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NRCC

NATIONAL RESOURCE FOR COMPUTATION IN CHEMISTRY

ANNUAL REPORT 1980-81

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SEPTEMBER 1981

LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA

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NRCC REPORT

1980-81

September 1981

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University of California
Berkeley, California 94720

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CONTENTS

Foreword iv
Introduction 1
Technical Progress 3
Workshops Conducted in 1980-81 3
Software 16
Cooperative Programs 18
National Theoretical Effort on Combustion 18
Daresbury Laboratory Interactions 20
CECAM Interactions. 20
Research by NRCC Staff 22
Collision Dynamics. 22
Crystallography 28
Graphics. 33
Quantum Chemistry 37
Statistical Mechanics 46
Proposal Program 56
Proposals Funded 56
Hardware Developments. 57
VAX Enhancement. 57
Graphics Hardware. 57
Appendix A 58
Seminars in 1980-81. 58
Visitors 62
Appendix B 65
Publications - Others. 65
Appendix C 72
Software Requests. 72
Appendix D 76
NRCC Staff and Directorate 76

FOREWORD

This report of the National Resource for Computation in Chemistry (NRCC) is the final one for the Division. It describes all aspects of the Division's activities for calendar 1980 and through the close of the NRCC on September 30, 1981. The report focuses on the workshops and research activities of the in-house staff and workers elsewhere supported by the NRCC.

Because the NRCC has been instructed by its funding agencies, the Department of Energy and the National Science Foundation, to terminate operation on September 30, 1981, I would like to reflect on our brief past as an organization, and comment on the future of computational chemistry in this country.

First, I thank those people who have worked hard to build the NRCC, helped support it, and given it a record of accomplishment of which we can all be proud. Indeed, I feel quite strongly that, within the time and budget constraints set by the funding agencies, the NRCC has made remarkable progress in fulfilling the mission set out for it by the Wiberg and Bigeleisen Committees. We of the NRCC take pride in the numerous workshops which we have held and in the various research and software development projects which they have spawned. We believe that the NRCC Software Library that we have developed, assembled, catalogued, and distributed is a significant contribution to the chemistry community. In addition, I feel that the outstanding record of the scientific staff both in service and in their own research activities should not go unrecognized. Certainly the burden of

establishing the service component of the NRCC's activities (workshops, software library, user assistance) has made the research efforts of these computational chemists all the more impressive. Needless to say, I am deeply disappointed by the decision of the DOE and NSF to halt funding of the NRCC. I feel that, given the record of the NRCC during its short existence and the growing need within the chemical community for just this type of activity, the decision is an unfortunate and untimely one.

Having the privilege of being a part of the nation's only center for computation in chemistry has given us a unique perspective from which to view a rapidly evolving and increasingly exciting symbiosis--that between scientific research and the computer. The nature of scientific information gathering, examination, and interpretation is changing dramatically. Computational technology is providing the tools that are effecting this transformation.

Along with this changing environment have come new needs within the chemical community--the need for information on, evaluation of, and access to rapidly advancing computational hardware; the need for access to ever expanding chemical data bases; the need for a means of sharing the increasing burden of software development; and the need for establishing standards to assure that developed software has a long, broadly useful lifetime independent of system hardware and software changes. Of course, individual research groups and organizations recognize what their computing needs are and will be; and they are taking individual steps to address those needs.

Although a diversity of approaches to research level problems is healthy and should be encouraged, there are drawbacks inherent in a "cottage industry" attitude. There are an increasing number of computational "workhorse" tasks for which programs need not be reinvented or readapted at each individual laboratory or computer site. The amount of scientific manpower presently devoted to this duplication of effort is large, wasteful, and still growing. The need here is for a coherent national policy for this type of software development in the sciences, a policy that recognizes the costs and eases the burden on the individual investigator. Centralization seems to be the most cost-effective and equitable way of providing information on, evaluation of, and access to the newest computational equipment. As awareness of computational capability grows within the chemical community a wealth of research ideas will be generated. A mechanism for exploration must be available that depends upon more than happenstance of location or connection. Other countries have been addressing these problems and have committed proportionately far greater resources to solutions than has this country in the NRCC experiment. Notable are the Daresbury Collaborative Computing Projects in the United Kingdom and the Institute for Molecular Science in Japan. If the United States is to maintain state-of-the-art capability in the changing environment of scientific research it must not let its efforts to establish a coherent national policy on computational technology in chemistry end with the closing of the NRCC.

William A. Lester, Jr.
Director, NRCC

INTRODUCTION

The NRCC was established to provide facilities and personnel dedicated to advancing chemistry and related sciences through widespread, and intensive use of high-speed computational equipment. This mission is accomplished by making appropriate facilities available to a wide group of scientists, by providing and developing software to expedite and upgrade computer use, by encouraging and supporting research efforts to build new and more effective computational methods, and by carrying out an informational and educational program to bring the benefits created through the Resource to the widest possible scientific public.

At the National Academy of Sciences conceptual workshop on the NRCC in the summer of 1976, the participants agreed that the NRCC, in addition to providing major computing hardware, should provide the manpower needed to ensure that existing chemical computing software be made more efficient, accessible, and widely usable. Moreover, there was a commonly expressed desire to cooperate in the creation of needed software and to set up means to facilitate such cooperation across areas of chemistry and within them, as well as between chemists, numerical analysts, and computer scientists. Through workshops and other interactions among users, the NRCC should promote agreement, without stifling innovation, on unification, standardization, and on clarification of codes used in chemical computation, thereby making them more readily comprehensible and transferable. The NRCC should

function catalytically to increase the productivity and long-term benefits of the present large investment in computational chemistry. Such a course of action has been pursued.

Many of the organizational and management requirements of the NRCC are similar to those that govern the use of high-energy accelerators and astronomical facilities. These include a Policy Board, a Program Review Committee, a User Association, and an administrative structure as part of the facility.

The responsibility for management resides with the Policy Board and an executive officer, the Director, who is selected by the Board. The Policy Board has the responsibility for determining the operating rules of the Program Committee, which is authorized to approve proposals for utilization of the NRCC and to recommend scientific priorities. The User Association consists of representatives from the group of outside users of the NRCC and from the resident scientific staff It is patterned after similar groups associated with national laboratories and has an elected Executive Committee that implements the program of the association. It provides feedback to the NRCC on matching operations to user needs. The Association also provides a means for exchange of information between scientists both in and outside the NRCC.

TECHNICAL PROGRESS

Efforts for 1980-81 focused on research and educational functions through the research workshop program staff assistance to software users, and in-house research projects. Because of the forthcoming closing of the NRCC, the software library was moved to the National Energy Software Center at Argonne National Laboratory and to the Quantum Chemistry Program Exchange at Indiana University in Bloomington.

A brief description of the workshops, software library, staff research, and other activities for 1980-81 follows.

WORKSHOPS CONDUCTED IN 1980-81

The workshops focused on identifying bottlenecks and posing solutions to problems in theoretical and computational areas. Our experience indicates that important considerations for a successful workshop of this type include a) identification of a timely topic, b) selection of a recognized leader in the subject area to help guide the development of the agenda and to identify active workers in the field to participate, c) detailed planning of the program in order to have focused discussion on the key items to be considered, and d) restriction of participants to those most likely to contribute, in order to maximize open discussion.

THE PROBLEM OF LONG-RANGE FORCES IN THE COMPUTER SIMULATION OF CONDENSED MEDIA

January 8-11, 1980 at the Vallambrosa Center, Menlo Park, California

Organizers: Profs. George Stell and Harold Friedman, State University of New York at Stony Brook
Dr. David Ceperley, NRCC, Lawrence Berkeley Laboratory

Simulation (both Monte Carlo and molecular dynamical) has become a powerful - and nearly routine - tool in the study of classical systems of particles interacting with short-range pair potentials, i.e., potentials that decay faster than r^{-d} as $r \to \infty$, here d is dimension and r the interparticle distance. (Prototypal examples are the Lennard-Jones and hard-sphere potentials.) The utility of much simulation hinges on the surprising fact that many of the interesting bulk properties of infinite systems can be inferred with remarkable accuracy from simulations involving a relatively small number of particles (typically between 25 and 1000) in a periodic box, interacting with a pair potential that is truncated beyond three particle diameters or less. To be sure, extrapolation procedures must often be used to safely infer the infinite-system untruncated-potential properties, but conceptually they are of a relatively rudimentary nature.

For systems involving long-range forces (e.g., Coulombic, dipolar, hydrodynamic) it is a different story. Relating infinite-system

properties to the results of computer simulation involving relatively small numbers of particles, periodically replicated, raises difficult and challenging problems. The purpose of the workshop was to bring together a group of scientists, all of whom share a strong direct interest in clearly formulating and resolving these problems. There were 46 participants, most of whom have been actively engaged in simulations of Hamiltonian models of condensed media. A few participants were scientists not primarily concerned themselves with simulation, but deeply involved in the theory of such models.

Many shades of opinion and degrees of optimism emerged at the workshop, but it seems safe to say that there was general agreement that

1) the full resolution of the problems noted above entails not simply more computational expertise (or hardware, or software, or funding), but a detailed understanding of the statistical mechanics of those systems actually being simulated (typically small, periodically replicated systems) as well as those systems (typically infinite, in a well-defined thermodynamic limit) that are traditionally of primary interest to theoreticians,

2) real progress is already being made,

3) this workshop helped.

DATA INTERFACES IN QUANTUM CHEMISTRY

January 15-17, 1980 at the NRCC, Lawrence Berkeley Laboratory

Organizer: Prof. Stanley Hagstrom, NRCC, Lawrence Berkeley Laboratory

The establishment of a small working group on "Quantum Chemistry Data Interfaces," consisting of ten-twelve scientists, was an outgrowth of a recommendation made at the NRCC Conference on "Software Standards in Chemistry" held July 25-27, 1979 in Salt Lake City. The essence of this recommendation was that a working group be established by the NRCC to "specify the structure, service functions and contents of data interfaces (logical and physical) between the basic modules of a general-purpose quantum chemical system."

The major quantum chemistry systems discussed were ALCHEMY, ATMOL3, ALIS, GAUSSIAN 80, GRADSCF, HONDO, MELD, MUNICH, and PROPAGATOR, with special emphasis on program task structure (integrals, SCF, MCSCF, CI, gradients) along with associated intra- and inter-task file interfacing requirements. The concept of a run-time random-access "master" file for tying together the various system modules received considerable discussion. Other aspects of the data interface problem covered were machine-independent input/output access routines portable random access I/O, data compression, archival files, and data base access protocols.

PORTABLE CRYSTALLOGRAPHIC CODE: MULTIPLE ISOMORPHOUS REPLACEMENT

June 1-8, 1980, Part II, at the NRCC, Lawrence Berkeley Laboratory

June 8-18, 1981, Part III, at the NRCC, Lawrence Berkeley Laboratory

Organizer: Dr. Arthur J. Olson, NRCC, Lawrence Berkeley Laboratory

Workshop II

The purpose of this workshop was to assemble, debug, test and document the multiple isomorphous replacement (MIR) phasing program that had been written during the first workshop held the previous November. Those scientists who participated in both workshops included: Jim Stewart and Robert Munn, University of Maryland; Steven Freer, University of California at San Diego; Keith Watenpaugh, University of Washington, Jurgen Sygush, University of Sherbrook; Steven Sheriff, UCLA; and Arthur Olson, NRCC.

