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NRCC NATIONAL RESOURCE FOR COMPUTATION IN CHEMISTRY

BULLETIN

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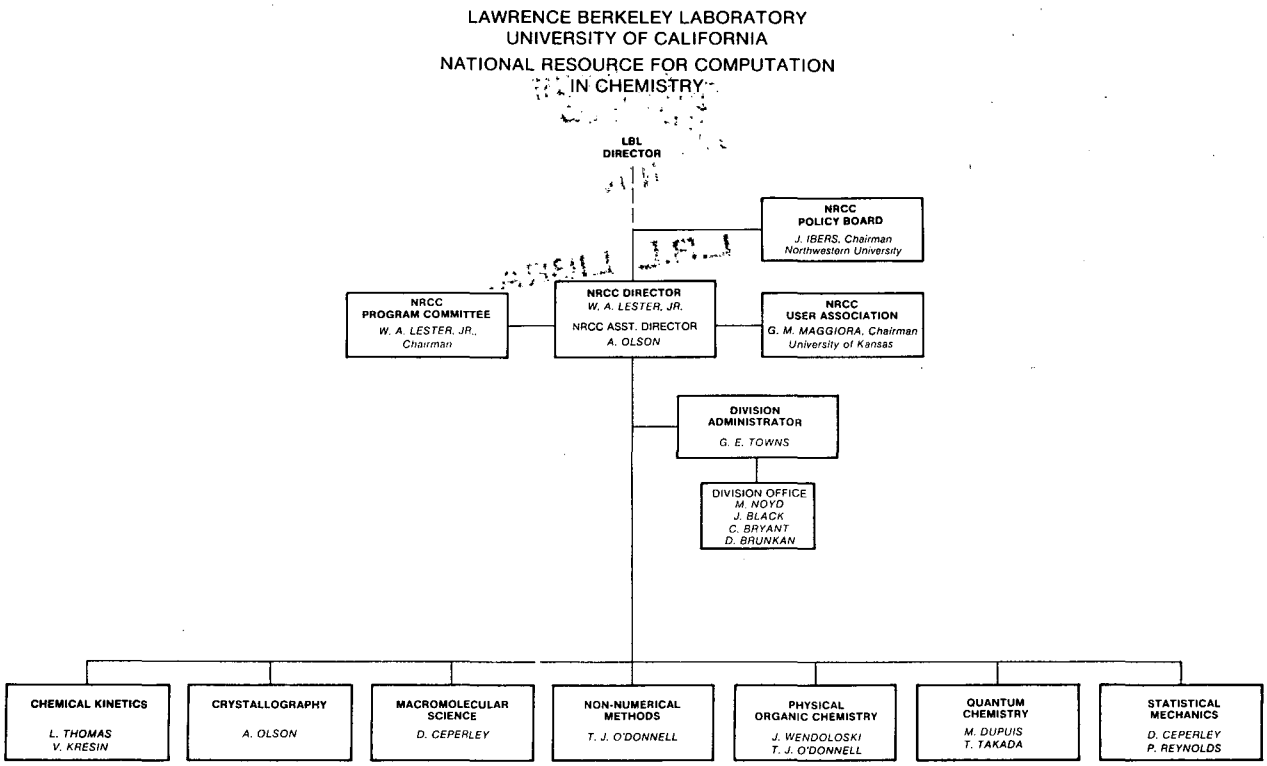

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Bulletin Editor:
John J. Wendoloski

PERSONNEL CHANGES

Dr. Dale Spangler of the scientific staff has left the NRCC to accept a position at SRI International, Menlo Park, California. Dr. Spangler, who was one of the first members of the scientific staff, played a key role in establishing the NRCC software library. Utilizing his expertise in the areas of chemistry and computer science, he contributed to making the library both transportable and efficient. In addition, he made significant improvements in many of the most important codes available from the NRCC including GAMESS, GIVEIS, MINDO/3 and MNDO.

Mr. Tim S. Clark of the administrative staff has left NRCC to continue his studies at the University of California, Berkeley.

Ms. Devon Brunkan has joined the NRCC administrative staff as program librarian.

NRCC PROPOSAL PROGRAM

The NRCC proposal Program is currently under review. Based on the recommendation of the NRCC Policy Board, no further calls for proposals will be announced in the Phase I period which ends September 30, 1981. The future direction of this part of the NRCC's program will be presented in a forthcoming issue of the BULLETIN.

WORKSHOP ANNOUNCEMENTS

Biological Software

The NRCC will hold a small workshop to discuss the development of software in the area of computer simulation of structural, energetic, and dynamic properties of organic and biologically active molecules. The goal of this workshop will be to define the desired capabilities of the software. This effort is being coordinated in the United States by Dr. Arnold T. Hagler, presently on sabbatical leave from the Weizmann Institute to the Chemistry Department, University of California at San Diego, La Jolla, California 92093. The meeting, to be held January 5-8, 1981 in Asilomar, California, will begin with an evening session on January 5th and conclude at noon on the 8th.

