

# INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY, KYOTO

Chemistry is a phenomenological and predictive science whose domain includes all substances and their structures, interactions, properties, and transformations. Theoretical chemistry can be described as a blend of applied physics and applied mathematics directed toward the problems of chemistry. The goals of theoretical chemists include explaining empirical observations, corroborating experimental measurements, and predicting new chemical results. Quantum chemistry evolved as a branch of theoretical chemistry in the late 1920's, shortly after the advent of quantum mechanics. Since then, quantum chemistry has advanced from an empirical field to the present stage where results in the domain of chemistry can be calculated from first principles governing the structure of atoms and molecules. The current status of theoretical developments was the concern of the Third International Congress of Quantum Chemistry, held in Kyoto, Japan, from 29 October to 3 November 1979 under the sponsorship of the Science Council of Japan, the Chemical Society of Japan, and the Commemorative Association for the Japan World Exposition of 1970.

With a week of sunny and balmy autumn weather, Kyoto offered an ideal location for the Congress. The magnificent meeting facilities of the Kyoto International Conference Hall provided a serene and modern setting, in contrast to the bustle of Kyoto's metropolis and the charms of its ancient gardens, temples, shrines, and palaces. The atmosphere of the conference was quite Japanese as evidenced by the highly efficient proceedings, the careful attention to every detail, and the extreme politeness. Although two-thirds of the 650 participants came from Japan, the character of the meeting was truly international, with 46 scientists coming from the United States, 20 from France, 16 from West Germany, and the remainder comprised of small delegations from 30 other countries on every continent.

The Congress was opened by a number of speakers who represented the official hosts. The chairman of the Organizing Committee, K. Fukui (Kyoto University), observed that quantum chemistry has assumed the role of strengthening the connections between subdivisions of chemistry by using concepts of molecular structure to unify the underlying theoretical basis for all chemical phenomena. In this way, it has led to new directions in experimental work as well as to a deeper understanding of the foundations of chemistry. K. Fusimi (President, Science Council of Japan) noted that chemistry used to be mostly an experimental field consisting of such activities as measuring rates of

chemical reactions and classifying properties of chemical substances and systems. Quantum mechanics has opened new avenues and, through the pioneering efforts of chemists, has fostered quantum molecular science, which now broadly spans chemistry, biology, pharmacology, electronics, and other related areas. The central revolutionizing tool has been the computer, which is responsible for the current quantitative abilities of theoretical work. Y. Yukawa (President, Chemical Society of Japan) expressed confidence that quantum mechanics has become the basis for all chemistry—now and in the future. The opening ceremony was followed by an elegant reception that featured a sumptuous buffet, abundant sake, and traditional Japanese entertainment.

The scientific sessions of the Conference were organized into five invited symposia, one each morning; contributed papers were presented in the afternoons. English was the official language of the meeting, which included some 350 papers presented at both oral and poster sessions. (I presented a paper titled "Application of Many-Body Perturbation Theory to the Calculation of Potential Energy Surfaces.") This brief account of the meeting focuses on the 17 invited lectures and therefore omits mention of the many illuminating and important contributions that filled the week in Kyoto.

**The first symposium** discussed New Approaches in Quantum Chemical Methodology. R. G. Parr (University of North Carolina) spoke on density functional theory and its application to the concept of electronegativity and gradient expansions of potential energy surfaces. W. Meyer (Kaiserslautern University, West Germany) reviewed recent developments in *ab initio* methods for determining computationally the electronic structures of atoms and molecules. Particular attention was paid to the degree to which variational pair theory, many-body perturbation theory, and direct configuration interaction approaches are converging toward mutually consistent and accurate representations of electronic energies of chemical systems. Propagator methods in quantum chemistry were discussed by O. Goscinski (Uppsala University), and the unitary group formulation of the many-electron problem was covered by F. A. Matsen (University of Texas, Austin).

**The second symposium**, on Bond Formation and Breaking, was chaired by M. Simonetta (Institute of Chemical Physics, Milan), who commented that its topic was close to the very heart of chemistry, since chemistry can be defined as the art of making and disrupting bonds. Such events have been used by both experimentalists and theoreticians to



describe chemical reactions. Recent attention has been given to changes in electronic charge distributions along chemical reaction paths.

In his lecture, K. Ruedenberg (Iowa State University, Ames) stated that change is the essence of chemistry and that chemical reactions are of central interest. Theory can contribute important information about reactions that cannot be derived by experiment. Using theoretical methods, individual reaction channels can be isolated and intermediate and transition states can be frozen and examined. Quantum chemistry can provide qualitative interpretations of changes in energy in terms of the rearrangement of orbital structure as well as quantitative predictions of activation energies. Moreover, cross sections can be calculated for chemical scattering, as in reactive collisions and energy transfer in inelastic collisions. However, these tasks are difficult because there is a mixing of structural configurations along reaction paths, electron correlation effects must be taken into account, and chemical accuracy is very demanding, being on the order of 1 kcal/mole ( $\sim 0.04$  eV) along a reaction path.

R. F. W. Bader (McMaster University, Ontario) described a formulation of quantum mechanics through which the topological properties of the electronic charge density can be used to define atoms, molecules, and bonds. These concepts lead to a definition of structure and to a qualitative analysis of structural stability.

**During the third symposium**, Molecular Interactions, R. A. Marcus (California Institute of Technology) discussed semiclassical mechanics as a bridge between quantum and classical results both for intramolecular motion and for collisional energy transfer. If vibrational energies are high enough, individual vibrational states of a molecule can become delocalized over the classical energetically accessible region of coordinate space, giving rise to a so-called stochastic vibrational state. The mechanism of the delocalization, which can be analyzed with the semiclassical approach, has implications for such phenomena as unimolecular reactions, infrared multiphoton dissociation, and energy disposal in molecular beam reactions involving complexes.