Participants joining the project for the second workshop were: Wayne Hendrickson, U.S. Naval Research Laboratory; Pella Machin, Daresbury Laboratory, Warrington, England; and Gerard Bricogne, Medical Research Laboratory, Cambridge, England.

The agenda outlined for the one week workshop was quite ambitious, since it involved checking the workings and intercommmunication of over forty individual routines.

As with the earlier workshop, tasks were parceled out to subgroups on the basis of expertise and previous experience. The modular nature of the XTAL80 system and the MIR code again aided in the parallel activity

of the cooperative project. By the end of the scheduled week all routines had compiled successfully and the program had been linked and run with both ideal and real test data. However, some bugs still persisted, and so a distributable program had not been produced within the alloted time. Participants carried tapes containing the "work in progress" back to their home laboratories for further debugging and testing.

Notable sidelights to the main workshop activity came from the two participants from England. Pella Machin, who works at the counterpart organization to the NRCC at the Daresbury Laboratory, came to the workshop primarily to observe the type of cooperative coding activity that the NRCC was sponsoring, and to examine the utilization of the XTAL Binary Data File as a standard crystallographic data format. Ms. Machin used her crystallographic and programming knowledge to contribute significantly to the week's progress.

Gerard Bricogne came to the NRCC from Cambridge, England, for a six-week period primarily to implement a new method he was developing for solving the MIR phasing problem. His new method involves treating the most probable phases as implicit functions of all the parameters of all the isomorphous derivatives. After presenting the method to the group, it was agreed that once tested, the method would be worthwhile incorporating into the XTAL80 MIR Program. His interaction with the other workshop participants was mutually valuable. Through participation in the workshop, Dr. Bricogne became familiar enough with the existing MIR program to outline the means of dove-tailing his new algorithm into the program.

Workshop III

The final workshop was set up to critique the running program and to refine macromolecular data sets in a "production" setting. Calculations were carried out which formed phases and refined the heavy-atom parameters for actual protein structures. The main effort was final debugging, documentation, clean up of the printed output, planning the enhancement of the code to include the phase refinement method of Bricogne.

Alder, Freer, Sheriff, and Watenpaugh had spent considerable time in the inter workshop period rewriting and debugging the codes produced at Workshop II. This effort along with the concomitant development of XTAL system led to a more relaxed, but productive third workshop. The third workshop was what the end of the second workshop had been hoped to be.

RECENT DEVELOPMENTS AND APPLICATIONS OF MULTICONFIGURATIONAL HARTREE-FOCK (MCHF) METHODS

July 14-16, 1980 at Texas A & M University

Organizers: Dr. Michel Dupuis, NRCC, Lawrence Berkeley Laboratory
Dr. Danny L. Yeager, Texas A & M University

The goals of the workshop were to foster discussion of ideas in multiconfigurational methodology which might lead to better methods and computer codes, and to consider chemical applications which would benefit from the availability of MCHF wavefunctions. Thirty-five scientists involved in the development of MCHF methods and their applications attended the workshop and reported on their work. The Fock operator approach developed in the early 1970's, the "super-CI" approach, and the recently introduced exponential unitary transformation approach were analyzed in detail. The view emerged from the attendees that the convergence behavior for ground and excited state wavefunctions was well understood. Speakers discussed applications of MCHF methods to response functions, effective hamiltonian methods, potential energy surface calculations, and symmetry breaking problems. One question still to be resolved is the selection of configurations to be included in the MC wavefunctions in order to assure a reliable description of chemical systems.

COMPUTER SIMULATION OF ORGANIC AND BIOLOGICAL MOLECULES

January 5-8, 1981 at Asilomar Conference Center, Pacific Grove

Organizer: Prof. A. J. Hagler, University of California at San Diego

The workshop brought together a variety of scientists with, at first glance, very different interests and outlooks, ranging from gas phase electron diffraction to NMR spectroscopy of proteins. This variety was also evidenced by the range of molecules which occupied the interest of the various participants. These ranged from the cyclohexane and IF_7, to polynucleotides, proteins, and aqueous solutions. It might be interesting to ponder that, irrespective of the size of the molecule, the investigator was not completely satisfied with his understanding of the intramolecular forces which determined its properties. The diversity of interests was, in fact, a major contribution to the success of the meeting, as it brought out very different perspectives, and allowed exchange of views between people who might otherwise not cross paths.

The aspect common to each participant was that each one had struggled with the problem of determining the properties of his or her molecular system from the nature of its inter- or intramolecular forces. This struggle was carried out with the aid of a computer. In general the computer was given a set of coordinates, a potential energy function, and, of course, a program (software) to tell it what to do with the energy functions and coordinates, and was expected to yield the desired

properties. Both the science and the software were presented, and the variety stimulated lively and interesting discussion.

Seven sessions were held, followed by a round table discussion. The first day's sessions were divided roughly into discussion of (1) molecular mechanics applied to smaller molecules; (2) conformational studies of nucleotides and (3) dynamics and energetics of small peptides. The second day's discussion moved on to still larger systems including proteins, and protein hydration. The final session continued the theme of introducing solvent with two talks on Monte Carlo simulations of hydration.

The round table discussion focused on the desirability of writing a general software package for calculating the properties of molecular systems using methods of classical mechanics e.g., molecular mechanics, Monte Carlo, and molecular dynamics using an analytical representation of the energy. Although there was general agreement that the larger number of individual software packages discussed at the meeting represented considerable duplication of many man-years of effort, there were mixed feelings expressed about creating a standard package. There was a consensus that a small group of experts convene in a mini-workshop to determine the value of such a package. A variety of extremely useful and potentially valuable suggestions were made for consideration in this proposed effort. These were: the need for transportability; use of RATMAC; conflicting demands between transportability and efficiency; need for clear, adequate documentation; mechanism for user feedback; problems in defining programming modules and assigning modules to individuals who would need to anticipate communication between modules and consider

problems which would arise in debugging; assessment of existing programs as a nucleus for proposed package; establishment of a common data format among workers in field; need for consultants on data base management and for experts in programming.

EFFECTIVE POTENTIALS IN QUANTUM CHEMISTRY

June, 15-17, 1981 at the Los Alamos National Laboratory

Organizers: Dr. P. Jeffrey Hay, Los Alamos National Laboratory
Dr. Willard Wadt, Los Alamos National Laboratory

The prime focus of this workshop was to explore ideas for removing the major source of ambiguity in ab initio effective potentials, namely, the construction of pseudo-orbitals. Other areas of discussion included the choice of core orbitals, the dependence of the potential on the parent atomic configurations including oxidation state, and extensions of the technique needed to (1) incorporate relativistic and correlation effects, (2) calculate properties other than the energy, and (3) derive effective potentials for molecular fragments. Thirty-two of the leading workers in this field, including five from outside the U. S., met in a format that permitted talks by all participants. Each session was highlighted by two to three extended presentations followed by shorter prepared comments by other workers on the session topic. Because of limitations imposed by the NRCC's closing and uncertainties of support staffing, no workshop proceedings volume was prepared.

PERTURBATION METHODS IN QUANTUM CHEMISTRY

July 7-10, 1981 at the University of Washington, Seattle, Washington

Organizer: Prof. Ernest Davidson, Department of Chemistry, University of Washington

The purpose of this workshop was to bring together active workers in perturbation methods to present recent advances and to explore factors limiting the use of perturbation theory for calculations of, for example, ground state potential energy surfaces near equilibrium and at large bond lengths, vertical excitation energies and oscillator strengths, and excited state potential energy surfaces for polyatomic systems. Speakers were asked to divide their 45-minute presentations equally between their novel approaches to the basic theory, successful applications of their approaches, methods and difficulties in implementation, and other difficulties and limitations of their methods. This format permitted discussion to focus primarily on inherent problems and possible solutions. Twenty four of the leading researchers in this field, including six from outside the U.S., engaged in 3 1/2 days of intensive exchange on various aspects of the subject. Informal notes were prepared beforehand for review by the participants. Unlike earlier workshops, however, no proceedings volume summarizing the individual talks and discussion were possible because of the limitations of time imposed by the NRCC's closing, and uncertainties of support staffing.

SYMPOSIUM ON SUPERCOMPUTERS AND CHEMISTRY

A symposium on Supercomputers and Chemistry was held in Las Vegas as part of the National Meeting of the American Chemical Society during the week of August 24-29, 1980. This symposium was jointly sponsored by the ACS's Division of Computers in Chemistry and Physical Chemistry and by the NRCC. Co-chairmen for the symposium were Dr. Isaiah Shavitt of Battelle Columbus Laboratory and Professor Peter Lykos of the Illinois Institute of Technology, Chicago, Illinois.

The symposium was highlighted by discussions of the state-of-the-art and future trends in large scale scientific computers. Representatives of several major computer manufacturers outlined both present and planned capabilities. A novel approach to large scale computing utilizing a user-made micro vector processor was also described.

Several experiments in the conversion of codes to vector processing machines were discussed by representatives of the Daresbury Laboratory and the NRCC. They found that, while a significant increase in speed over non-vector machines could be obtained without major rewriting of programs, a much larger increase was possible by redesigning and improving existing algorithms.

Many applications of vector processing machines were also described. A major conclusion of these talks was that there are several areas of computational chemistry, such as artificial intelligence and graphics, where the real-time use of high-speed vector processing machines is critical.

SOFTWARE

The GAUSSIAN 80 series of programs developed by Professor J. A. Pople and co-workers at Carnegie-Mellon University was made available for distribution through the NRCC. GAUSSIAN 80 is a connected system of programs capable of performing ab initio molecular orbital (MO) calculations within the linear combination of atomic orbitals (LCAO) framework. It represents further development of the GAUSSIAN 70 and GAUSSIAN 76 systems already published.

The system contains programs for the calculation of the required one- and two-electron integrals using basis sets of s, p, or d cartesian gaussian functions. Programs are included for the determination of Hartree-Fock (HF) single-determinant wavefunctions and associated total energies. Closed-shell singlet states are computed following the restricted Hartree-Fock (RHF) procedure of Roothaan. Wavefunctions and energies for open-shell states are obtained by the unrestricted Hartree-Fock (UHF) procedure. Also incorporated is the capability for computing the Mulliken population analysis, the electric dipole moment, spin densities at the nuclear coordinates, first derivatives of the Hartree-Fock energy with respect to all nuclear coordinates, and control programs for energy minimization.

There are several methods included for going beyond the Hartree-Fock level. The electron correlation energy may be calculated by Moller-Plesset perturbation theory carried to second order (MP2) or third order (MP3). Programs are also provided to perform configuration interaction (CI) calculations with double substitutions.

PROGRAMMER'S GUIDE FOR XTAL80 SYSTEM OF CRYSTALLOGRAPHIC PROGRAMS

As part of its effort to foster the generation of portable code for chemical computation, the NRCC, in cooperation with the University of Maryland Computer Science Center, published a manual for the XTAL system of crystallographic programs. The XTAL system, developed by Professor James Stewart of the University of Maryland and co-workers, is the outgrowth of a collaborative development effort. For example, the NRCC's multiple isomorphous replacement (MIR) code will be an element of the XTAL system.

