

QUANTUM CHEMISTRY SUMMER INSTITUTE

By Albert Gold

LANGUAGE differences have long presented a barrier to communication which is as troublesome as it is difficult to surmount. Further, it seems that modern scientific research has developed a second language barrier of its own to compound the difficulties encountered when national boundaries are crossed and to cause confusion and misunderstanding even among those sharing the same native tongue. For example, some readers may find it strange that an institute in quantum *chemistry* is the subject of a report to physicists, while, on the other hand, these same readers would find nothing inappropriate in the topic if it were alternately called an institute on atomic, molecular, and solid-state *physics*.

In a sense, it is quite trivial to observe that the traditionally drawn borders between various scientific disciplines have lost much, if not all, of their meaning in contemporary research. On the other hand, it seems quite important to point this out so that workers in the various sciences may become more keenly aware of the pertinent accomplishments and literature produced by those designated by dissimilar disciplinary titles. The quantum mechanical study of atoms, molecules, and solids is pursued by physicists, chemists, and mathematicians. Yet each of these groups largely persists in using its own jargon and neglecting much useful information which could be obtained from the others. Examples of the lack of communication are legion. In passing, one need only pause to consider the history of

such things as those which physicists refer to as the Bloch theorem (discovered years earlier by the mathematician Floquet) or the Wentzel-Kramers-Brillouin approximation (first worked on by Liouville in 1837).

It can certainly be said that one of the objectives of the Third Summer Institute in Quantum Chemistry was the removal of both national and scientific language barriers. The institute, held in Uppsala, Sweden, from July 17 through August 21, 1960, provided an opportunity for some one hundred participants (representing twenty nations and such varying backgrounds as experimental chemistry, theoretical chemistry, experimental and theoretical physics, and mathematics) to work and live in close association for five weeks. This, the third effort in the series, was arranged by the Quantum Chemistry Group of the University of Uppsala and the Quantum Theory Group of the University of Florida and was directed by Professor Per-Olov Löwdin of Uppsala and Florida. The remainder of the staff of the institute consisted of Laurens Jansen (Battelle Memorial Institute, Geneva, Switzerland), Ruben Puncz (Technion, Haifa, Israel), Joseph de Heer (University of Colorado, Boulder, Colorado), Roy McWeeny (University of North Staffordshire, Keele, England), Tadashi Arai (University of Tokyo, Tokyo, Japan), and Anders Fröman, Lars Hedin, Jan Nordling, and Yngve Öhrn (all of Uppsala).

The institute's role was twofold. First, it played the part of a school, educating in and reviewing the fundamentals and foundations of the theory of atomic and molecular systems, up to the level of techniques used in current research. Second, it was a symposium on new

Participants, International Summer Institute in Quantum Chemistry, University of Uppsala. Left to right, first row: Margery Fort, Laurens Jansen, Ruben Puncz, Joop de Heer, Ian Boswarva, W. J. Orville-Thomas, Per Löwdin; second row: C. H. Langford, Irving Day, Günther von Büнау, Joyce Kaufman, L. Forster, Kenneth Miller, A. R. Blythe, Fritz Klein, Karin Ericson, Jan Nordling, Martin Klessinger; third row: John Bickel, Tadashi Arai, Brian Sutcliffe, Peter Davies, Asgar Ali, Ralph Deal, Sam Faulkner, J. Brown, Dick Wood, Tom Brown, J. Dubois; fourth row: Karin Löwdin, Arthur Rotenberg, Chuck Weiss, Karl-Fredrik Berggren, Torbjörn Lagerwall, W. S. Merville, Gerhard Hanisch, Al Gold, Ludwig Bruch, Rune Pettersson, Jim Brown, Phillip Myhre, Göran Löfroth; top row: Lars Hedin, Yngve Öhrn, Bill Adams, Lawrence Lohr, Werner Kutzelnigg, W. H. Phillips, Alf Loftus. Photo by Olaf

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research, both theoretical and experimental, offering an opportunity for informal scientific discussion. Accordingly, it was divided into two parts. The introductory course filled the first three weeks and consisted of formal lectures by the staff and problem-solving sessions. The introductory work continued on a one-lecture-per-day basis through the final two weeks which were, however, primarily devoted to the advanced course. The advanced course contained both longer papers reviewing rather broad areas of current research and shorter reports (of the sort familiar in society meetings) of recent work.

THE principal material of the introductory course was presented in series of lectures by Professors Löwdin, Jansen, Pauncz, and de Heer. Löwdin's lectures covered an introduction to the many-electron Schrödinger equation and associated wave functions, the superposition of configurations, the problems of the choice of variational parameters, scaling and the virial theorem, density matrices and their applications to the calculation of expectation values and the formulation of the Hartree-Fock scheme, excitation and ionization energies, analytic Hartree-Fock functions and Slater-type orbitals, the correlation problem, and extensions of the Hartree-Fock scheme to include different orbitals for different spins, and so-called natural spin-orbitals, the valence-bond method, and exchange phenomena.

Jansen spoke on Hilbert-space formalism, the matrix formulation of the Schrödinger equation, the variational principal, the problem of upper and lower bounds for eigenvalues, complete sets, coordinate systems, prob-

lems arising from nonorthogonality of basis sets and orthogonalization procedures, stationary perturbation theory in both the Schrödinger and Brillouin-Wigner forms, the variation-perturbation method of Löwdin, and time-dependent perturbation theory.

The lectures of Professor Pauncz discussed matrix calculus and its applications in eigenvalue problems, the general theory of angular momentum, spin, the construction and applications of projection operators, atomic states, and numerical methods.

