DISCLAIMER

NRCC NATIONAL RESOURCE FOR COMPUTATION IN CHEMISTRY

BULLETIN

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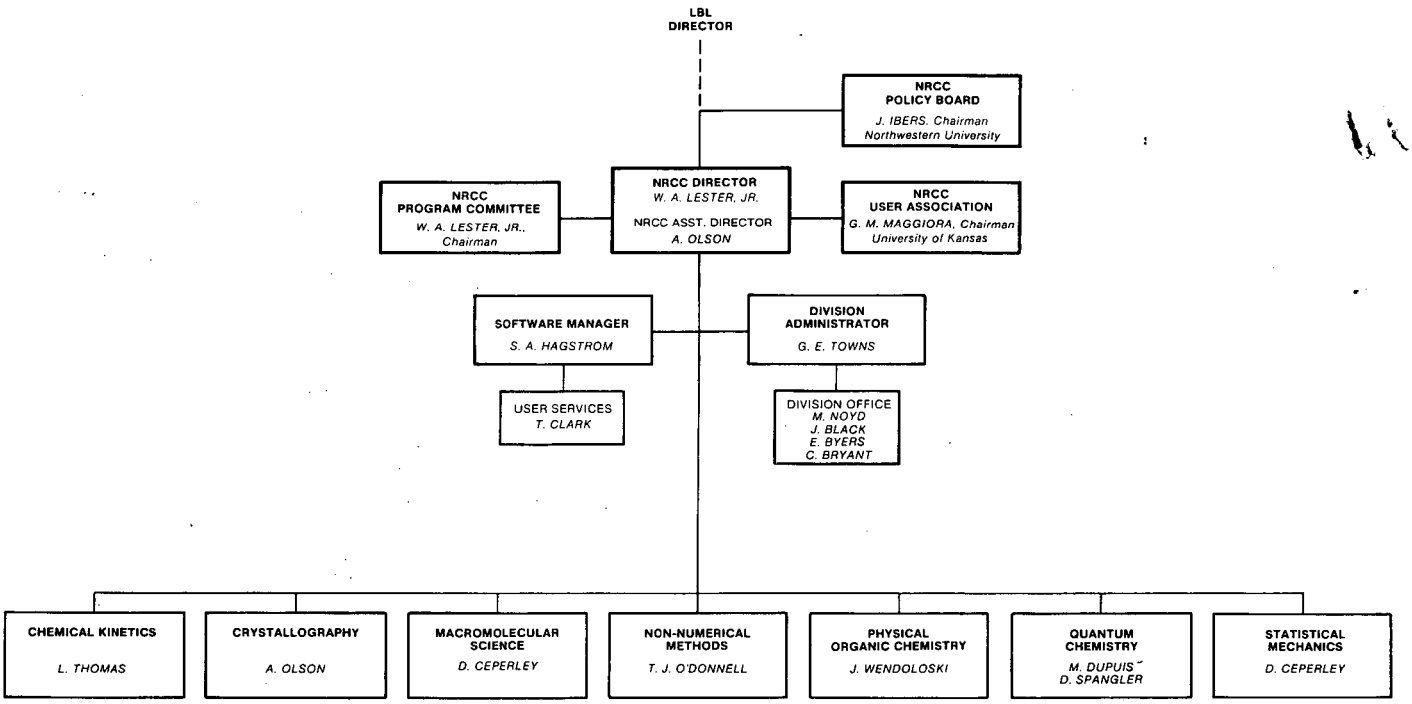
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
NATIONAL RESOURCE FOR COMPUTATION
IN CHEMISTRY



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Messages may be left at Extension 6722.

Bulletin Editor:
John J. Wendoloski

PERSONNEL CHANGES

Vladimir Kresin has joined the NRCC as a member of the scientific staff in the area of π-electron systems and molecular spectroscopy. His present interests involve the applications of methods of the quantum theory of many-body systems (Green's function methods, theory of finite Fermi systems) to study properties of π-electron systems of complex molecules: correlation effects, optical activity, charge transfer, electron-vibration interaction. His previous research activity utilized the methods of quantum field theory to study problems of solid state physics and the properties of the superconducting state.

Selected Publications

1. V. Kresin, V. Litovchenko, A. Panasenko. "Effects Related to Pair Correlation of π-electrons." J. Chem. Phys. 63, 3613 (1975).