The Programmer's Manual details the structure of the XTAL system and describes the following XTAL tools, conventions, and restrictions:

1. XTAL nucleus routines which provide essential primitives.
2. Program naming conventions which provide unique names for routines and permit easy assembly of the XTAL system.
3. A storage allocation scheme which provides for efficient utilization of memory.
4. Intercommunication protocol which insures proper communication between XTAL routines.
5. A template for a typical program which illustrates use of the communications protocol.
6. SYSTEM common blocks which provide inter-routine communication within a single program.
7. OVERLAY common blocks which provide communication between different XTAL program segments.
8. Specifications for integer and floating point words.

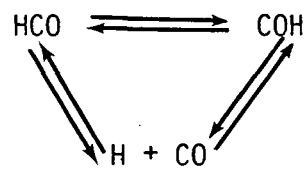
9. Word packing convention and utility macros.
10. Bit, byte, word, integer, real, and character manipulation macros.
11. The QXDATA common block which provides storage for all I/O buffers and large arrays.
12. A procedure for dynamic core allocation.

COOPERATIVE PROGRAMS

NATIONAL THEORETICAL EFFORT ON COMBUSTION

The third meeting of participants in the national theoretical effort on combustion took place at the NRCC on February 21, 1980. This group, which is involved in a collaborative effort on the chemistry of combustion, is currently pursuing a course of research to elucidate the electronic structure and collision dynamics of a system of reactions involving carbon, hydrogen, and oxygen. Progress in the following areas was described at the meeting.

1. Ground-state potential energy surface calculations for the reactions



2. Valence bond pictures and potential curves of molecular states arising from

$$CH\ (^2\Pi,\ ^4\Sigma^-) + O\ (^3P).$$

3. An approach for dealing with the reaction dynamics of polyatomic systems.
4. Application of semiclassical methods to the unimolecular decomposition of HCO.

As a result of this meeting, several participants decided to look in more detail at the reaction

$$H + CO \rightleftharpoons HCO$$

The goals associated with this subproblem are:

1. To refine the calculation of the energy barrier to within 1-2 kcal/mole;
2. To calculate the vertical excitation energies;
3. To determine the anharmonicity effects for use in vibrational energy transfer and unimolecular dissociation processes; and
4. To examine the feasibility of calculating the potential energy surface to a high level of accuracy for reliable estimation of the lifetime, and to explore the effect of the fourth body.

Because of the added costs of travel and current budget limitations, it was deceided that future meetings of the group be held only as a part of the DOE Combustion Contractor's meeting. The final meeting of the Theoretical Combustion Interest group under NRCC aegis was held on 29 October 1980 as a part of the aforementioned meeting at Argonne National Laboratory.

DARESBURY INTERACTIONS

During 1980-81 there were continuing contacts between Daresbury workers involved in Collaborative Computational Projects (CCP) collaborations and the NRCC. As a result of these contacts, Daresbury staff arranged two visits to the NRCC.

During August 1980, Dr. M. F. Guest visited for discussions on the current status of quantum chemistry codes at the NRCC. He arranged for several widely used programs to be forwarded to Daresbury. These included the latest versions of ALCHEMY, GAMESS, GRADSCF, MELD, and XASW.

Dr. P. A. Machin attended the second MIR (Multiple Isomorphous Replacement) workshop to initiate collaboration and exchanges between crystallographers in the United States and at Daresbury. It is indicated that the final XTAL program including the new MIR code will be implemented.

CECAM INTERACTIONS

In 1980 the Centre European de Calcul Atomique et Moleculaire (CECAM) (European Center for Atomic and Molecular Calculations) and the NRCC collaborated in support of a workshop on "Laser Excitation and Dynamics of Highly Excited Polyatomics." This joint workshop effort was carried out under a cooperative agreement between CECAM and the NRCC.

The U. S. participants in this workshop were M. Goodman (University of Southern California), K. Kay (Kansas State University), R. Marcus (California Institute of Technology), D. Noid (Oak Ridge National Laboratory), and E. Thiele (University of Southern California).

The workshop was held at the University Paris-Sud, Orsay, under the guidance of CECAM director C. Moser. Its focus was the construction and critical evaluation of theories of intramolecular relaxation in complex polyatomic molecules. Questions of energy localization versus ergodicity in polyatomics excited by laser light were considered together with a re-examination of the applicability of RRKM theory to unimolecular decay of molecules excited above the dissociation threshold by multiphoton absorption of infrared laser photons.

RESEARCH BY NRCC STAFF

COLLISION DYNAMICS

1. Rainbow Scattering in Inelastic Molecular Collisions L. D. Thomas

This subject has been reviewed with particular emphasis on the rainbow structures in rotational state distributions of differential cross sections at fixed scattering angle (rotational rainbows). The classical analysis has been extended for atom-rigid rotor collisions. In particular 1) it has been shown that rainbows occur at points where both the scattering angle and final rotational angular momentum are extrema, 2) in the region of an attractive potential well two or more rainbows can coalesce, and 3) double rainbows in the total differential cross sections are due to an asymmetry in the anisotropic potential.

2. Theory of Photodissociation of Polyatomic Molecules V. Z. Kresin and W. A. Lester, Jr.

An adiabatic theory of polyatomic photodissociatioon has been developed that explicitly treats the interaction between the relative and internal motion and leads to an expression for the nuclear wavefunction of the final dissociative state which differs considerably from the zeroth-order distorted-wave approximation. The vibrational frequencies ω_i of the fragments are found to depend on the interfragment distance. In the evaluation of the matrix element needed to describe the energy distribution of the fragments, it is found necessary to use values of ω_i different from the frequencies of the free fragments. These values of ω_i can be expressed in terms

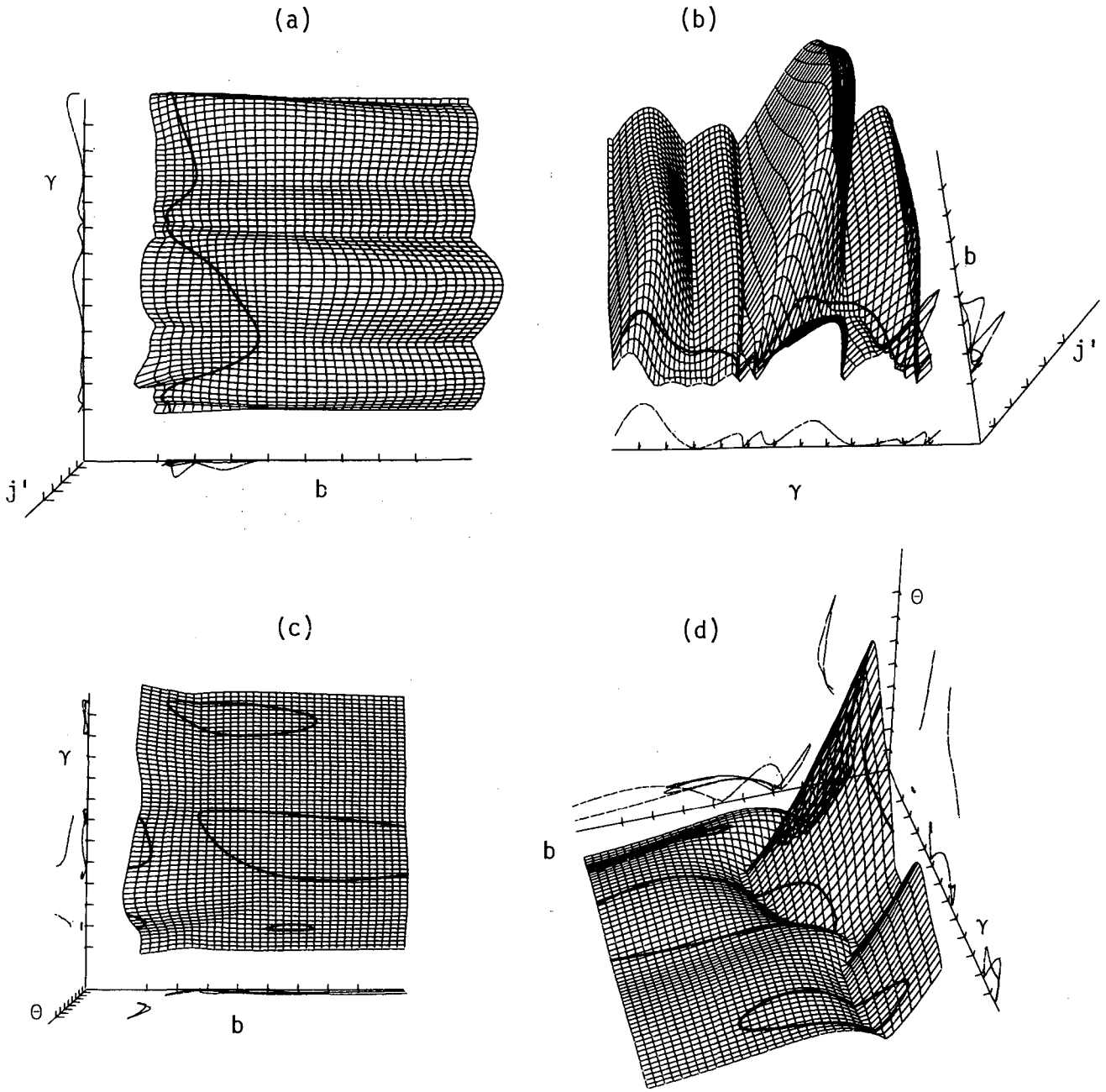


Figure 1. Surfaces of final rotational angular momentum, j', and scattering angle θ for classical, coplanar scattering of Li^+ from CO.
(a) j'(b,γ). The j'-axis is directed outward in front of the page. The view is down on the top of the surface. The heavy line on the surface is a trace of a θ = 10° contour. Projections of this line are shown in the (j',γ) and (j',b) planes. (b) A different view of the same surface as in (a). The j'-axis is directed outward in front of the page. (c) θ(b, γ). The θ-axis is directed outward in front of the page. The heavy lines on the surface are traces of the j' = 12.17 contours. Projections of these lines are shown in the (θ, b) and (θ, γ) planes. (d) A different view of the same surface as in (c).

of the force constants of the precursor system. Inverse vibrational distributions are obtained from this theory in accord with recent experimental data.

3. Iterative Method for a Single Column of the S-Matrix L. D. Thomas

Two different algorithms have been developed and tested for an improved version of the iterative method for solving the close coupling equations of inelastic molecular collision theory for a single initial state. With this method the potential energy matrix is divided into $V=V^0+V^1$. The Green's function is computed for the unperturbed V^0. Then Kato's variational method is used to accelerate the convergence of Born's series. The improvement over the original method is to include off-diagonal elements of V in V^0. The new work has been in the computation of the non-diagonal Green's function. The problem with this approach is connected with the irregular function which is divergent in the non-classical region. The first algorithm attempted to avoid this difficulty by computing the wavefunction ratio, $\Psi(r_i)\ \Psi^{-1}(r_{i+1})$, rather than the wavefunction itself. This was partially successful, but numerical instabilities were still troublesome for some problems. Therefore, a second algorithm was developed. This method uses the log derivatives, $\Psi'\Psi^{-1}$, and numerical stability is achieved through use of the matrix Wronskian relation between the regular and irregular solutions. This algorithm is stable for all problems attempted to date. Satisfactory tests of up to 360 coupled equations have been completed for the He-CO systems. Five hundred channel problems will be possible with this program. The increase in computer time appears to be linear in the

number of coupled equations. Preparations are underway for the application of this method to N_2-N_2 and HF-HF collisions.

