time for the accession to the WTO convention on 1 January 2005.

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MEETING REPORT

Refresher course in quantum chemistry*

Quantum chemistry is considered to be one of the dreaded subjects in the M Sc programme in chemistry in most of the universities. Many students look upon this field as a final hurdle that they have to overcome, so that the course can be completed. This is a serious drawback, because a large percentage of research publications in experimental chemistry these days have a quantum-chemistry component. Advances in computer hardware and software have made numerical solutions to Schrödinger equation practical, albeit with many approximations. These developments help in relating the equations to observables in chemistry. In addition, application of ideas based on symmetry, overlap of orbitals and perturbation theory has brought a novel conceptual framework in chemistry. It was reasoned that students would be more receptive to quantum chemistry if, in addition to the formalistic treatment, numerical studies of specific problems and qualitative arguments to convert the outputs of computer programs to 'understanding' are simultaneously provided. With this idea in mind, a refresher course in quantum chemistry for teachers was conducted.

Basic quantum chemistry, with all its mathematical background, is available in textbooks and also on the web. Worked-out assignments and problem-solving sessions are also available. Despite all of these, enough connection is not established in the minds of students between quantum chemistry and the rest of chemistry. Our emphasis in this course, therefore, was to teach the basics of quantum mechanics in the morning lectures and provide hands-on sessions on the use of quantum chemistry in obtaining further insights on experimental problems in chemistry in the afternoon sessions. To achieve this, we considered laboratory components where participants will be putting into practice, with the help of PCs, the quantum chemical methods that they learn in the lectures. Lectures on quantum chemistry and the mathematical background along with group theory were arranged, so that the relationship between wave function and symmetry of the molecular system is used in the most optimal way in understanding chemistry. There were attempts to show how the electronic structure methodologies discussed in the lectures are useful in designing molecules, materials and drugs. We also had some classes on molecular mechanics, which is often used in combination with semi-empirical and *ab initio* electronic structure theory. We wanted to

*A report on the Academy Refresher Course in Quantum Chemistry held during 16 February–2 March 2003 at the University of Hyderabad and jointly organized by the Indian Academy of Sciences, Bangalore and the School of Chemistry, University of Hyderabad.

make this a unique experience, where resource persons and participants stay together as long as possible. For this reason, essentially all the resource persons were from Hyderabad.

Topics covered in the lectures and in the practical sessions were as follows: Failure of classical mechanics and advent of quantum mechanics, Postulates of quantum mechanics, Exactly solvable problems and their relevance to chemistry, Ad hoc introduction of spin and indistinguishability of electrons, Variation and perturbation theories, Huckel and other one-electron theories, Hartree–Fock theory–LCAO–MO–SCF method, Approximations to *ab initio* methodologies, Density functional theory, Molecular electron densities and electrostatic potential mappings, Comparison of MO and VB methods, Conservation of orbital symmetry, Walsh diagram and molecular geometries, Walsh orbitals and strained rings, Anomeric effect and hyperconjugation, Fragment molecular orbitals and isolobal analogies, Aromaticity, Molecular mechanics and molecular modelling, Quantum chemistry in design of molecules and materials. The attempt at every point was to bring the connection between what is taught in various topics in B Sc/M Sc and quantum chemistry.

The course started in the afternoon of 16 February 2003, where we discussed the expectations and requirements of the course. The projected computational laboratory courses already brought up the issue of familiarity with computers. Participants (four of them) who did not have any interaction with computers were given crash lessons on Windows Operating System and word processing, and editors on the first day itself, so that they will not be lagging behind when the program started the next day. The exactly solvable problems of quantum mechanics were covered in the first few lectures, with the mathematical background as well as group theory following in parallel. The concept of electron spin and its many implications in chemistry was also introduced. Once perturbation and variation methods were proved, approximate ways in which quantum mechanics can be used in chemistry were introduced. The laboratory courses in the afternoon started with the calculation of molecular orbitals of H_2 using a semi-empirical method, with programs that have been installed on eight PCs available to the participants. The program was taken from the *Resonance* CD, a copy of which was provided to each participant. In addition, a textbook on quantum chemistry by I. Levine was also provided. There were several initial hurdles in the process of doing computations. Once the specifying of the internal coordinates of small molecules was mastered by the participants, they learned to select a Hamiltonian and a basis set to do calculations using the program. The output of the program (wave functions, energies, Mulliken and other overlap population analyses, where the electrons in the molecule were partitioned to different atoms and bonds) was analysed by the participants. The process of converting the coefficients of atomic orbitals to conventional molecular orbital pictures found in textbooks and publications, was tedious in the beginning. It took far more time than anticipated for most participants, so that they had to take extra laboratory lessons.

The response to this laboratory course has been overwhelming, with the result that the resource persons had to stay on for longer periods of time. The idea behind these laboratory courses was to make the teacher participants confident in using the programs given in the CD once they get back to their colleges and universities. The qualitative ideas that we taught, such as the Walsh diagram for the geometric distortion of a molecule, influence of frontier orbitals on structure and reactivity and so on, were drawn from the calculations and immediately compared with the morning lectures.

Emphasis was given to understand molecular orbitals by giving several examples starting with water, CH_2, CH_3, CH_4, C_2H_6, $CH_3CH_2^+$, anomeric effect, hyper conjugation and other concepts of electronic structure popular among chemists. Reactions such as 4 + 2-cycloaddition were studied using semi-empirical molecular orbital theory. The participants were encouraged to locate the transition state and through a frequency calculation, establish the transition state as a true one. At the same time, they also convinced themselves that correlation diagrams can be seen from the outputs of calculations. The participants also did calculations on inorganic complexes such as ferrocene, examined the resulting electronic structures, and compared them with what would be obtained from a symmetry-adapted linear combination method which is taught in group theory in chemistry course. Electron correlations beyond the Hartree–Fock method were included in the program in two lectures. Density functional theory, which is now becoming popular, was also introduced in two lectures.

N. Mukunda gave a lecture on the philosophy of quantum mechanics, giving a historical evolution of the subject with many personal anecdotes. He also gently reminded the largely chemical audience that, while molecular orbitals may be useful to interpret chemistry, MO theory is essentially a model and nothing more. On Sunday, 22 February 2003 the participants were taken on a tour of the twin cities, first to Qutub Shahi tombs and Charminar and then to Silparamam for an evening programme. On the afternoon of 1 March 2003 the participants went to the town. There were two general meetings in the evening on 22 February and 1 March 2003 so that they could meet other teachers of the School and other Fellows of the Academy of the University. There were no formal inaugural and valedictory functions for the programme but on 1 March 2003 at an evening dinner, the Vice-Chancellor of the University of Hyderabad, Kota Harinarayana gave away the participation certificates.

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