2. V. Kresin, A. Panasenko. The Oscillator Model in the Theory of Complex Molecules." Sov. Phys.-Doklady-Physical Chemistry 227, 336 (1976).

3. V. Kresin. "The Pair π-Electron Correlation of the Superconducing Type in the Complex Molecules." J. de Phys. 39, C6-479 (1978).

4. B. Geilikman, V. Kresin. "Kinetic and Nonstationary Phenomena in Superconductors," John Wiley and Sons, New York (1974).

Dr. George Zahr of the scientific staff has left the NRCC to accept a position at E. I. duPont de Nemours and Company, Inc., Wilmington, Delaware.

Ms. JoAnn Kim of the administrative staff has left NRCC to accept a position at the University of California, Berkeley.

PROPOSALS FUNDED

The NRCC is pleased to announce awards totaling $17,000 for proposals funded from the fifth NRCC proposal review. A brief description of the funded proposals follows:

T. Keyes and J. W. Lyklema, Sterling Chemistry Laboratory, Yale University, Yale University, "Monte Carlo Calculations of Light Scattering from Simple Liquids." Support the calculation of the intensity of depolarized light scattering by simple liquids, in the dipole-induced dipole approximation, via Monte-Carlo simulation. ($10,000 for 12 months).

T. Valencich, Department of Chemistry, California State University, Los Angeles, "Reactive Dynamics and Electronic Transitions in the $(NH_2)^+$ System." Support computational studies of the competitive dynamics of abstraction and insertion/decomposition processes for $(NH_2)^+$. ($7,000 for 24 months).

CALL FOR PROPOSALS

The deadlines for receipt of proposals for the next round is July 15, 1980. Proposals are sought of the highest scientific quality and therefore fundable by the criteria of federal agencies such as the NSF and the DOE. However, it should be remembered that because of its mission, size, and budget, the NRCC is not another federal funding agency. It is an organization created to assist research in chemistry using computational methods in ways not presently possible under federal agency practices. An example worth noting is the support of joint proposals involving researchers across (1) areas (e.g., crystallography and quantum chemistry), (2) subdisciplines (e.g., analytical and physical chemistry, (3) departments (e.g., chemistry and biochemistry), (4) disciplines (e.g., chemistry and physics), and (5) institutions (e.g., corporation x and university y). Clearly there are other possibilities. Do not hesitate to contact the NRCC Director to discuss alternatives of interest.

Besides serving as an information resource, the NRCC scientific staff can participate in collaborative research efforts. There may be problems of appropriate scope for support by the NRCC that need additional computational expertise for implementation. The NRCC staff is a possible resource for filling such gaps. Inquiries concerning collaborative projects with NRCC staff should be directed to the NRCC Director.

Under present NRCC policy, awards are made to cover the cost of computer time at the LBL Computer Center and at other institutions. In the latter case approval of both the NRCC Program Committee and the NRCC Policy Board is required. Proposals may be from any field of chemistry and should promote the development of chemistry through: the advancement of computational methods; the innovative application of existing methods to problems in some frontier areas of chemistry; the study of problems of significant scientific merit that cannot be carried out in the proposer's institution due to lack of large-scale computational facilities; the resolution of intradisciplinary computational methodology issues; and the development of interdisciplinary approaches to forefront problems in chemistry.

Awards from past rounds might lead to the impression that only proposals requiring modest amounts of computer time will be funded. On the contrary the NRCC has increased the funds available for awards, but the NRCC Program Committee has stated that the majority of proposals reviewed to date were for the most part only modest departures from proposals normally received by federal funding agencies. Thus the NRCC Program Committee repeats its request presented in Vol. II, No. 1 of the NRCC BULLETIN that we receive proposals of broad scope and effort.

Directions for proposal preparation follow. The LBL computer system is a complex consisting of a CDC-7600, CDC-6600, and CDC-6400. Further information on the LBL computer system, its rate structure, and details on using it may be obtained by writing to the NRCC.

Directions for Proposal Preparation

The NRCC has established the following guidelines for the submission of proposals. These guidelines supersede those previously provided.