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CRYSTALLOGRAPHY

Crystallographic research at the NRCC has focused on the area of macromolecular structure determination and interpretation. The application of diffraction techniques in this realm has grown dramatically in the past decade and is demanding increasing computer resources. The computational methodology used in analyzing molecular structures of this size is still very much in the development state. By concentrating effort on virus structure - among the largest crystallographic problems yet to be undertaken - not only will important information be gained about basic molecular biological processes but also new computational techniques will be developed that

will have considerable impact on future crystallographic investigations that are at the frontier of structural knowledge.

1. Interpretation of Macromolecular Structural Assemblies A. J. Olson

Crystallographic research has been, since its inception, one of the most computationally intensive branches of experimental chemistry. Present crystallographic techniques allow investigation of macromolecular structures such as proteins and nucleic acids. Analysis of structures of this size present very demanding tasks to the crystallographer. The interpretation of complex structural information is one task that can be greatly facilitated by the appropriate scientist-computer interface. Work is presently underway at the NRCC to develop graphical methods for examining assemblies of macromolecular structures.

The atomic level interpretation of supra-molecular aggregates such as viruses, multi-subunit enzymes, and organelles, is critical to a detailed understanding of fundamental cellular processes such as self-assembly, regulation and recognition. Since the acquisition of the Evans and Sutherland Multi-picture System in May of 1980, work has progressed on the development of general purpose software for graphical analysis of three dimensional structures. The graphics interpreter language GRAMPS[1] has been developed and implemented, and used in the study of multi-subunit macromolecular structures. The ability to easily generate symmetry related elements using GRAMPS has greatly facilitated the analysis of intermolecular contacts in virus structures. Work is continuing on developing both GRAMPS and

additional software written to interface with GRAMPS for higher level application.

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1. T. J. O'Donnell, and A. J. Olson, "GRAMPS a graphics language interpreter for real-time interactive, three-dimensional picture editing and animation." Computer Graphics 15 1981.

2. The Structure of Tomato Bush Stunt Virus At 2.9 Angstroms Resolution A. Olson and S. Harrison (Harvard)

The structure of tomato bushy stunt virus (TBSV) has now been solved to near atomic resolution.[1] By several measures this is the largest crystal structure to be solved to date (600,000 daltons in the crystallographic asymmetric unit, 383 angstrom cubic unit cell axis). Work is presently underway on the refinement and interpretation of the structural results. The size of the structure necessitates new developments in the techniques of structure interpretation. Concurrent work is proceeding along these lines.

As analysis progresses, we are learning more about the nature of flexibility of proteins in supra-molecular assemblies. In the TBSV structure, 180 chemically identical proteins pack to form the icosahedrally symmetric coat of the virus particle. As a result of the particle geometry, the proteins occupy three distinct symmetry environments. Important structural and functional differences exist between the three distinguishable versions of the coat protein molelcule. The virus structure thus gives three distinct pictures of the same molecule, and shows the flexibility that has been built-in by

evolution to enable the process of self-assembly. Using the interactive graphics system, work has progressed on the analysis of several protein-protein interfaces and several modes of structural flexibility. The interaction of protein "arms" around the particles three-fold axes seems to be implicated in correct particle sizing and assembly. In addition to conformational changes between the symmetrically distinct versions of the protein subunits, new conformations arising from data on a swollen form of the virus particle have been examined.

Using GRAMPS a nine-minute film describing the structure of tomato bushy stunt virus has been produced.

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1. S. C. Harrison, A. J. Olson, C. E. Schutt, F. K. Winkler, and G. Bricogne, Nature, Vol. 276, pp. 368-73 (1978).

3. Antigenic Peptides in the Structure of the Influenza Virus Haemaglutinen A. Olson and R. Lerner (Research Institute of Scripps Clinic)

The structure of haemaglutinen has recently been solved to 3 Å resolution[1]. It is this molecule that is the major surface antigen of the influenza virus. Concurrently, work has been carried out on the synthesis and immunological analysis of peptide fragments of the haemaglutinen molecule. These fragments have been used to produce antibodies, which in turn have been tested against the intact haemaglutinen complex (a trimer). Using the NRCC interactive molecular graphics facility, we have examined these peptide fragments within the

context of the 3-dimensional structure of the haemaglutinen trimer. We have correlated antigenic response of each peptide fragment to its position in the intact structure. The results of the analysis have implications both for the understanding of immunological activity and for further structural knowledge regarding the packing of the haemaglutinen trimer on the surface of the intact influenza virus.

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GRAPHICS

1. Interactive Graphics in Chemistry T. J. O'Donnell

The use of computer graphics in chemistry has been rapidly growing in recent years, not only in the production of publication graphics, such as plots and contour-diagrams, but also in sophisticated interactive real-time systems for macromolecular structure determination and drug design.[1,2] As chemical systems become more complex there will be an even greater need for computer graphics tools

to aid the researcher in visualizing large amounts of data, constructing and evaluating models, and in presenting results to other scientists and to the public. For these purposes, computer graphics software has been developed principally in an ad hoc manner, with a single graphics task in mind. Rather than further develop or collect a set of single purpose graphics programs, the graphics work at NRCC has focused on the development of a general purpose interactive graphics language to form the basis for a multitude of differing chemical applications.

The NRCC's graphics system consists of an Evans and Sutherland Multi-Picture-System interfaced to a VAX 11/780 computer. The software system developed at the NRCC is called GRAMPS (GRAphics for the Multi-Picture-System). GRAMPS is written entirely in FORTRAN IV and consists of two main parts. The large part is run as a background process on the VAX and manages the graphics data base and the display cycle. This part also contains the command language interpreter through which the user controls the graphical data base and specifies interaction with the data base. The second part, which is run as a foreground process, accepts commands, passes the commands to the interpreter, and governs the synchronization of the display list update and other display list functions occurring in the background.

The command language and display list functions of GRAMPS were designed for great flexibility and ease of use. The command language has a simple format consisting of a VERB (such as ROTATE, SCALE, SAVE) followed by ARGUMENTS specifying names of objects to be manipulated and functions describing the type of manipulation desired. GRAMPS

also contains features useful for constructing animated sequences of image manipulation for future playback or eventual filming.

GRAMPS has been used by members of the NRCC staff in a variety of chemical applications.

1) The Tomato Bushy Stunt Virus (TBSV) particle geometry has been extensively modeled by A. J. Olson. The dynamic model constructed by Olson presents aspects of the TBSV particle ranging from an alpha carbon trace of a protein subunit of the particle to a surface representation of the icosohedral symmetry of the virus envelope.

2) The representation of three and four dimensional potential surfaces has been investigated by T. J. O'Donnell. By sequentially paging through many three dimensional plots of potential energy, it is possible to investigate a four dimensional surface in real-time.

3) David Ceperley of the NRCC has used GRAMPS to display the dynamics of molecules in a Monte Carlo simulation of polymer chains.

4) R. Mathies of the Department of Chemistry, University of California, Berkeley, in conjunction with A. J. Olson and T. J. O'Donnell has used GRAMPS to dynamically display the atomic motion in the normal modes of retinal, the chromphore of the visual pigment rhodopsin.

5) T. J. O'Donnell has graphically investigated some of the bond angle and torsional angle changes in strands of double helical DNA that lead to unwinding in model structures.

Recently two films have been produced demonstrating the features of the TBSV particle model and the unwinding of the double helical DNA model.

The development of GRAMPS is continuing in two major directions. Manipulation of images, currently controlled by a command language interpreter which requires a knowledge of GRAMPS commands and syntax, will be governed by system extensions which will enable the user to select options from a menu of available items displayed on the graphics screen. The second direction aimed at aiding molecular modeling and structure manipulation, will enable the independent manipulation of subsections of a molecule. Currently, a molecular structure is displayed in GRAMPS as a rigid line drawing which can be manipulated only as a whole.

O'Donnell and Olson presented a paper describing GRAMPS at the Special Interest Group in Graphics of the Association for Computing Machinery Meeting, SIGGRAPH '81, Dallas, Texas, August 3-7, 1981.

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QUANTUM CHEMISTRY

1. Theoretical Study of the Reaction of $O(^3P)$ with Olefins

M. Dupuis, J. Wendoloski, and W. A. Lester, Jr.

The reactions of oxygen atoms with olefins play an important role in combustion processes and photochemical oxidation. Although global reaction rates have been measured for many of these reactions, very little is known about the elementary steps and the free radical intermediates formed in these important reactions.

Two significant routes were originally proposed by Cvetanovic for the simplest case

$$O(^3p) + C_2H_4 \rightarrow CH_3 + HCO \qquad (95\%)$$

$$O(^3p) + C_2H_4 \rightarrow H_2 + H_2C_2O \qquad (4\%)$$

In a crossed molecular beam experiment using photoionization mass spectrometry detection, Gutman was able to observe the various

products above. The dominant mechanism has long been assumed to involve the electrophilic addition of $O(^3P)$ to the double bond to form a diradical which then rearranges to form vibrationally hot acetaldehyde and ethylene oxide. The rearrangement is presumably followed by unimolecular fragmentation to various radicals.

Recent independent experiments by Y. Lee (LBL and UCB), H. Hunziker (IBM-San Jose), and by A. Luntz (IBM-San Jose) indicate that the substitution mechanism for the formation of the CH_2CHO radical plays an important role in the reaction of oxygen atoms with olefins and call for a reassessment of the reaction mechanisms. With LBL Director's Program funds, we undertook a theoretical study to determine the molecular structure of reactants, intermediates, and products of the $O(^3p)$ + C_2H_4 reaction. Both <u>ab initio</u> Hartree-Fock (HF) and configuration interaction (CI) wavefunctions were used in conjunction with a double zeta plus polarization basis set. The calculated energy diagram is shown in Fig. 1. The energies are estimated to be accurate to within 15 %. The following results were obtained:

1. Oxygen addition to the olefin double bond is exothermic by ~ 15 Kcal/mol.
2. The structure of the diradical CH_2CH_2O is similar to the structure of the ethyl radical.
3. H-atom elimination to form CH_2CHO + H has an energy barrier of less than 10 kcal/mol.
4. H-atom migration in CH_2CH_2O to form CH_3CHO has an energy barrier of ~ 50 Kcal/mol on the triplet surface.