The workshop will be built around presentations by leaders in the biological software field, summarizing their research efforts and interests, with emphasis on those areas where computer simulation plays a significant role. The final session will be devoted to a roundtable discussion in which the de-

sired capabilities and possible mode of implementation of the software are addressed explicitly.

The number of workshop participants is restricted by the format; interested scientists may apply to the NRCC to attend. They should supply information to support their probable contribution to the workshop. Selection of the participants will be determined from supporting data provided by the candidate.

Please see page 15 for further information on application submission.

WORKSHOP CALENDAR

January 5-8, 1981: Biological Software

Chairman: Dr. Arnold T. Hagler
Weizmann Institute, Israel

Location: Asilomar, California

REPORTS ON NRCC WORKSHOPS

Portable Crystallographic Code II: Multiple Isomorphous Replacement

A second workshop on portable crystallographic code was held from June 1-8 at the NRCC. 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 Sygusch, University of Sherbrook; Steven Sheriff, U.C.L.A.; 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 intercommunication 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 suc-

cessfully 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.

At present, the XTAL80 Program has been run successfully on both ideal and real test data. There exists some remaining work to be done on "user-friendly" input and output, and complete documentation. The present hope is for distribution of the program some time this fall.

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 is 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. With his 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.

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

On July 14-16, the NRCC sponsored a workshop on "Recent Developments and Applications of Multiconfigurational Hartree-Fock (MCHF) Methods" at Texas A&M University. Cochairmen for this workshop were Professor Danny L. Yeager of Texas A&M and Dr. Michel Dupuis of the NRCC. The goal of the workshop was to foster discussion of ideas on multiconfigurational methodology which might lead to better methods and computer codes, and on 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 feeling emerging from these discussions was that the convergence process for ground and excited state wavefunctions was well understood. Applications of MCHF methods to response functions, effective hamiltonian methods, potential energy surface calculations, and symmetry breaking problems were presented. One question still to be resolved is the selection

of configurations to be included in the MC wavefunctions in order to obtain a reliable description of chemical systems.

The proceedings of this workshop will be available by the end of 1980.

NEW PROCEEDINGS AVAILABLE

The Problem of Long-Range Forces in the Computer Simulations of Condensed Media

Copies of the proceedings of the NRCC conference on Long-Range Forces, which was held January 8-11 in Vallambrosa Center, Menlo Park, California, are now available from the NRCC. This conference, which was organized by Professors Harold Friedman and George Stell of the State University of New York at Stony Brook, dealt with problems arising in the simulation of systems that have a potential energy of interaction which decays slowly with distance. Two common examples are coulombic and dipolar interactions. The focus of the workshop was on how to relate infinite system properties to the results of computer simulations involving relatively small numbers of periodically replicated particles. These proceedings also contain several applications to ionic and dipolar systems.

NRCC SOFTWARE CATALOG AVAILABLE

Volume 1 of the NRCC Software Catalog is now available for distribution. Copies have been sent to everyone on the current NRCC mailing list. Additional copies may be requested using the form on Page 5.

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 annaully. Special software updates will be issued at irregular intervals as the need arises.

USER ASSOCIATION NEWS

The Executive Board of the NRCC User Association convened the second annual meeting of the User Association August 25-29 in conjunction with the fall meeting of the American Chemical Society. Due to a scheduling change by the ACS, this meeting was moved to Las Vegas, Nevada. A summary of the proceedings of this meeting will be published in the next BULLETIN.

SEMINARS

* Dr. John Hepburn, Lash Miller Chemical Laboratories, "Vacuum UV Laser Induced Fluorescence Studies in Chemical Dynamics," April 11, 1980.

Dr. Richard Blint, General Motors Research Group, "Theoretical and Experimental Investigations Relating to Methane Flames," April 18, 1980.

Prof. Jack Tossell, University of Maryland, "Quantum Mineralogy," May 27, 1980.

Prof. Anthony C. Hearn, University of Utah, "The Coming Revolution in Scientific Computation," May 28, 1980.

Dr. Gerard Bricogne, The Medical Research Council, Cambridge, England, "An Improved Formulation of MIR Phase Refinement," July 9, 1980.

Dr. Gerhard E. Hahne, private consultant, "Incorrect Weak Coupling Limit of an Effective Potential Method," July 9, 1980.

Prof. Peter Reynolds, Boston University, "Large Cell Monte Carlo Renormalization Group for Percolation," August 13, 1980.