General

1. One-inch left margin on all pages.

2. Pagination on all sheets.

3. Ten copies required.

Cover Page

The following information must appear on the cover page:

1. Name of principal investigator(s) submitting proposal.

2. Name of submitting organization (including department).

3. Address (including building and room where appropriate).

4. Telephone number.

5. Title of proposed research.

6. Computing time on (model of computer); desired level: ____ hours; estimated cost ____; threshold level: ____ hours; estimated cost ____; method of estimating cost.

7. Proposed starting date.

8. Proposed duration of research.

9. Previous anniversary date and account number (for renewal of continuing award request).

Abstract

A brief summary of the proposed research, including significance to science and impact for the NRCC.

Proposal Narrative

The narrative should be no more than ten double-spaced typewritten pages and include the following information:

1. A description of the work being proposed, including the objectives, significance, and nature of the calculations.

2. A general plan for achieving these objectives, including an explanation of the methods to be used.

3. Relation of the proposed work to the current status of the topic addressed.

4. Outline (with pertinent references) of what has been done on the topic to date.

5. Explanation of how this research will advance understanding in the subject area of chemistry.

6. Justification of requested hours of computer time.

7. A bibliography of pertinent literature.

Budget

The financial statement section should include the following information:

1. Detailed line item budget for the grant monies required, including computer time and communication costs (if any).

2. Other agencies, if any, to which the proposal will be submitted.

3. All current support: title of project, funding period of award(s), agency and annual budget levels.

4. Other proposals (including renewal applications) which are currently pending (including DOE and NSF).

Staffing

The statement of staffing should include the following documentation:

1. List of all collaborators who will be computing on the research outlined in the proposals (include names, titles, and telephone numbers).

2. Curriculum vitae of the principal investigator(s).

3. Principal publications of other senior personnel during the past five years on the subject matter covered by the proposal.

Computer Information

1. Briefly describe the available equipment, policies, and capabilities of the computer center at your home institution. If the computations proposed are not to be carried out at LBL or your home institution computer center, provide the above information for the system to be used.

3. Have you ever computed at LBL before? If not, skip 4-5, and answer 6-7.

4. If so, are you currently connected to the LBL computer system?

5. What is your access code (account number)?

6. What type of equipment is currently available to you for connection with the LBL Computer Center ?

   (a) REC Terminal (make _____ model _____
   (b) RJE (make _____ model _____
   (c) Other (make _____ model _____

7. Briefly describe the hardware and communications software available, if any, for remote access to the LBL Computer Center.

Go to Next Section

8. Give institution at which computations will be done and reasons for carrying out computations at institutions.

9. Briefly indicate how computer codes extended or developed under an NRCC award would be made available to the chemistry community through the NRCC.

Communication Availability (for Computing at LBL)

1. LBL has provided communication systems (TYMNET, ARPANET and FTS) for toll-free access to the LBL computers for interactive (RECC) calculations. If you are planning to compute via the Remote Job Entry System (RJE), have you made provisions, either in the proposal or elsewhere, for communication costs? If so, please explain in detail.

2. Is your computer terminal connected to any other leased phone line system? If so, what kind?

3. Do you have a teletype (TWX) machine available to you? If so, what is the phone number of the machine?

4. Do you have a telecopier available to you? If so, list the make, speeds, type (automatic or manual), machine telephone number, and confirmation telephone number.

WORKSHOP ANNOUNCEMENTS

Recent Developments and Applications of Multiconfigurational Hartree-Fock (MCHF) Methods

The National Resource for Computation in Chemistry (NRCC) is sponsoring a workshop entitled: "Recent Developments and Applications of Multiconfigurational Hartree-Fock (MCHF) Methods." The workshop will be held July 14-16, 1980 at Texas A&M University in College Station, Texas, U.S.A. Serving as cochairmen for this workshop are Dr. Michel Dupuis of the NRCC and Professor D. L. Yeager of Texas A&M University.

A consensus from the 1978 NRCC workshop "Post Hartree-Fock: Configuration Interaction (CI)," was that CI calculations can be most efficiently and reliably performed based on a multiconfigurational reference space. In addition, recent developments have also occurred in multiconfiguration time-dependent Hartree-Fock methods and effective hamiltonian methods.

For these reasons, the organization of a workshop on multiconfiguration methodology appears timely. The purpose of the workshop is to foster discussions of ideas which might lead to better methods and computer codes. Chemical applications will be discussed which can benefit from the availability of multiconfigurational wavefunctions, such as excited state calculations, symmetry breaking problems, and time-dependent Hartree-Fock calculations.