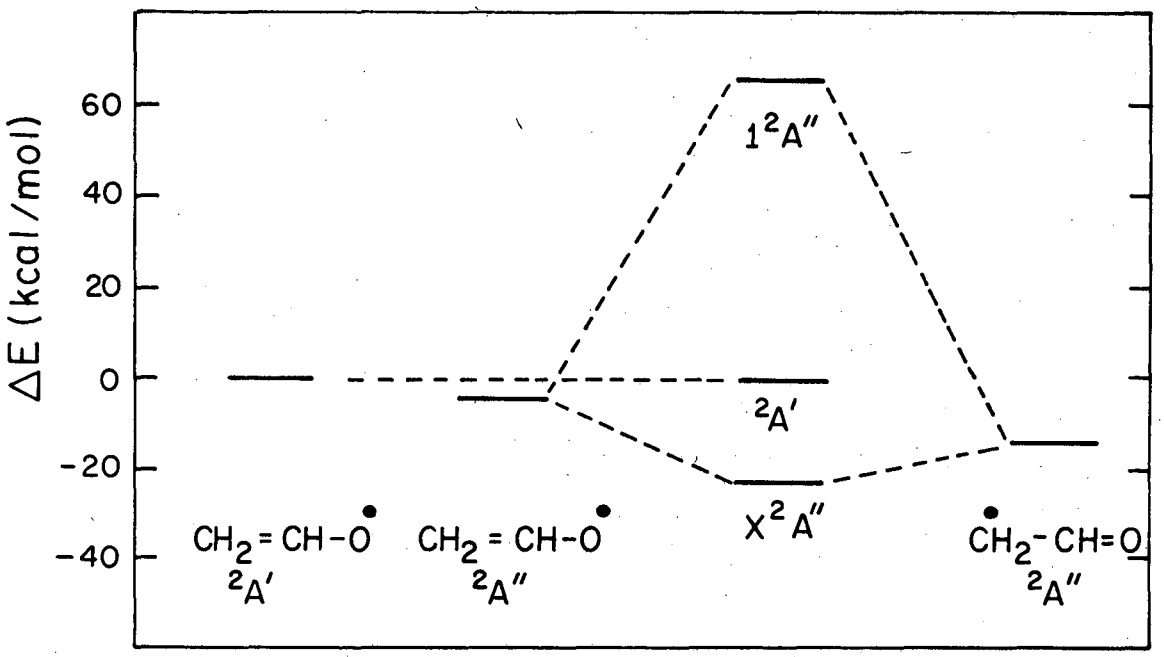

Figure 2. Resonance correlation diagram for the $^2A''$ and $^2A'$ structures of the CH_2CHO radical.

5. H-atom migration in CH_2CH_2O to form CH_3CHO has an energy barrier of ~ 10 Kcal/mol on the singlet surface.

The above results lead to the following significant conclusions:

i. The reaction $O(^3p) + C_2H_4 \rightarrow CH_3 + HCO$ proceeds through an intersystem crossing involving the diradical intermediate CH_2CH_2O.

ii. The vinoxy radical CH_2CHO is a product of the reaction of $O(^3P) + C_2H_4$.

2. <u>Special Projects in Molecular Spectroscopy</u> M. Dupuis, J. J. Wendoloski, T. Takada

Theoretical investigations of molecular structure and spectra as well as chemical reactions, such as $O(^3p) + C_2H_4$, require powerful computer codes to obtain accurate descriptions of molecular reactants, intermediates and products. The HONDO program, developed originally in part by Dupuis, is specifically designed for the study of chemical reactions. Over the past couple of years, the NRCC staff has extended the capabilities of the code. It is useful for present purposes to present a brief description of HONDO here; see also the Annual Report of the NRCC Division for 1979, p 24.

For a variety of wavefunctions [restricted and unrestricted Hartree-Fock (HF) generalized valence bond (GVB)], the program can generate directly the energy gradients, and from this information determine the minimum energy structure and complete vibrational spectrum of a molecules. The Graphical Unitary Group Approach (GUGA) computer code for configuration interaction calculations developed by H. F. Schaefer (LBL and UCB) and coworkers has been incorporated in HONDO to provide a quantitative description of electron correlation. Many molecular properties can be calculated from the wavefunctions. In the last year, partially supported by Director's Program Funds, three very important features were added to the code:

1) automatic determination of transition states (saddle points) on potential energy surfaces; 2) use of multiconfiguration Hartree-Fock (MCHF) wavefunctions for molecules not well

represented by HF wavefunctions; and 3) analytic evaluation of the second derivatives of the energy with respect to nuclear coordinates for HF, MCHF, and CI wavefunctions. Items 2) and 3) are the implementation of novel computational methods developed by Dupuis assisted by Takada.

The importance of these three features can not be overemphasized. The determination of reaction saddle points contribute greatly to the understanding of chemical reaction mechanisms, as shown in the $O(^3p)$ + C_2H_4 study. In many chemical reactions the HF model is known to break down, while a compact electronic description can be obtained with an MCHF wavefunction. Finally, with analytical evaluation of second derivatives of the energy, more powerful search methods for stationary points can be implemented. In addition it can be shown that the analytical evaluation of a force field is ~ 10 to 100 times more efficient than the usual method which uses numerical differences of the energy gradient.

3. Collective Excitations in π-Electron Systems V. Z. Kresin

Collective excitations can be defined as states, absent in a system of non-interacting particles, which may be interpreted as bound states. The many-body theory of finite Fermi systems has been applied to find the collective excitations in π-electron systems of complex molecules. Collective levels correspond to the poles of the vertex function describing the effective electron-electron interaction. Different groups of collective levels were found. One of them is analogous to plasmons in a solid and is located high in the electronic manifold.

The most interesting group is located below the usual first-excited electronic energy level. The existence of this group results in a specific multiplet structure in the spectrum.

The pair correlation of π-electrons also leads to the appearance of collective levels. The existence of low-lying exciton-type collective levels is determined to be a general feature of large π-electron systems.

4. Superconducting Materials V. Z. Kresin

It is well known that new specific effects, not observed in bulk samples, can appear in thin films. An interesting direction of research is connected with the study of films which are characterized by the quantization of the transverse motion (i.e., size quantization). This phenomenon is very sensitive to the quality of the film. The best conditions for its observation are realized in semimetal and semiconductor films, where a number of factors cause the de Broglie wavelength to exceed greatly the atomic distance, and it is this property which makes a surface specular.

A very interesting phenomenon has been observed by several independent groups in superconductor-semiconductor and superconductor-semimetal systems. It turns out that T_c oscillates if the thickness of a normal non-metallic film is changed. The mean value of T_c depends on the composition of the system. Some systems are characterized by the relation $\overline{T}_c > T_{co}$, where T_{co} is the critical temperature of the isolated superconducting film.

I have developed a theory of this phenomenon. It is based on the following considerations:

- A proximity effect which results in the appearance of the induced superconductivity of semiconductors (or semimetals).
- The size quantization of semiconducting film.
- The appearance of additional attraction in the superconducting film which is due to the interaction of its electron systems with the phonon modes of the (semiconductor or semimetal) covering.

By studying superconductor-semiconductor and superconductor-semimetal systems, it is possible to obtain information about the structure and electron-phonon interaction in semiconductors and semimetals.

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STATISTICAL MECHANICS

Research in statistical mechanics has been concentrated in the area of simulation of quantum mechanical systems. For the last several years we have been developing Monte Carlo methods to simulate a many Fermion system at zero temperature. Within the past year we have begun application of this method to important physical and chemical systems and are in the process of developing the method for quantum systems at finite temperature. A smaller effort has been

maintained on classical phase transitions in disordered systems, and polymer statistics. A brief description of these projects follows.

1. Simulation of Cold Bulk Hydrogen and Deuterium at High Pressures

D. M. Ceperley and B. J. Alder (LLNL)

Hydrogen is the simplest of all substances. As such, it has been extensively studied both theoretically and experimentally. However, its behavior at high pressure (~1MBAR) is still only crudely known. In the experimentally accessible region (< 100 KBAR) it is known that bulk hydrogen is a molecular quantum crystal in which the molecules undergo almost unhindered rotation. At some higher pressure the molecules become aligned, the solid becomes a conducting metal, and the structure changes from a molecular crystal to an atomic crystal. In principle, hydrogen can undergo three separate transitions. It has been conjectured that metallic hydrogen will be a room temperature superconductor and metastable at zero pressure. In addition, the equation of state of compressed hydrogen is an ingredient of theories of planetary interiors. We are attempting to simulate this system because there is good experimental information available at low pressure, and thus we can check our Monte Carlo method, and because there are many theoretically interesting and unresolved questions concerned with the behavior of hydrogen at high pressures.

The quantum Monte Carlo method assumes only the nonrelativistic Schroedinger equation and the Coulomb interaction between protons and electrons. The many-electron correlations and the zero point motion of the protons are accurately accounted for by the "fixed-node" diffusion Monte Carlo algorithm. Surface effects are minimized with

the use of periodic boundary conditions and the Ewald image potential. We have been able to simulate systems of up to 256 electrons and 256 protons. We have reproduced experimental results at low pressure. At high pressures, our results show that most existing calculations have given an equation of state that is much too soft. In the metallic phase, harmonic lattice theory is shown to give adequate results only at low pressures. The molecular atomic phase transition is located at approximately 3MBars. We are currently extending our calculations to study the insulator-metal transition as well as the molecular ordering transition.

2. Simulation of Quantum Systems at Finite Temperature

D. M. Ceperley and E. L. Pollock (LLNL)

The Monte Carlo algorithms useful at zero temperature can also be applied at finite temperature. The Bloch equation, which describes the temperature evolution of the quantum density matrix is a diffusion equation. In contrast to ground state problems, the random walks in configuration space must return to their starting positions, (since one typically wants only the diagonal portion of the density matrix), or to a permutation of the origin for indistinguishable particles.

In this Monte Carlo procedure, it is necessary to make use of a trial density matrix, to guide the random walk, and to estimate the energy. This year we have explored the use of a pair product trial density matrix for two systems; liquid helium 4 and the one component plasma. In both cases we found a lambda transition (as evidenced by an explosion in the lengths of permutation cycles) and agreement with

ground state properties to about 5%. We are currently testing exact Monte Carlo methods on these systems.

3. Simulation of a Metallic Surface L. J. Johnson and D. M. Ceperley

The description of the behavior of electrons near a metal surface is an important problem in many areas of physics and surface chemistry. We have developed a variational and a "fixed-node" Monte Carlo program to simulate the electrons confined by a slab (infinite in two dimensions but finite in the third dimension) of positive charge. Using this program, we have tested various choices of trial wavefunctions and are now in the process of using the program to benchmark density functional theory on this inhomogeneous electronic system.

4. Application of Monte Carlo in Quantum Chemistry P. Reynolds, D. Ceperley, B. Alder (LLNL), and W. A. Lester, Jr.

We have undertaken the computation of the ground-state properties of selected molecules. Our goal is to calculate the energies of large molecules to the exceedingly exacting precision required for chemical studies, without recourse to the complex basis sets and huge configuration interaction expansions used by other workers.