VISITORS

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

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

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

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

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

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

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

H. Jones, Division of Natural Sciences and Mathematics, Florida A & M University, Tallahassee, Florida, June 31-August 29, 1980.

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

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

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

M. Bishop, Division of Science and Mathematics, Fordham University at Lincoln Center, July 14-August 22, 1980.

D. Yarkony, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland, august 2-27, 1980.

A. Lupkis, Department of Chemistry, University of Rochester, Rochester, New York, August 11-31, 1980.

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

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

MANUSCRIPTS RECEIVED--RESEARCH PARTIALLY SUPPORTED BY THE NRCC

Millard H. Alexander, University of Maryland, "Close-Coupling Studies of Rotationally-Inelastic HF-HF Collisions at Hyperthermal Energies," to appear in J. Chem. Phys., November 1, 1980.

Millard H. Alexander, University of Maryland, Eugene F. Jendrek, Monsanto Research Corporation, Miamisburg, Ohio, and Paul J. Dagdigian, University of Maryland, "Validity of Energy Gap Representations of Rotationally Inelastic Cross Sections between Polar Molecules," to appear in J. Chem. Phys., October 15, 1980.

Marvin Bishop, Fordham University at Lincoln Center, David Ceperley, NRCC, and Harry L. Frisch, State University of New York at Albany, Malvin H. Kalos, New York University, "Investigations of Static Properties of Model Bulk Polymer Fluids," J. Chem. Phys. 72 (5), March 1, 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. Macromolecular Science, 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).

Robert R. Lucchese and Vincent McKoy, California Institute of Technology, "Application of the Schwinger Variational Principle to Electron-Ion Scattering in the Static-Exchange Approximation," Phys. Rev. A, 21 112 (1980).

Robert R. Lucchese and Vincent McKoy, California Institute of Technology, "Application of the Schwinger Variational Principle to Electron-Molecular on Scattering," Physica Scripta, 21, 366 (1980).

Lawrence R. Pratt, Harvard University (present address: University of California, Berkeley), "Effective Field of a Dipole in Nonpolar Polarizable Fluids," Mol. Phys., to be published 1980.

Lawrence R. Pratt, University of California, Berkeley, Effective Intramolecular Potentials for Molecular Bromine in Argon. Comparison of Theory with Simulation," J. Chem. Phys., to be published 1980.

J. C. Sun, B. H. Choi, and R. T. Poe, University of California, Riverside, and K. T. Tang, Pacific Lutheran University, "Quantum Theory of D + H_2 Rearrangement Collision: Effects of Vibrational Excitation," Phys. Rev. Letts. 44, 1211 (1980).

J. C. Sun, B. H. Choi, and R. T. Poe, University of California, Riverside, and K. T. Tang, Pacific Lutheran University, "Reactive Scattering of Rotationally Excited Target Molecules with Adiabatic Theory," accepted by J. Chem. Phys., November 1980.

J. C. Sun, B. H. Choi, and R. T. Poe, University of California, Riverside, and K. T. Tang, Pacific Lutheran University, "Three-Dimensional Quantum Mechanical Studies of D + H_2 → HD + H Reactive Scattering. IV. Cross Sections and Rate Constants with Rotationally Excited Target Molecules," submitted to J. Chem. Phys.

FINAL PROJECT SUMMARIES OF RESEARCH SUPPORTED BY THE NRCC

Title of Project: "Computational Studies of Laser-Assisted Molecular Rate Processes"

Duration: November 1978 - September 1980

Amount: $5,000

Principal Investigator: Thomas F. George

Address: Department of Chemistry, University of Rochester, Rochester, New York 14627

Summary

Close-coupling calculations were carried out for Na + Xe collisions in the presence of two lasers: the rhodamine 110 dye laser (0.55-μm line) and the Nd:glass laser (1.32-μm line).[1,2] The electronic degrees of freedom were represented in terms of potential energy curves for the four energetically lowest states of the NaXe system ($X^2\Sigma$, $A^2\pi$, $B^2\Sigma$ and $C^2\Sigma$), where these curves and the transition dipole moments were constructed from ab initio (pseudopotential) data. The two lasers are not resonant with the asymptotic atomic states, although they do come into resonance with the molecular states for finite internuclear separations. Assuming the radiation from both lasers to be perfectly monochromatic and linearly polarized in the same direction, we used the orientational average approximation to derive a set of nine coupled equations to be solved for each partial wave.