WORKSHOP CALENDAR

June 1-7, 1980 — Portable Crystallographic Code II: Multiple Isomorphous Replacement

Chairman: A. J. Olson, NRCC

Location: NRCC

July 14-16, 1980 — Recent Developments and Applications of Multiconfigurational Hartree-Fock (MCHF) Methods

Chairman: Michel Dupuis, NRCC
D. L. Yeager, Texas A&M

Location: Texas A&M, College Station, Texas

SYMPOSIA SCHEDULED FOR NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY

Supercomputers and Chemistry

A Symposium on Supercomputers in Chemistry will be held as part of the National Meeting of the American Chemical Society during the week of 24-29 August 1980 in San Francisco. This symposium is jointly sponsored by the American Chemical Society's Divisions of Computers in Chemistry and of Physical Chemistry, and by the National Resource for Computation in Chemistry. The symposium is co-chaired by Dr. Isaiah Shavitt of Battelle Columbus Laboratories and Professor Peter Lykos of the Illinois Institute of Technology, Chicago, Illinois.

The primary purposes of this symposium are:

1. To discuss the state of the art and current trends in the development--and in the sharing--of very large scale scientific computers.

2. To explore their expected impact on the type of large scale calculations typical of several areas of chemical research (for example theoretical chemistry and crystallography).

3. To compare and contrast this with the opposite trend toward the use of dedicated "mini"-computers, which are often more powerful than yesterday's "large" computers.

4. To bring together the two groups, computer system designers and large scale computer users (from other disciplines as well as from chemistry), in order to improve communication between them.

Papers will be presented on the design of modern large-scale computers and on current trends and plans for the future, as well as papers on large scale applications expected to be impacted strongly by such machines. It is expected that this symposium will help prepare chemists for the changes taking place in the supercomputer field, and will also help the designers of such computers to understand the users needs.

Regional and National Facilities in Chemistry

A symposium on Regional and National Facilities in Chemistry will be held at the August 1980 meeting of the American Chemical Society in San Francisco. The symposium is jointly sponsored by the American Chemical Society's Divisions of Nuclear Chemistry and Technology, Inorganic Chemistry, Organic Chemistry, and Physical Chemistry. Chairman for this session is Professor Victor E. Viola, Jr. of the University of Maryland.

This will be a one-day symposium consisting of two sessions. The first will be a poster session dealing with the design of regional facilities, with representatives of the existing regional facilities on hand to answer questions. The second session will consist of invited talks on the NIH, NSF, and DOE regional facility program, followed by a panel discussion on the role of the outside user in the regional national facilities.

Additional information on scheduling can be obtained by consulting the detailed meeting schedule published by the American Chemical Society in Chemical and Engineering News.

NRCC TO SPONSOR A TOUR OF ITS NEW FACILITIES

In conjunction with the 1980 fall meeting of the American Chemical Society in San Francisco, the NRCC and the NRCC User Association are jointly sponsoring a tour of the NRCC and the Lawrence Berkeley Laboratory in Berkeley, California. This tour will include the new NRCC building, the Lawrence Berkeley Laboratory (LBL) computer center, and other LBL facilities.

Transportation from San Francisco to LBL will be provided. Information on the tour registration and dates can be obtained at the ACS tour center during the meeting or by contacting the NRCC.

NEW SOFTWARE

The GAUSSIAN 80 series of programs developed by Professor J. A. Pople and co-workers at Carnegie Mellon University is now 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 and 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 calculations (CI) with double substitutions.

The Gaussian 80 system is available from NRCC as a program number QH03.2 (GAUSS80). The program is also available directly from Professor Pople or from the Quantum Chemistry Program Exchange.

The present version is the VAX version as implemented on the VAX 11/780 at Carnegie-Mellon University.

The NRCC does not provide any consulting or program support for the GAUSSIAN 80 system (support level C). However, any user problems will be relayed to the program originators.

NRCC SOFTWARE CATALOG

Volume 1 of the NRCC Software Catalog is now available for distribution. Everyone on the current NRCC mailing list will be mailed copies of this catalog and updates. Additional copies may be requested using the form on Page .