Our method is a Monte Carlo approach to the solution of the Schroedinger equation. Choosing a relatively simple trial function, consisting of a Slater determinant of molecular orbitals multiplied by a Jastrow factor (a product of pair correlation functions), we first use variational Monte Carlo to optimize the parameters of this wavefunction. This step provides an upper bound to the energy of the system. Next, in order to converge to the exact solution, this trial

function--used now as a guiding function--is sampled by a "walk" (Markov chain) of the electrons through configuration space. The dynamics of this walk are governed by the Schroedinger equation interpreted as a diffusion equation. Depending on local values of the trial function and its derivatives, a given electron will diffuse as well as drift under the influence of a local "quantum force." Initially, an entire ensemble of systems is constructed. After all the electrons in a particular constituent system have been moved, the entire system may be duplicated or eliminated from the ensemble. As time evolves, this process forces the electrons to approach an equilibrium probability distribution proportional to the exact Bose ground state. The nodes of the trial function define regions in which this solution is exact. The true Fermi ground state may be obtained by "relaxing the nodes". That is, the nodal surfaces are no longer fixed by the trial function, and configurations can now cross these nodes.

We have carried out this procedure for He, H_2, LiH, Li_2 and H_2O. With only moderate computing effort we are able to account for most of the correlation energy of these molecules. Thus far only the variational and the fixed node procedures have been completed. We are working to improve our results by a better choice of variational wavefunction, by further optimization, by choosing somewhat larger basis sets, by including electron-nuclear Jastrow functions, and by releasing the nodes. Our present results are most encouraging, for we are often able to equal or achieve lower energies than traditional approaches with only modest effort. The algorithm is also suitable

for calculations of systems with significantly more electrons, since computational effort increases only as the square of the number of electrons.

5. Phase Transitions in Disordered System P. Reynolds

Percolation serves as a model for numerous disordered systems, from fluid flow through porous rock, randomly disordered magnets, and gels, to conduction in mixed media, such as conductor-superconductor matrices, or the strength of materials such as ceramic-metal mixtures. Percolation also exhibits a phase transition, common to all these systems. Because of the essential simplicity of the model, and its explicit probabilistic nature, it sheds light on the process of phase transformations in general.

I have been studying a percolation model in which bonds are oriented with respect to an external direction. In other words, flow along any given path is possible in one and only one direction. This models, for example, the gelation transition in a flowing solvent, or flow (e.g., oil recovery) through porous rock in the presence of gravity. This is also a model of an insulator-to-diode transition. Every bond may be thought of as a diode, allowing conduction in only one direction. The entire macroscopic system will behave as an insulator when the concentration of diode elements is less than a critical value. Above this concentration the system is a macroscopic diode. With the introduction of an external electric field opposing the orientation of the diodes, one obtains a phase diagram with two lines of transitions separating three distinct phases: insulator, macroscopic diode, and at sufficiently large values of the field where

a "breakdown" occurs, a macroscopically conducting phase. I have calculated the location of these phase boundaries as well as the critical exponents associated with these transitions using a position-space renormalization group which I had developed earlier. I have also studied a model with "forward-pointing" diodes, "backward-pointing" diodes, conductors (bi-directional elements) and insulators, and obtained its phase diagram, and critical behavior. Of particular theoretical interest is that the phase transition of these oriented models is in a different universality class than ordinary percolation.

6. Polymer Statistics P. Reynolds and S. Redner (Boston University)

We have developed a large-cell position space renormalization group to study the scaling properties of polymer chains. In order to implement the procedure, we needed to first develop a Monte Carlo method to sample chains of all sizes within a b x b cell, for b up to 150. To do this we studied chains in the grand canonical ensemble. Rather than study chains at fixed monomeric length N, we calculated $\langle N \rangle$ for chains at fixed fugacity p. At p near its critical value, chains could be grown to almost any length.

The results of our work were to (1) provide a new Monte Carlo procedure for studying polymers, (2) examine alternative (and more physical) renormalization group transformations, and evaluate their performance, and (3) calculate an accurate value for the exponent ν describing the way the radius of gyration of a polymer scales with the number of monomers.

PUBLICATIONS

1. D. M. Ceperley and B. J. Alder, "Ground State of the Electron Gas by a Stochastic Method," Phys. Rev. Letts. 45, 566 (1980).
2. D. M. Ceperley and B. J. Alder, "The Low Density Phases of the Electron Gas," Journal de Physique C-7, 295 (1980).
3. M. Bishop, D. Ceperley, H. L. Frisch and M. H. Kalos, "Investigations of the Static Properties of Model Bulk Polymer Fluids," J. Chem. Phys. 75, 3228 (1980).
4. H. L. Frisch, M. Bishop, D. Ceperley, M. H. Kalos, "Computer Simulation of Chains in Solution and Bulk State," J. Macromolecular Science, Phys. B18(3), 453-459 (1980).
5. M. Bishop, D. Ceperley, H. L. Frisch and M. H. Kalos, "Investigation of Static Properties of Two Dimensional Bulk Polymer Systems," submitted to J. Chem. Phys.
6. D. M. Ceperley, M. H. Kalos and J. L. Lebowitz "The Computer Simulation of the Static and Dynamic Properties of a Polymer Chain," in press, Macromolecules 1981.
7. D. M. Ceperley, "The Relative Performances of Several Scientific Computers for a Liquid Molecular Dynamics Simulation," to be published in the ACS symposium series as Supercomputers in Chemistry, ed., P. Lykos, 1981.
8. M. Bishop, H. L. Frisch, M. H. Kalos and D. Ceperley, "Supercomputers for Time Dependent Polymer Simulation," to be published in the ACS symposium series as Supercomputers in Chemistry, ed. P. Lykos, 1981.

9. D. M. Ceperley and B. J. Alder, "The Calculation of the Properties of Metallic Hydrogen Using Monte Carlo," Proceedings of the XVI International Conference on Low Temperature Physics, Los Angeles, California, 1981.

10. D. Ceperley, "The Stochastic Solution of the Many-Body Schroedinger Equation For Fermions," in Recent Progress in Many Body Physics, pg. 262 Springer Verdag Lecture Notes 142, 1981, ed. J. G. Zabolitzky, et al.

11. P. Reynolds, D. Ceperley, B. Alder, and W. A. Lester, Jr., "High Accuracy Quantum Monte Carlo for Molecules," to be submitted to J. Chem. Phys.

TALKS/PRESENTATIONS

D. M. Ceperley, "Brownian Dynamics of Polymers," Joint U. S.-France Workshop on the Dynamics of Polymer Solutions, May 1980.

D. M. Ceperley, Workshop on Monte Carlo Methods in Physics, Aspen Institute for Physics, August 1980.

D. M. Ceperley, "A Molecular Dynamics Benchmark on Several Scientific Computers," Symposium on Supercomputers in Chemistry, Las Vegas meeting of the ACS, August 1980.

P. J. Reynolds, "Overview of phase transitions and critical phenomena," NRCC Policy Board Meeting, November 1, 1980.

D. C. Ceperley, "Exact Monte Carlo Methods for the Ground State of Many-Fermion Systems," International Conference on Recent Progress in Many-Body Theory, Oaxtepec, Mexico, January 1981.

D. M. Ceperley, "Simulation of Many Fermion Systems," University of Michigan, April 1981.

D. M. Ceperley, "Fixed-Node Monte Carlo Methods for Molecules," New York University, May 1981.

D. M. Ceperley, "Simulation of Many Fermion Systems," Massachusetts Institute of Technology, May 1981.

P. R. Reynolds, "High-Accuracy Quantum Monte Carlo for Molecules," American Conference on Theoretical Chemistry, University of Colorado, Boulder, June 22, 1981.

D. M. Ceperley, "Monte Carlo Simulation of Metallic Hydrogen," International Low Temperature Conference, Los Angeles, California, August 1981.

OTHER

W. A. Lester, Jr., "Recent Progress at the National Resource for Computation in Chemistry," Conference on Computers and Chemistry, Florida State University, Tallahassee, Florida, March 1981.

W. A. Lester, Jr., "The National Resource for Computation in Chemistry: A Service to the Chemistry Community," Meeting of the Society of Black Physicists, Stanford University, April 1980.

W. A. Lester, Jr., "Some Computational Trends in Theoretical Chemistry," Keynote Lecture, 28th Congress of the International Union of Pure and Applied Chemistry, Vancouver, British Columbia, August 1981.

PROPOSAL PROGRAM

The NRCC's proposal program was directed toward the advancement of new computational methods, the innovative use of existing methods, the study of problems of significant scientific merit, the resolution of intradisciplinary computational issues and the development of interdisciplinary approaches to forefront problems in chemistry. In response to the 1980 calls for proposals, 16 proposals were received and five approved. The total costs allocated for these proposals was $50,000. There were no calls for proposals in 1981.

PROPOSALS FUNDED

LASER-STIMULATED SURFACE PROCESSES, Thomas F. George, Department of Chemistry, University of Rochester, $10,000.

DEVELOPMENT OF COMPUTATIONAL EFFICIENT SPLIT-VALENCE BASIS SETS FOR THIRD-ROW ELEMENTS, Warren J. Hehre, Department of Chemistry, University of California, Irvine, $20,000.

MONTE CARLO CALCULATIONS OF LIGHT SCATTERING FROM SIMPLE LIQUIDS, T. Keys and J. W. Lyklema, Sterling Chemistry Laboratory, Yale University, $10,000.

APPLICATIONS OF DISTANCE GEOMETRY TO COMFORMATIONAL ANALYSIS, Irwin D. Kuntz, Jr., Department of Pharmaceutical Chemistry, University of California, San Francisco, $3,000.

REACTIVE DYNAMICS AND ELECTRONIC TRANSITIONS IN THE $(NH_2)^+$ SYSTEM, Trina Valencich, Department of Chemistry, California State University, Los Angeles, $7,000.

VAX ENHANCEMENT

In February 1980 the fast memory on the NRCC VAX 11/780 was increased to 2.5 megabytes with the installation of 2 megabytes of Trendata memory. Also during this month, a second 176 megabyte RP06 disk drive was installed to increase the amount of local file space available to large jobs and to provide a removable pack capability. It is now possible to run several large batch jobs simultaneously without seriously impacting interactive users of the system, a capability not possible prior to these acquisitions.

GRAPHICS HARDWARE

In May 1980, the NRCC chemical graphics facility came on-line with the installation of the Evans and Sutherland multi-picture system. The graphics hardware consists of a central graphics processor with 48K words of picture memory, monochrome caligraphic (random stroke) picture display, data tablet, control dials and a three axis joy stick for graphical input, and an interface to the NRCC's VAX 11/780. The picture system allows pictures composed of up to 15,000 lines to be manipulated and transformed in real-time by the graphics user.

The NRCC's interactive chemical graphics facility is used both in development and application of graphical analysis in chemical research. Software development has focused on the production of general purpose graphical tools for enabling easy and rapid application of the hardware to a wide range of chemical problems.

