Meetings

Quantum Chemistry and Solid State Physics

Something of a mile-marker has been reached in the area of testing and applying quantum theory. This was the feeling of many who attended the Symposium on Quantum Chemistry and Solid State Physics, 27 August to 1 September 1962, as they listened to W. Kolos (Polish Academy of Science) describe a successful and precise calculation of the four-body problem that is the H_2 molecule (two electrons and two protons), a calculation which accounted for nuclear motion and incorporated 80 terms.

The symposium was sponsored by the Quantum Chemistry Institute at Uppsala University under the stimulating guidance of Per-Olov Lowdin. It was held at Rättvik, a tiny Swedish resort town. The topics of discussion were numerous, from the four-body problem already mentioned, to 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 the tunneling of protons that could affect gene, DNA, RNA, and protein synthesis. It was apparent in the discussions that the means of application, and even to some extent the quantum theory itself, in certain of its details and in its time dependency, is still being tested. Much work that was reported dealt with the means available now to circumvent the considerable mathematical and computational difficulties which beset the quantum chemist.

Progress in solving problems with the Schrödinger equation has been made on several fronts. J. Coleman, P. O. Löwdin and F. Sasaki described advances in the density matrix approach in many-body theory, while N. Bazley and D. W. Fox told of new methods for determining lower limits of the energy levels of atomic and molecular systems. The problem of electron–electron interaction (correlation) was discussed in terms of the alternant molecular orbital scheme (different orbitals for different spins) by R. Pauncz for hydrocarbons, by G. 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 R. Gaspar. The evaluation of zeta-function expan-

sions 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 compounds containing heteroatoms by H. Looyenga of Nederlandse Centrale Organisatie, T.N.O., Delft.

In masterful presentations, B. and A. Pullman described the considerable progress in understanding the relative reactivity and natural selection of many molecules of biological importance. Quantum chemistry has been helpful in interpreting the role of enzyme constituents important in oxidation reduction reactions, in the calculation of stability to ultraviolet radiation, in evaluation of 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 faulty storage of information could occur. This then has direct implications in the problems of mutations, evolution, ageing, and tumor inception.

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

There are new areas where quantum chemistry is being used to solve major problems. The determination of the cage-like structure of the many new polyhedric organic and inorganic molecules was discussed by R. H. Hoffman, and the many-electron approach of Naziere-Pines to the treatment of the dielectric constant of a solid and the consequent estimation of London intermolecular force terms was developed by Jan Linderberg. H. A. Pohl discussed the nature of carrier transport vis-à-vis molecular overlap in molecular solids with special reference to conductivity and to piezoresistivity; the existing gap in the theory of carrier mobility in solids in the transition range between that well described by wave-packet "drifting," and that describable by "hopping" processes (between about 500 and 0.01 cm^2/volt sec); the much needed extension of theory using random coordinate spacings to the problems of electronic transport processes in amorphous solids and liquids; and the problem of the near identity of the activation energy of conduction to the lowest triplet energy in molecular solids of organic nature. Finally, Coleman made a laudatory reference to the equation of Wentzel for many particles which is relativistically invariant; and Löwdin presented a 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, who came 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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Forthcoming Events

January

18–19. **Blood**, annual symp., Detroit, Mich. (G. F. Anderson, Dept. of Physiology and Pharmacology, Wayne State Univ., 1401 Rivard St., Detroit 7)

21–23. Chemistry and Biochemistry of **Seed Proteins**, intern. conf., New Orleans, La. (C. H. Fisher, Southern Utilization Research and Development Div., Agricultural Research Service, U.S. Dept. of Agriculture, P.O. Box 19687, New Orleans 19)

21–23. Institute of the **Aerospace Sciences**, annual, New York, N.Y. (IAS, 2 E. 64 St., New York 21)

21–24. American **Meteorological** Soc., annual, New York, N.Y. (R. L. Pfeffer, Lamont Geological Observatory, Columbia Univ., Palisades, N.Y.)

21–24. Advances in **Gas Chromatography**, intern. symp., Houston, Tex. (A. Zlatkis, Chemistry Dept., Univ. of Houston, Houston)

22. Infectious Diseases of the **Heart and Circulation**, conf., New York, N.Y. (C. A. R. Connor, New York Heart Assoc., 10 Columbus Circle, New York 19)

22–24. **Reliability and Quality Control**, natl. symp., San Francisco, Calif. (L. W. Ball, Boeing Co., P.O. Box 3707, Seattle 24, Wash.)

23–25. **Elevated Temperature Mechanics**, intern. conf., 3rd Navy Structural Mechanics Symp., New York, N.Y. (by invitation). (A. M. Freudenthal, 624 Mudd Bldg., Columbia Univ., New York 27)

23–26. American Assoc. of **Physics Teachers**, New York, N.Y. (R. P. Winch,