MEETINGS

Quantum Chemistry and the Solid State

Like the ever-widening ripples from a pebble dropped into a pond, the clarifying concepts of quantum mechanics spread wider through the years into all problems of science and life. This was particularly evident at the recent conference sponsored by the Quantum Chemistry Institute at Uppsala University and held at the tiny Swedish resort town of Rättvik in picturesque Dalecarlia, August 27 through September 1. The Quantum Chemistry Institute, with the stimulating guidance of Per-Olov Löwdin, specializes in attacking those problems in chemistry and solid state which may be formulated at the outset in terms of the Schrödinger equation.

The symposium dealt with a wide range of problems, ranging from the four-body problem for the H_2 molecule, considerations of density matrices in many-body theory, solid-state theory, and ligand-field theory, to recent work in "quantum biology", including suggestive considerations of protonic tunneling as affecting gene, DNA, RNA, and protein synthesis.

It was clearly apparent in the discussions that the means of application, and even to some extent the quantum theory itself in its furthest details and in its time dependency, is still under test. Much of the effort reported upon at the symposium dealt with the means available now to circumvent the considerable mathematical and computational difficulties which now beset the quantum chemist. W. Kolos of the Institute for Nuclear Research, Polish Academy of Science, Warsaw, described a successful and precise calculation of the H_2 molecule as a four-body problem, including nuclear motion and involving eighty terms. This was regarded by many attending as something of a mile-marker in testing and applying quantum theory.

Headway in attacking problems with the Schrödinger equation was disclosed on several fronts. J. Coleman, P. O. Löwdin, and Fukashi Sasaki described advances in the density matrix approach in many-body theory, whereas Norman Bazley and David W. Fox gave new methods for determining lower bounds to the energy levels of atomic and molecular systems. The electron-electron interaction (correlation) problem was also discussed in terms of the alternant molecular orbital scheme (different orbitals for different spins) by R. Pauncz for hydrocarbons, by George Dermit for diamond, and by J. W. Moskowitz for the interesting hypothetical molecule, annular H_6.

A statistical theoretical study along the lines of the Fermi-Thomas approach was described for atoms by Rezso Gaspár. The evaluation of zeta-function expansions for molecular integrals was described by Moskowitz. Remarks on linked-cluster expansions were presented by Löwdin. An interesting extension of density-matrix theory in a Hückel-type approximation was made and applied to conjugated hydrocarbons and benzenoid hydrocarbons containing heteroatoms by H. Looyenga of TNO, Delft, Holland.

On hearing the grave and complex computational difficulties facing present-day quantum chemists, and of their need to deal with many high-order determinants of complex integrals, etc., one is repeatedly struck with the hope that a way out will be found. Perhaps it will be analogous to the invention of nonunit numerators for fractions which so greatly eased the problems faced by early Egyptians who had conceived only the use of sums of fractions of numerator, 1, to express a given fractional value.

Bernard and Alberte Pullman, in masterful presentations, described the considerable progress made in accounting for the relative reactivity and natural selection of many molecules of biological importance. Particular success has been had in the interpretation of the role of enzyme constituents important in redox reactions, in calculating stability to ultraviolet radiation, in evaluating the role of functional molecular *portions* (as opposed to whole molecules) in carcinogen action, and in the evaluation of hydrogen bonding through the amino acid residues as potential pathways for electron transfer. Löwdin presented an interesting and potentially fruitful notion of protonic tunneling between the doubly hydrogen-bonded base pairs of the double-stranded DNA molecule. If such a process did occur, it was pointed out, then inversion of pairing and other information misstorage could occur. This then has direct implication in the problems of mutations, evolution, aging, and tumor inception.

Rembrance was given the perennial problem of phase determination in electron and x-ray diffraction determinations, by K. Hedberg.

New areas for quantum chemistry considerations were seen in (1) the discussion by Ronald Hoffmann of the many new polyhedric organic and inorganic molecules of cage-like structure; (2) in the development by Jan Linderberg of the Naziere-Pines many-electron approach to the treatment of the dielectric constant of a solid and the consequent estimation of London intermolecular force terms; (3) in the discussion by H. A. Pohl of (a) the nature of carrier transport vis-a-vis molecular overlap in molecular solids with special reference to conductivity and to piezo-resistivity, (b) the existing gap in the theory of carrier mobility in solids in the transition ranges between that well described by wave-packet "drifing", and that describable by "hopping" processes (i.e., between about 500 and 0.01 cm^2/volt sec), (c) the much-needed extension of theory using random coordinate spacings to the problem of electronic transport processes in amorphous solids and liquids, (d) the problem of the near identity of the

activation energy of conduction to the lowest triplet energy in molecular solids of organic nature, (4) Coleman's laudatory reference to the equation of Wentzel for many particles which is relativistically invariant; (5) Löwdin's challenging discussion of the reaction-rate problem in terms of the wave-mechanical *evolution operator* for the time-dependent Schrödinger equation. Löwdin urged a fresh consideration of the evolution operator in treating kinetic problems and expressed confidence that it would become a powerful tool.

The attending scientists, from many nations, united in expressing their deep appreciation for the hospitality extended them by their Swedish hosts, and for the stimulating approaches in quantum chemistry presented at the symposium.

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Calorimetry Conference

The seventeenth annual Calorimetry Conference was held August 22–24 at the University of California in Berkeley. Hosts for the occasion were the Inorganic Materials Research Division of the Lawrence Radiation Laboratory and the College of Chemistry. Local arrangements were made by a committee consisting of N. E. Phillips (chairman), R. Hultgren, D. N. Lyon and I. Pratt.

In keeping with the traditions of previous conferences, a wide variety of calorimetric topics was discussed, ranging from techniques, through results, to interpretation. Thirty-seven papers were presented, the principal one being that given as the Huffman Memorial Lecture by E. F. Westrum, Jr. (University of Michigan). Professor Westrum, whose topic was the thermodynamics of globular molecules, offered a lucid discussion of the problems of understanding the behavior of the so-called plastic crystals. Thermodynamic measurements on these substances can yield valuable information about transitions, and about rotation of molecules and molecular groups in the solid. Much of the available experimental information has been obtained by Professor Westrum and his students.

Invited papers were given by M. L. McGlashan (University of Reading), D. Patterson (University of Montreal), and A. M. Karo and A. W. Searcy (University of California). Each of the papers served to keynote a particular part of the program. For example, McGlashan's discussion of the calorimetric determination of the change of enthalpy of vapors with pressure and Patterson's application of the Prigogine theory to the explanation of heats of mixing of polymer solutions introduced a series of contributions on measurements of heats of mixing, solution, and dilution.

Karo described the information about lattice vibrations which is obtainable from an understanding of the thermodynamic properties of crystalline solids, illustrating his theme with examples of alkali-halide crystals. In particular, he showed that accurate experimental heat capacities are sufficient to distinguish be-