APPENDIX A

SEMINARS IN 1980-81

February 25, 1980:	SENSITIVITY ANALYSIS IN MOLECULAR DYNAMICS AND CHEMICAL KINETICS Prof. Herschel Rabitz, Princeton University
February 28, 1980:	AN UNMANNED COMPUTER SYSTEM AND LARGE SCALE MO COMPUTATION AT THE IMS COMPUTER CENTER Dr. Hiroschi Kashiwagi, Institute for Molecular Science, Japan
March 5, 1980:	DISSOCIATION OF VAN DER WAALS MOLECULES* Dr. J. A. Beswick, University of Paris
March 20, 1980:	THE ALCHEMY-CI METHOD: THE SYMBOLIC MATRIX METHOD FOR DETERMINATION OF FORMULAS OF MATRIX OPERATORS Dr. Bowen Liu, IBM Research Laboratory, San Jose
March 27, 1980:	MULTIPLE TRANSITION STATES IN CHEMICAL REACTIONS: A UNIFIED STATISTICAL THEORY APPROACH AND APPLICATION TO C_4H_8* Prof. Mike Bowers, University of California, Santa Barbara
March 27, 1980:	COMPUTER-GENERATED REPRESENTATION OF THE STRUCTURE OF BIOLOGICAL-MACROMOLECULES: A METHOD AND ITS APPLICATIONS Dr. Michael Liebman, Institute for Cancer Research, Philadelphia
April 7, 1980:	IR CHEMILUMINESCENCE STUDIES OF REACTIVE DYNAMICS* Prof. Stephen R. Leone, JILA, University of Colorado
April 11, 1980:	VACUUM UV LASER INDUCED FLUORESCENCE STUDIES IN CHEMICAL DYNAMICS* Dr. John Hepburn, Lash Miller Chemical Laboratories
April 18, 1980:	THEORETICAL AND EXPERIMENTAL INVESTIGATIONS RELATING TO METHANE FLAMES Dr. Richard Blint, General Motors Research Group

May 27, 1980:	QUANTUM MINERALOGY Prof. Jack Tossell, University of Maryland
May 28, 1980:	THE COMING REVOLUTION IN SCIENTIFIC COMPUTATION Prof. Anthony C. Hearn, University of Utah
July 9, 1980:	AN IMPROVED FORMULATION OF MIR PHASE REFINEMENT Dr. Gerard Bricogne, The Medical Research Council, Cambridge, England
July 9, 1980:	INCORRECT WEAK COUPLING LIMIT OF AN EFFECTIVE POTENTIAL METHOD Dr. Gerhard E. Hahne, private consultant
August 13, 1980:	LARGE CELL MONTE CARLO RENORMALIZATION GROUP FOR PERCOLATION Prof. Peter Reynolds, Boston University
August 19, 1980:	A NEW METHOD FOR OBTAINING INFORMATION OF POTENTIAL ENERGY SURFACES FROM EXPERIMENTAL DATA Dr. Jonathan N. L. Connor, University of Manchester, England
August 20, 1980:	MCSCF WAVEFUNCTIONS Prof. David R. Yarkony, Johns Hopkins University
September 5, 1980:	ARRAY PROCESSORS AND CRYSTALLOGRAPHY Dr. William Furey, University of Pittsburgh
September 29, 1980:	INFRARED LASER MOLECULAR BEAM SPECTROSCOPY* Dr. Roger Miller, University of Waterloo, Canada
October 15, 1980:	MODIFIED HELIOCENTRIC COORDINATES FOR MOLECULAR FRAGMENTS WITH ONE HEAVY CENTER Dr. Felix Smith, SRI International
October 16, 1980:	APPLICATIONS OF QUANTUM CHEMISTRY TO PROBLEMS IN CHEMICAL MUTAGENESIS AND PHOTOSYNTHESIS Dr. Lester Shipman, Argonne National Laboratory
October 22, 1980:	ROTATIONAL RAINBOWS IN INELASTIC SCATTERING Dr. Reinhard Schinke, Max-Planck Institut fur Stromungsforschung, Federal Republic of Germany
October 24, 1980:	FORMATION AND DECAY OF QUASI-BOUND CLUSTERS OF Ar ATOMS* Prof. Donald L. Thompson, Oklahoma State University

October 27, 1980:	CROSSED BEAM STUDIES OF PROTON TRANSFER REACTIONS AT LOW ENERGY* Prof. James Farrar, University of Rochester
November 17, 1980:	BEAM SCATTERING EXPERIMENTS ON ROTATIONAL AND VIBRATIONAL EXCITATION* Prof. J. Peter Toennies, Max-Planck-Institut, Federal Republic of Germany
November 17, 1980:	LASER DISSOCIATION OF IODINE AND THE CAGE EFFECT Mr. Alan Lipkus, University of Rochester
February 11, 1981:	LASER INVESTIGATION OF PHOTODISSOCIATION DYNAMICS* Prof. William Jackson, Howard University
February 19, 1981:	THE VIBRATIONAL STATES OF RETINAL Prof. Richard Mathies, University of California, Berkeley
February 23, 1981:	MULTIPLE MOMENTS AND LONG-RANGE INTERMOLECULAR FORCES OF ROTATING, VIBRATING MOLECULES Prof. Joseph O. Hirschfelder, University of Wisconsin
March 25, 1981:	CLASSICAL TRAJECTORY STUDIES OF MOLECULAR BEAM REACTIONS WHICH PROCEED THROUGH REACTION COMPLEXES* Prof. William Hase, Wayne State University
April 9, 1981:	RECENT WORK ON INELASTIC AND REACTIVE COLLISION DYNAMICS Dr. Michael J. Redmon, Chemical Dynamics Corporation
April 29, 1981:	SCATTERING OF RARE GAS ATOMS WITH Na_2* Dr. Patrick L. Jones, Universitat Kaiserslautern
June 3, 1981:	DYNAMICS OF UNIMOLECULAR DECOMPOSITION* Prof. Robert Gilbert, University of Sydney
June 23, 1981:	THE RESONANT PHOTOELECTRON APPEARANCE POTENTIAL SPECTROSCOPY AND ITS APPLICATIONS* Prof. Z. Y. Hua, Fudan University, China
July 8, 1981:	RECENT STUDIES ON ELECTRONIC TO VIBRATIONAL, ROTATIONAL AND TRANSLATIONAL ENERGY TRANSFER* Prof. Dr. I. Hertel, Freie Universitat Berlin

July 13, 1981:	ACCURATE MEASUREMENTS OF TOTAL SCATTERING CROSS SECTIONS FOR RARE GAS SYSTEMS* Dr. H.C.W. Beijerinck, Eindhoven University of Technology
July 17, 1981:	AB INITIO STUDY OF ELECTRONIC STATES OF CHLOROPHYLL AS THE LEADING PART OF THE REACTION CENTER OF PHOTOSYNTHESIS AND THE COMPUTER SYSTEM AND ITS UNMANNED OPERATION OF THE COMPUTER CENTER OF THE INSTITUTE FOR MOLECULAR SCIENCE Prof. Hiroshi Kashiwagi, Institute for Molecular Science, Japan
August 24, 1981:	MOLECULAR ION PHOTOFRAGMENT SPECTROSCOPY* Dr. Philip C. Cosby, SRI International
September 21, 1981:	MOLECULAR BEAM STUDIES OF GAS SURFACE DYNAMICS* Dr. Daniel Auerbach, IBM Research Center

*Joint seminar with the Materials and Molecular Research Division, Lawrence Berkeley Laboratory and the Department of Chemistry, University of California, Berkeley.

VISITORS

R. Alden, Department of Chemistry, University of California, San Diego, June 8-13, 1981.

K. Amano, Hokkaido University, Japan, August 5, 1981.

N. H. F. Beebe, Department of Physics, University of Utah, January 15-20, 1980.

R. Blint, General Motors Reserach Group, April 18, 1980.

M. Bishop, Division of Science and Mathematics, Fordham University at Lincoln Center, July 14-August 29, 1980 and July 16-August 14, 1981.

G. Bricogne, Unit for Molecular Biology Medical Research Council, Trinity College, Cambridge, England, May 31-July 14, 1980 and June 14-21, 1981.

A. Cutler, Department of Chemistry, Princeton University, June 30-July 11, 1980.

A. P. de Ruiter, North-Holland Publishing Company, The Netherlands, August 13, 1981.

D. DeTar, Department of Chemistry and Institute of Molecular Biophysics, Florida State University, August 17-September 17, 1980.

R. Eades, Department of Chemistry, University of Minnesota, June 1-27, 1981.

M. Faubel, Max-Planck-Institut, Gottingen, Federal Republic of Germany, June 20-25, 1980.

S. Freer, Department of Chemistry, University of California, San Diego, May 19-30, 1980 and June 9-18, 1981.

A. Hagler, Department of Chemistry, University of California, San Diego, May 5, 1980.

G. Hahne, Olympia, Washington, July 9, 1980.

W. Hendrickson, Naval Research Laboratories, Washington, D. C., May 19-30, 1980 and June 9-13, 1981.

H. Jones, Division of Natural Sciences and Mathematics, Florida A & M University, June 31-August 31, 1980.

W. Jorgensen, Department of Chemistry, Purdue University, January 11-14, 1980 and November 20-24, 1980.

M. Kalos, Courant Institute of Mathematical Sciences, New York University, May 12-17, 1980.

H. Kashiwagi, Institute for Molecular Science, Myodaiji, Japan, February 28, 1980 and July 17, 1981.

J. Kaufman, Johns Hopkins University, August 10-21, 1981.

W. Kraemer, Max-Planck-Institut fur Physik und Astrophysik, Munchen, March 12, 1980.

D. E. Kranbuehl, Department of Chemistry, College of William and Mary, February 2-June 15, 1981.

L. Lewis, Department of Chemistry, Clemson University, July 9-31, 1980.

M. Liebman, Institute for Cancer Research, Philadelphia, March 27, 1980.

A. Lipkus, Department of Chemistry, University of Rochester, August 11, 1980-September 30, 1981.

B. Liu, IBM Research Laboratory, San Jose, March 20, 1980.

G. Loew, SRI International, January 28, 1981.

J. Maggiora, Department of Chemistry, University of Kansas, December 9, 1980.

A. D. McLean, IBM Research Laboratory, San Jose, March 20, 1980.

K. G. Morokuma, Computer Center, Institute for Molecular Science, Myodaiji, Okazaki, Japan, June 24-25, 1980.

G. R. Moss, Department of Chemistry, State University of New York at Buffalo, January 20-31, 1980.

R. Munn, Department of Chemistry, University of Maryland, May 19-30, 1980.

J. Nichols, Department of Chemistry, Texas A & M University, August 15-29, 1980.

W. C. Nieuwpoort, Theoretical Chemistry Group, University Groningen, The Netherlands, June 24, 1980.

K. Ohno, Hokkaido University, Japan, March 27-29, 1980.

R. Schinke, Max-Planck Institut fur Stromungsforschung, Federal Republic of Germany, October 15, 1980.

J. Sun, Department of Chemistry, University of California, Riverside, May 21, 1981.

J. Sussman, Weitzman Institute, Tel Aviv, May 5, 1980.

J. Stewart, Department of Chemistry, University of Maryland, May 19-30, 1980 and June 15-18, 1981.

T. Story, Department of Chemistry, Atlanta University, July 1-August 31, 1981.

L. TenEyck, Department of Computer Science, University of North Carolina, June 10-18, 1981.

J. Tossell, Department of Chemistry, University of Maryland, May 23-29, 1980.

K. Watenpaugh, Department of Biological Structure, University of Washington, May 19-30, 1980 and June 11-16, 1981.

I. Wilson, Department of Chemistry, Harvard University, April 27-May 8, 1981.

D. Yarkony, Department of Chemistry, Johns Hopkins University, August 2-27, 1980.

D. Yeager, Department of Chemistry, Texas A & M University, July 2, 1980.

APPENDIX B

PUBLICATIONS - OTHERS

Listing of papers acknowledging NRCC support. Alphabetical by author supported by the NRCC.