Chiral discrimination in the interaction between two optically active molecules was discussed by D. P. Craig (Australian National University, Canberra). Theories of discriminating forces between molecules bear on the appearance of induced circular dichroism in achiral molecules and on the theory of the liquid state, for example, through knowledge of the orientational freedom of coupled chiral molecules as a function of separation distance. R. E. Wyatt (University of Texas, Austin) and Y. T. Lee (University of California, Berkeley) described theoretical and experimental aspects, respectively, of reactive scattering and the dynamics of atom-molecule collisions. Here quantum mechanics has pro-

vided the impetus to pursue an understanding of the influence of electronic, vibrational, and rotational states by examining state-to-state transitions.

**The subject of the fourth symposium** was New Fields of Molecular Spectroscopy. S. Nagakura (University of Tokyo) discussed the effect of magnetic fields on fluorescence from molecules in excited states. In carbon disulfide, for example, the effect consists of two components. The lower magnetic field component is explained in terms of resonance between the fluorescence state and appropriate triplet states through spin-orbit and vibronic interactions. The higher magnetic field component is caused by the electronic Zeeman interaction between the fluorescence state and higher rovibronic levels of the ground state. Another area concerns the external magnetic field effect on chemical reactions of radical-pair systems as exemplified in the singlet sensitized photolysis of dibenzoyl peroxide.

T. Oka (National Research Council of Canada) reviewed the status of infrared lasers as radiation sources in spectroscopy. Five general properties of lasers that have already been exploited are that lasers are monochromatic, pulsed, intense, collimated, and polarized. A further property—lasers are coherent, which is a statement about the statistical nature of the beam—has yet to be exploited and is something to be considered for the future. P. W. Atkins (Oxford University) described spectroscopic processes from the point of view of molecules as sources. When the underlying quantum-mechanical basis of photon scattering and absorption processes is explored on the basis of Schwinger's theory of sources, the fundamental primitive concepts of causality and space-time uniformity can be used as constructive principles in the discussion of optical birefringent and spectroscopic properties.

**The final symposium** considered Large Molecules of Biological Importance. Such systems are closely related to one-dimensional lattices, which are treated in solid state theory. The essential difference is that the large biological molecules lack the strict periodicity of the lattices. Some unresolved difficulties are caused by the nearly degenerate ground state, by solvent effects, and by temperature-dependent phenomena.

A. Veillard (Louis Pasteur University, Strasbourg) described *ab initio* calculations at the Hartree-Fock self-consistent-field level on hemoglobin to determine the position of the iron atom at various stages of oxidation. K. Ohno (Hokkaido University) described detailed calculations that included correlation effects in metal porphyrin complexes to evaluate excitation energies and oscillator strengths. M. V. Basilevsky (Karpov Institute, Moscow) described calculations on the mechanism of cation polymerization in crystals. The distinctive feature of these systems is the influence of the crystal field contribution to the potential energy surfaces. The propagating polymer chain moves inside the crystal lattice under the combination of crystal-



line and chemical forces. The role of nonclassical conformations is important for chain termination; this provides some insight for biological analogies. Finally, E. Clementi (G. Donegani Institute, Novara, Italy) described various techniques for calculating the effects of reactivity, solvents, and temperature on proteins and biopolymers.

The activities of the meeting were concluded by P. O. Löwdin (Uppsala University) who will be the local host of the next (1982) Congress in Uppsala. He noted that the traditional approach of quantum chemistry has been to seek an understanding of fundamental principles underlying a particular application in order to extend our knowledge to additional applications. Despite the progress that quantum chemistry has achieved, there is a long way to go before a full understanding of all of chemistry can be reached.

In conjunction with the Kyoto Congress, five satellite meetings were arranged on related but more specialized topics. One was a three-day symposium on Many-Body Theoretical Approaches to Electron Correlation in Molecules, held in Kobe. Attendance was limited to 80 participants, half of whom were from Japan. Eight of the 25 lectures were presented by Japanese scientists. (I presented an invited lecture, "Electron Correlation and Interaction Energies Between Closed Shell Systems Using Many-Body Perturbation Theory".) The meeting was supported by the Chemical Society of Japan and was financially aided by the Yamada Science Foundation and the Commemorative Association for the Japan World Exposition of 1970. The meeting was extremely well organized and offered a stimulating scientific program. Funding was also at a high level. For example, each invited speaker from out-

side Japan was provided a generous stipend to cover international travel expenses plus room and board at the Inter-University Seminar House of Kansai, the conference residence.

The remaining four meetings were smaller and of two days' duration each. One was held in Nara on Future Aspects of the Education of Theoretical Chemistry in Asia. Another met in Okazaki to discuss Theoretical Aspects of Molecular Interaction and Chemical Reaction. The other two met separately in Kyoto and covered the Design of Inorganic and Organic Materials of Technological Importance and Quantum-Chemical Aspects of Biomolecules—Their Structures and Functions.

An adjunct activity for some of the attendees from outside Japan was an invitation to visit a university or laboratory. (For instance, I was invited to present a seminar, "Electron Correlation in Simple Chemical Systems," at the Department of Materials Science of the University of Electro-Communications in Tokyo.) Such visits provided an excellent way to make closer contact with scientists and their facilities in Japan.

In conclusion, the Third International Congress of Quantum Chemistry and its affiliated meetings were enjoyable and rewarding considering the depth and breadth of the presentations. Of course, the occasion promoted interactions within the international community of scientists but, equally important, it afforded the participants from abroad the opportunity to explore parts of Japan and glimpse its customs and culture.

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## DEPARTMENTS

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