The remaining series of lectures in the introductory course was given by Professor de Heer and dealt primarily with problems in the theory of conjugated hydrocarbons (those "classically" having alternating double and single C—C bonds). Topics discussed included hybridization, localized bonds, perfect pairing, the principal of maximum overlap, conjugation, σ - π separation, simple LCAO-MO calculations, resonance energies, population analysis, self-consistent field methods, and configuration interaction. Other lectures in the introductory course were given by J. Nordling, who discussed the application of electronic computers, and A. Fröman, who spoke on $1/Z$ expansions.

The introductory course lectures, together with the supplementary exercise-solving meetings, provided an excellent foundation for the understanding of current research in quantum chemistry. The care in preparation and general excellence of these lectures on the part of the staff as a whole were indeed notable and praiseworthy. Though the primary orientation of the course was in the direction of molecular problems, the topics covered, most particularly those of a fundamental, for-

malistic nature, were of interest and benefit to participants with a wide variety of backgrounds. Though it involved some strain on the part of the participants having weaker theoretical training, a great quantity of material was quite successfully presented in a very short time.

AS previously noted, the advanced course took the form of a symposium lasting two weeks. The formal sessions covered the following topics: nuclear motion and molecular vibrations, bond lengths and isotope effects; the correlation problem; spin resonance; mathematical aspects of quantum chemistry; ligand field theory; many-body theory; conjugated systems and hyperconjugation; molecular structure and spectra; atoms in molecules; computational methods; exchange and superexchange; solid-state theory. In addition to the regular sessions, there were informal group meetings during the evenings, discussing such topics as mathematical techniques, many-particle theory and Brueckner method, conjugated systems, molecular structure and spectra, electronic computation, electron spin resonance, and the biochemical applications of quantum chemistry.

Since a full report on the proceedings of the symposium will be issued by the Quantum Chemistry Group at Uppsala, it seems unnecessary to treat the individual papers presented in detail here. However, it does seem appropriate to mention some of the work which appeared to be of particular novelty and interest. R. Dandel (Paris) discussed the electronic structure and vibrations of molecules and presented an explanation of negative spin densities in hydrocarbon radicals as a correlation effect, using the method of alternate molecular orbitals, which was discussed by R. Pauncz (Haifa), J. de Heer (Colorado), and Löwdin (Uppsala and Florida). A. Fost (Northwestern) reviewed the local-energy method for molecular calculations. D. Fox (Maryland) and N. Bazley (Maryland) presented an extensive discussion of the "method of intermediate problems" for establishing lower bounds in eigenvalue theory and explored computational techniques and the application of the theory to quantum mechanics. A. J. Freeman (MIT and OMRO, Watertown) spoke on atomic magnetic form factors and the a priori determination of crystal field strengths in crystal field theory. J. I. Horvath (Szeged) presented a summary of work on the many-body problem and discussed its application to problems in quantum chemistry.

Lively and lengthy discussions pervaded the final two weeks. Ample time was provided for them during the sessions and, in addition, discussion groups of specialized interests met during the evening. On the whole, however, it would seem that the advanced course was less successful than the introductory. This was, perhaps, in part due to the flagging of some participants after the first three weeks. It was, perhaps, due in part to the arrangement of sessions which placed all papers in a given area on the same day and had the effect of making some participants want to attend meetings from 9:00 a.m. to 9:00 p.m. on one day and none the next.

Nonetheless, a significant amount of scientific information was exchanged and propagated, and the balance was safely on the side of profit.

THE host institution, the Quantum Chemistry Group of the University of Uppsala, is a most active group of about twenty workers engaged in research on problems in the theory of atoms, molecules, and solids and is directed by Professor P.-O. Löwdin. The group is spaciouly quartered in modern facilities, including twenty-five offices, two lecture rooms, and a computing center equipped with a Logistics Research ALWAC III 8000-word magnetic drum computer. The group's staff, on the whole, did an admirable job of making all arrangements for the institute.

Lectures were held in the halls of the main building of the university. Excellent meals were provided at Smålands Nation, an institution equivalent to an American students' "eating club". Though some participants who traveled with their families stayed in apartments in the town, most were housed in a newly built dormitory, in light and well-appointed private rooms. The small, quiet university town of Uppsala was suited to such a meeting and provided much of the proper atmosphere, including the small coffee shops (*konditori*) for the all-important coffee-break discussions. The non-academic life of the participants was also looked after: the young ladies of Uppsala graced the social evenings; tours were arranged through the nearby countryside and Stockholm; a visit was made to a performance at the beautiful Drottningholm Opera House.

The summer institute set itself a prodigious task, bringing together scientists and students of varying background and attempting both to educate and stimulate research on an international scale in the short space of five weeks. In admirable part, it succeeded in this effort. Professor Löwdin and his colleagues are to be lauded and encouraged in their efforts to overcome both the national and scientific language barriers.

These efforts were continued with a winter institute sponsored by the University of Florida and directed by Professor Löwdin. The winter institute consisted of an introductory course given in Gainesville (December 12-31, 1960) followed by an advanced course held on Sanibel Island in the Gulf of Mexico (January 1-14, 1961). The courses were at the postdoctoral level and placed emphasis on solutions of the Schrödinger equation of interest in quantum chemistry and solid-state physics.

In closing, it should be noted that the summer institute was made possible by partial support from the following: The U. S. National Science Foundation; King Gustaf VI, Adolf's 70-Years' Fund for Swedish Culture; Knut and Alice Wallenberg's Foundation; the Swedish National Science Research Council, the Swedish Technical Research Council; and the Aeronautical Research Laboratory, Wright Air Development Division of the Air Research and Development Command, U. S. Air Force, its European office.