The catalog contains a description of all of the NRCC's software holdings, along with extensive descriptions of other software libraries available at LBL which are of interest to computational chemists.

The catalog will appear annually. Special software updates will be issued at irregular intervals as the need arises.

USER ASSOCIATION NEWS

The Executive Board of the NRCC User Association unanimously voted to hold its first annual meeting in conjunction with the 1980 fall meeting of the American Chemical Society, to be held 25-29 August in San Francisco. Further details will appear in the fall meeting issue of Chemical and Engineering News.

In conjunction with the 1980 fall meeting of the American Chemical Society in San Francisco, the NRCC and the NRCC User Association are jointly sponsoring a tour of the NRCC and the Lawrence Berkeley Laboratory in Berkeley, California. This tour will include the new NRCC building, the Lawrence Berkeley Laboratory (LBL) computer center, and other LBL facilities.

Transportation from San Francisco to LBL will be provided. Information on the tour registration and dates can be obtained at the ACS tour center during the meeting or by contacting the NRCC.

MINICOMPUTER NEWS

The fast memory on the NRCC VAX 11/780 has been increased to 2.5 megabytes with the installation of 2 megabytes of Trendata memory. A second 176 megabyte RP06 disk drive has also been 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 which was not possible prior to these acquisitions.

A 600 line/minute impact printer has been ordered with an expected June delivery. This will release the Versatec printer/plotter from its current role as a line printer, making it available as a hardcopy plot device to complement the Evans and Sutherland Picture System.

AUTOMATIC PROGRAM TIMING PROFILES ON THE CDC 7600

One of the basic problems in improving the execution speed of large and time-consuming programs is determining which subprograms are ripe for scrutiny and optimization. Following a suggestion be NRCC scientific staff, Richard Friedman of the Computer Center Systems Group has developed a package on the 7600 that uses the FTN4 compiler to produce program timing profiles automatically, without requiring any changes to the source code.

The package, called FTN4TRA, is a FORTRAN-callable procedure that compiles the user's program with special timing code inserted automatically by the compiler around each subprogram CALL and RETURN. On program termination, a table is generated which automatically displays the time spent in each called subprogram compiled with FTN4TRA. This profile table lists each routine by name, the number of times called, the total time spent in the routine, both in seconds and as percent of the total program running time, and the average time spent in the routine (per call). An estimate of the overhead involved in doing the timing is also given.

Using this profile, the programmer can easily identify which routines merit improvement. FTN4TRA is still under development, but is expected to be released soon to the LBL user community. A program description is in preparation, and will be announced in the Computer Center Newsletter and the weekly BKYNEWS.

PROGRAMMERS' 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, is publishing a manual for the XTAL system of crystallographic programs. The XTAL system, developed by Professor James Stewart 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 conventions 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

A copy of this manual may be obtained by returning the form on Page 19.

INTERACTION WITH CECAM

For 1980, the Centre European de Calcul Atomique et Moleculaire (CECAM) (The European Center for Atomic and Molecular Calculations) and the NRCC are participating in a workshop on "Laser Excitation and Dynamics of Highly Excited Polyatomics." This joint workshop interaction is part of the cooperative agreement between CECAM and the NRCC.

The U. S. participants for this workshop are Professors J. Ackerholt, M. Goodman, K. Kay, R. Marcus, and E. Theile.

The workshop will be held at the University Paris-Sud, Orsay, and will be hosted by the CECAM director Dr. C. Moser. Its focus will be on 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 will be considered along 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.

NEW REPORTS

Attached Scientific Processors for Chemical Computations

Copies of the report, "Attached Scientific Processors for Chemical Computations: A Report to the Chemistry Community," by Neil S. Ostlund, is now available from the NRCC. This NRCC sponsored report surveys the field of attached scientific processors ("array processors") and describes their present and possible future use in computational chemistry. Information is provided to assist chemists considering the use of an array processor for their computations. It also describes the general ideas and concepts involved in using array processors, the commercial products that are available, and the experiences reported by those currently using them.

In conjunction with the generation of this report, a small 1-1/2 day meeting "Array Processors for Chemical Computations," was held at the NRCC on July 20-21, 1979. The above report abstracts many of the points discussed in that meeting.

To request this report, see Page 19.