Arie Aizman and David A. Case, University of California, Davis, "An Xα Multiple Scattering Study of Hexacyanoferrate (III)," Inorg. Chem., in press.

Millard Alexander, University of Maryland, "Close-Coupling Studies of Rotationally-Inelastic HF-HF Collisions at Hyperthermal Energies," J. Chem. Phys. (1980).

Millard H. Alexander and Eugene F. Jendrek, University of Maryland, and Paul J. Dagdigian, Johns Hopkins University, "Validity of Energy Gap Representations of Rotationally Inelastic Cross Sections between Polar Molecules," J. Chem. Phys. (1980).

Marvin Bishop, Fordham University at Lincoln Center, David Ceperley, NRCC, Harry L. Frisch, State University of New York at Albany, and Malvin H. Kalos, New York University, "Computer Simulation of Chains in Solution and Bulk State," J. Macromol. Sci., in press.

Marvin Bishop, Fordham University at Lincoln Center, David Ceperley, NRCC, H. L. Frisch, State University of New York at Albany, and M. H. Kalos, New York University, "The Need for Supercomputers in Time Dependent Polymer Simulations," to be published in the ACS Symposium of Supercomputers, Las Vegas, August 1980.

Marvin Bishop, Fordham University at Lincoln Center, M. H. Kalos, New York University, and H. L. Frisch, State University of New at Albany, "Molecular Dynamics of Polymeric Systems," J. Chem. Phys. 70, 1299, (1979).

Marvin Bishop, Fordham University at Lincoln Center, David Ceperley, NRCC, H. L. Frisch, State University of New York at Albany, and M. H. Kalos, New York University, "Investigations of Static Properties of Two Dimensional Bulk Polymer Systems," submitted to J. Chem. Phys.

Weston Thatcher Borden, Ernest R. Davidson, and David Feller, University of Washington, "The Potential Surface for the Cyclobutadiene Radical Cation," submitted to J. Am. Chem. Soc.

David A. Case, University of California, Davis, and Cary Y. Yang, Surface Analytic Research, Inc., "Stable and Efficient Algorithms for Xα Multiple Scattering Calculations," Int. J. Quantum Chem. XVII, 1091 (1980).

David A. Case, University of California, Davis, and Cary Y. Yang, Surface Analytic Research, Inc., "Relativistic Scattered Wave Calculations on UF_6," J. Chem. Phys. 72, 3443 (1980).

J. W. Chinn, Jr. and M. B. Hall, Texas A & M University, "Generalized Molecular Orbital Theory: The Electronic Structure and Photoelectron Spectrum of Cyclobutadienetricarbonyliron," submitted to Inorg. Chem.

William F. Coleman, University of New Mexico, Michael G. Prisant and Richard N. Zare, Stanford University, "A Laser-Induced Transient Photovoltaic Effect Using Blocked Electrodes," J. Phys. Chem. 84, 2685 (1980).

DeLos F. DeTar, Florida State University, "Computation of Enzyme-Substrate Specificity," Biochem. 20, 1730 (1981).

Paul L. DeVries and Thomas F. George, University of Rochester, "Effect of Laser Frequency on a Collision-Induced Radiative Process," to appear in Potential Surfaces and Dynamics Calculations ed. by D. G. Truhlar, Plenum, in press.

Paul L. DeVries, C. Chang, and Thomas F. George, University of Rochester, Bernard Laskowski and James R. Stallcop, NASA-Ames Research Center, "Computational Study of Alkali-Metal-Noble-Gas Collisions in the Presence of Nonresonant Lasers: Na + Xe + $h\omega_1$ + $h\omega_2$ System," Phys. Rev. A 22, 545 (1980).

Randall N. Diffenderfer, Johns Hopkins University, Charles W. Bauschlicher, Polyatomics, Research, Inc., Byron H. Lengsfield, III, IBM Research Center, and David R. Yarkony, Johns Hopkins University, "A Systematic Study of the State Averaged MCSCF Procedure: Application to MgO and CaO," submitted to J. Chem. Phys.

D. E. Ellis and Ziva Berkovitch-Yellin, Northwestern University, "Charge and Spin Distributions of Copper and Silver Porphine," J. Chem. Phys. 74, 2427 (1981).

Glenn T. Evans and Donald C. Knauss, Oregon State University, "Brownian Dynamics Simulation of Alkane Chain Reorientation: A Comparison of Models," J. Chem. Phys. 72, 1504 (1980).

David Feller, Ernest R. Davidson, and Weston Thatcher Borden, University of Washington, "A Theoretical Study of Concerted Versus Stepwise Fragmentation of 2-Carbena-1, 3-dioxolane," submitted to J. Am. Chem. Soc.

K. E. Foley and B. J. Garrison, Pennsylvania State University, "Mechanisms of Particle Ejection from Cu(001) Induced by Directional Orientation of the Bombarding Primary Ion," J. Chem. Phys. 72, 1018 (1980).

B. J. Garrison, Pennsylvania State University, "Mechanisms of Ejection of Organic Molecules from Surfaces by keV Ion Bombardment," J. Am. Chem. Soc. 102, 6553 (1980).

B. J. Garrison, Pennsylvania State University, "Mechanisms of Ejection due to Ion Bombardment: c(4x4) Overlayer of Benzene C_6H_6, on Ni(001)," Le Vide, le Couches Minces, 201, 1411 (1980).

B. J. Garrison, Pennsylvania State University, "Classical Trajectory Studies of keV Ions Interacting with Solid Surfaces," in Potential Energy Surfaces and Dynamics Calculations, ed by D. G. Truhlar, Plenum, in press.

B. J. Garrision, S. P. Holland, and N. Winograd, Pennsylvania State University, "Angle-resolved SIMS - A New Technique for the Determination of Surface Structure," Springer Sieries in Chemical Physics, Vol. 9, p. 44, Springer-Verlag (1979).

M. B. Hall, Texas A & M University, "Generalized Molecular Orbital Theory: A Simple Multiconfiguration Self-consistent-field Method," Int. J. Quantum Chem. 14, 613 (1978).

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APPENDIX C

SOFTWARE REQUESTS

Name	Identifier	Title	Number Requested
ABCD	KC05	Atom-Triatomic Classical Trajectory Program	16
ABCRR	KC01	A + BC Classical Trajectory Program	15
ABCRRJ	KC01	A + BC Classical Trajectory Program	15
ALIS/CDC	QM01	*Ab Initio* MCSCF Program for Atomic and Molecular Electronic Structure Calculations	42
ALIS/IBM	QM01	*Ab Initio* MCSCF Program for Atomic and Molecular Electronic Structure Calculations	48
CLAMPS/CDC	SS01	Classical Many Particle Simulator	43
CLAMPS/VAX	SS01	Classical Many Particle Simulator	51
CLASTR	KC04	Reactive A + BC Classical Trajectory Program	17
DEVOG	KQ11	Coupled Channel Scattering Program (Devogelaere's Algorithm)	19
EHT	QE02	Extended Hueckel Theory	9
FSGOMF	QH05	*Ab Initio* Hartree-Fock Self-consistent Field Program Using Floating Spherical Guassian Orbitals	18
GAMESS	QG01	General Atomic and Molecular Electronic Structure System	42

Name	Identifier	Title	Number Requested
GORDON	KQ05	Inelastic Atom-Diatom Quantum Scattering (Modified Version of QCPE No. 187.)	22
GRADSCF	QH04	*Ab Initio* Gradient Program System	38
HOND05/CDC	QH02	*Ab Initio* Hartree-Fock Self-consistent Field Program	20
HOND05/IBM	QH02	*Ab Initio* Hartree-Fock Self-consistent Field Program	44
INSCAT	KQ08	Coupled Channel Scattering Program (Integral Equations Method with Piecewise Analytic Influence Potentials	18
KAPPAS	KS01	Semiclassical 1-D Transmission Probabilities	15
LOGD	KQ06	Coupled Channel Scattering Program (Log Derivative Method)	19
L2RMAT	KQ13	Coupled Channel Scattering Program (L^2 Approach to R-Matrix Propagation Method)	17
MELD	QC04	*Ab Initio* SCF-CI System of Programs	52
MIEHM	QE01	Modified Iterative Extended Hueckel Method	9
MINDO	QZ02	Modified Intermediate Neglect of Differential Overlap	22
MNN	KQ12	Coupled Channel Scattering Program (Numerov Method)	18
MOLSCAT	KQ01	Molecular Scattering Program	25
MULTAN78/CDC	XS01	X-ray Diffraction Structure Solving Package	19

Name	Identifier	Title	Number Requested
MULTAN78/VAX	XS01	X-ray Diffraction Structure Solving Package	28
PC	KQ10	Coupled Channel Scattering Program (Predictor-Corrector Method)	11
PFORTV	TV01	Portable FORTRAN Verifer	43
PLUTO/VAX	GM01	A Program for Plotting Molecular and Crystal Structure	38
PRETTY	TC01	Convert FORTRAN to Prettier Format	57
QLEVEL	KQ02	Bound States of 1-D Potentials	15
RANNUM/CDC	NR01	A FORTRAN IV Routine for Matrix Bi-orthogonalization	10
RANNUM/VAX	NR01	A FORTRAN IV Routine for Matrix Bi-orthogonalization	13
RMAT	KQ09	Coupled Channel Scattering Program (R-Matrix Propagation Method)	16
RMATOM	KE01	R-matrix Method for Electron-atom Scattering	9
SAMS	KQ07	Coupled Channel Scattering Program (Sams-Kouri Integral Equation Method)	22
SPDFG/IBM	KH03	*Ab Initio* Hartree-Fock Self-consistent Field Program	34
TDELAY	KQ03	Phase Shifts and Time Delays for 1-D Potentials	12
VIVAS	KQ04	A-BC (Vib-rotor) Coupled Channel Scattering Program (Variable-Interval, Variable-step Method)	22

Name	Identifier	Title	Number Requested
XASW	QX01	X-alpha Scattered Wave Program	58
ALCHEMY	QC03	*Ab Initio* Electronic Structure Calculations Package	26
DIAG	ND03	Iterative Calculation of a Few of the Lowest Eigenvalues and Eigenvectors of Large Real-symmetric Matrices	16
GAUSS80		*Ab Initio* Electronic Structure Package	11

APPENDIX C

NRCC STAFF AND DIRECTORATE 1980-81

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Arthur J. Olson, Assistant Director
George E. Towns, Division Administrator

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Devon Brunkan (to 9/11/81)
Evelyn Byers (to 7/18/80)
Gervaise Christiansen
Timothy R. Clark (to 8/1/80)
L. C. Jordon (to 8/31/81)
JoAnn Kim (to 2/29/80)
Maudie Noyd

NRCC Policy Board

Terms of Appointment
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