ROSTER OF MINICOMPUTER USERS

One of the purposes of the National Resource for Computation in Chemistry (NRCC) is to provide information to the chemistry community on recent developments in computational chemistry. In response to the current strong interest of chemists in minicomputers, we have compiled a roster of minicomputer users to facilitate exchange of information between individuals and groups on this timely subject. The present roster has been compiled in response to a recent solicitation in the NRCC BULLETIN. Copies of the roster are available upon request; see the order form on Page 19.

MANUSCRIPTS RECEIVED--RESEARCH PARTIALLY SUPPORTED BY THE NRCC

Glenn T. Evans and Donald C. Knauss, Department of Chemistry, Oregon State University, "Brownian Dynamics Simulation of Alkane Chain Reorientation: A Comparison of Models," J. Chem. Phys. 72, 3 (1980).

David A. Case, University of California, Davis, and Cary Y. Yang, Surface Analytic Research, Inc., and NASA-Ames Research Center, "Stable and Efficient

Algorithms for Xα Multiple Scattering Calculations," submitted to Int. J. Quantum Chem., February 1980.

Paul L. De Vries, C. H. Chang, Thomas F. George, Department of Chemistry, University of Rochester, Bernard Laskowski, and James R. Stallop, NASA-Ames Research Center, "Na + Xe Collisions in the Presence of Two Nonresonant Lasers," Chem. Phys. Lett. 69, 3 (1980).

David A. Case, University of California, Davis, and Cary Y. Yang, Surface Analytic Research, Inc., and NASA-Ames Research Center, "Relativistic Scattered Wave Calculations on UF_6," to appear in J. Chem. Phys. (1980).

SEMINARS

Prof. Herschel Rabitz, Princeton University, "Sensitivity Analysis in Molecular Dynamics and Chemical Kinetics," February 25, 1980.

Dr. Hiroschi Kashiwagi, Institute for Molecular Science, Myodaiji, "An Unmanned Computer System and Large Scale MO Computation at the IMS Computer Center," February 28, 1980.

*Dr. J. A. Beswick, University of Paris, "Dissociation of van der Waals Molecules," March 5, 1980.

Dr. Bowen Liu, IBM Research Laboratory, San Jose, "The ALCHEMY-CI Method: The Symbolic Matrix Method for Determination of Formulas of Matrix Operators," March 20, 1980.

*Prof. Mike Bowers, University of California, Santa Barbara, "Multiple Transition States in Chemical Reactions: A Unified Statistical Theory Approach. Application to $C_4H_8^+$," March 27, 1980.

Dr. Michael Liebman, Institute for Cancer Research, Philadelphia, Computer-Generated Representation of the Structure of Biological-Macromolecules: A Method and Its Applications," March 27, 1980.

*Prof. Stephen R. Leone, JILA, University of Colorado, "IR Chemiluminescence Studies of Reactive Dynamics," April 7, 1980.

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

Abstracts of Presentations and Papers of the NRCC Staff

D. Spangler, J. J. Wendoloski, M. Dupuis, NRCC, and M. M. L. Chen and H. F. Schaefer III, Department of Chemistry, University of California at Berkeley and Lawrence Berkeley Laboratory, "Geometry and Electronic Structure of $(CO)_3NiCH_2$. A Model Transition Metal Carbene," LBL-10650, submitted to The Journal of the American Chemical Society.

Abstract: The first application of nonempirical molecular electronic structure theory to a realistic transition metal carbene complex is reported. The system chosen was $(CO)_3NiCH_2$, methylene(tricarbonyl) nickel(0). All studies were carried out at the self-consistent-field (SCF) level of theory. A large and flexibly contracted basis set was chosen, labeled Ni(15s 11p 6d/11s 8p 3d); C,O(9s 5p/4s 2p); H(5s/3s). In addition, the importance of methylene carbon d functions was investigated. The critical predicted equilibrium geometrical parameters were R[Ni-C (methylene)] = 1.83Å, θ(HCH) = 108°. The sixfold barrier to rotation about the Ni-C (methylene) axis is small, ~0.2 kcal. The electronic structure of $(CO)_3NiCH_2$ is discussed and compared with those of the "naked" complex $NiCH_2$ and the stable $Ni(CO)_4$ molecule.

S. Hagstrom, NRCC, and H. Partridge III, NASA Ames Research Center, "Fourier Transform Method for Evaluation of Multicenter Slater Integrals," LBL-10814, presented April 1980 at the Second West Coast Theoretical Chemistry Conference.

Abstract: The formulation and implementation of the Fourier transform method for the evaluation of multicenter two-electron Slater integrals over s-, p- and d-type Slater orbitals will be presented. The algorithm is charge distribution based and becomes progressively more efficient as the basis set size increases. Numerical experience accumulated over the last few years will be reported along with prospects for future enhancements.

J. J. Wendoloski, NRCC, "Determination of the Charge Distribution in Molecules: An Analysis of the Infrared Intensities in Methane, Ethylene, and Acetylene," LBL-10710, presented April 1980 at the Second West Coast Theoretical Chemistry Conference.

Abstract: The nature of the charge distribution and charge rearrangement in methane, ethylene, and acetylene has been examined using restricted Hartree-Fock methods plus Boys localization and also within the Generalized-Valence Bond (GVB) framework. It was found that the intensities could not be explained by considering the magnitude of the atomic charge shifts themselves, but that account must be taken of the vector direction both of the bond dipoles and the lone pair-like atomic dipoles which form during vibration. Mulliken population results were found to lead to misleading conclusions about the nature of the infrared intensities.

J. J. Wendoloski, NRCC, "Calculation of the Force Fields and Infrared Intensities of Organic Molecules Using Analytic GVB Gradients: Methane, Ethylene, and Acetylene," LBL-10709, presented June 1980 at the 35th Symposium on Molecular Spectroscopy, Ohio State University, Columbus, Ohio.

Abstract: Energy optimized geometries for methane, ethylene, and acetylene have been calculated using analytic energy gradients (Force Method) within the generalized valence bond (GVB) perfect pairing framework. The full force field and normal mode frequencies were then calculated using the GVB Force Method. The infrared intensities associated with each normal mode were also obtained from the numerical differencing of the GVB dipole moments. Basis set dependencies for all of these quantities were also examined. A detailed comparison between these results and the restricted Hartree-Fock results is presented, along with a comparison with experimental data.

D. M. Ceperley, NRCC, and B. J. Alder, Lawrence Livermore Laboratory, "The Low Density Phases of the Electron Gas," LBL-11032, submitted to Journal de Physique.

Abstract: We have generalized the quantum Monte Carlo method for Bosons of Kalos, Levesque, and Verlet to exactly simulate the ground state of many-Fermion systems. We have carried out such simulations on the one component plasma with up to 250 electrons and determined the equation of state in three phases: the normal (unpolarized) Fermi liquid, the polarized Fermi liquid, and the Wigner crystal. Two phase transitions are seen: from the normal liquid to the polarized at $r_s = 75$, and from the polarized liquid to the Wigner crystal at $r_s = 100$ where r_s is the mean interparticle spacing in Bohr radii.

D. M. Ceperley, NRCC, and B. J. Alder, Lawrence Livermore Laboratory, "The Ground State of the Electron Gas by a Stochastic Method," LBL-10813. Submitted to Physical Review Letters.

Abstract: We have used an exact stochastic simulation of the Schroedinger equation for charged Bosons and Fermions to calculate the correlation energies, to locate the transitions to their respective crystal phases at zero temperature within 10%, and to establish the stability at intermediate densities of a ferromagnetic fluid of electrons.

D. M. Ceperley, NRCC, "The Relative performances of Several Scientific Computers for a Liquid Molecular Dynamics Simulation," LBL-8015 to be presented at the August 1980 meeting of the American Chemical Society in San Francisco.

Abstract: A statistical mechanics simulation package "CLAMPS" has been tested and timed on four scientific computers: CDC 7600, VAX 11/70, the VAX 11/70 with FPS array processor 120B, and CRAY-1. The simulation used for the timing studies was a molecular dynamics calculation for the Stillinger-Lemberg potential of water. The author will discuss the ease of programming the various machines to achieve high efficiency and the type of simulation, which in his opinion, each computer is best suited.

VISITORS

W. Jorgensen, Department of Chemistry, Purdue University, January 11-14, 1980.

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

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

H. Kashiwagi, Institute for Molecular Science, Myodaiji, Japan, February 28, 1980.

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

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

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

PUBLICATIONS REQUEST FORM

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