The equations were solved for collision energies ranging from 0.03 to 0.27 eV and for partial waves up to 310 to yield cross sections which were summed and averaged over degeneracies. For intensities of each laser as low as 10 MW/cm^2, the cross sections for the following three processes are as high as 0.3, 0.0008 and 0.03 Å^2, respectively:

$$Na(3s) + Xe + \hbar\omega_1 + \hbar\omega_2 \rightarrow Na^*(3p) + Xe + \hbar\omega_2$$

$$\rightarrow Na^*(4s) + Xe$$

$$Na(3p) + Xe + \hbar\omega_1 + \hbar\omega_2 \rightarrow Na^*(4s) + Xe + \hbar\omega_2$$

The first and third processes involve the absorption of a single photon [from rhodamine 110 ($\hbar\omega_1$) and Nd:glass ($\hbar\omega_2$), respectively] and the second involves the absorption of two photons. The cross section for the second process should be high enough for experimental detection of fluorescence from $Na^*(4s)$. The first and third processes are nearly linear in the laser intensity, and the second is nearly proportional to the product of the two laser intensities. Hence, for example, the cross section of 0.0008 Å^2 for the second process, which occurs around a collision energy of 0.06 eV, increases to 0.008 Å^2 when the intensity of the rhodamine 110 laser is increased to 100 MW/cm^2 (with that of the Nd:glass fixed at 10 MW/cm^2).

Calculations were also carried out for Na + Ar collisions in the presence of the rhodamine 110 and Nd:glass lasers.[3,4] In this case, five different frequencies of the tunable rhodamine 110 laser were considered: 18250, 18300, 18350, 18400 and 18450 cm^{-1}. [The line at 0.55 μm, corresponding to 18182 cm^{-1}, used in the Na + Xe calculations occurs at the peak of the intensity vs frequency spectrum of the laser.] A noticeable feature associated with varying the frequency is a double maximum in the total cross section vs. col-

lision energy for the process Na(3s) + Ar + $\hbar\omega_1$ + $\hbar\omega_2$ → Na*(3p) + Ar + $\hbar\omega_2$, which occurs for a frequency of 18,250 cm^{-1} but disappears as the frequency is increased. This is attributed to the coalescence of curve crossings in the electronic-field representation.

The particular algorithm used to solve the coupled-equations was the Light-Walker R-matrix method, and the computer code was developed by Dr. Paul L. DeVries. The basic code, designed to treat coupled electronic states, has existed in our research group for some time and has been thoroughly tested. Subroutines specific to alkali-metal-noble-gas systems in the presence of laser radiation, i.e., those treating angular momenta and the evaluation of electronic and radiative matrix elements, have been added. Due to the specific nature of the code, and hence its limited applicability, we suggest that anyone wishing to use it should contact us directly.

Papers Acknowledging NRCC Support

1. P. L. DeVries, C. Chang, T. F. George, B. C. F. Laskowski, and J. R. Stallcop, "Na + Xe Collisions in the Presence of Two Nonresonant Lasers," Chem. Phys. Lett. 69, 417 (1980).

2. P. L. DeVries, C. Chang, T. F. George, B. Laskowski and J. R. Stallcop, "Computational Study of Alkali-Metal-Noble-Gas Collisions in the Presence of Nonresonant Lasers: Na + Xe + $\hbar\omega_1$ + $\hbar\omega_2$ System," Phys. Rev. A 22, 545 (1980).

3. P. L. DeVries and T. F. George, "Effect of Laser Frequency on a Collision Induced Radiative Process" in Potential Energy Surfaces and Dynamics Calculations, ed. by D. G. Truhlar (Plenum Press, New York), in preparation.

4. P. L. DeVries and T. F. George, "Computational Study of Alkali-Metal-Noble-Gas Collisions in the Presence of Nonresonant Lasers. II. Na + Ar + $\hbar\omega_1$ + $\hbar\omega_2$ System," in preparation.

Abstracts of Presentations and Papers of the NRCC Staff

Investigations of Static Properties of Model Bulk Polymer Fluids, LBL-10149

M. Bishop, Division of Science and Mathematics, Fordham University at Lincoln Center, New York
D. Ceperley, NRCC, Lawrence Berkeley Laboratory
H. L. Frisch, Department of Chemistry and Center for Biological Macromolecules, State University of New York at Albany
M. H. Kalos, Courant Institute of Mathematical Sciences, New York University, New York

Abstract: The static properties of continuum, multichain systems are investigated by a "reptation" Monte Carlo algorithm. All beads interact via a repulsive (shifted) Lennard-Jones potential. In addition, nearest neighbors along chains are linked by a quasiharmonic potential which permits limited pair extensions. Chain lengths of 5, 10, 20, 32, 50, and 70 beads have been studied. Studies at densities of 0.1, 0.3, and 0.5 demonstrate that chain dimensions are compressed as the concentration is increased. Both the mean square end-to-end distance, $\langle R^2 \rangle$, and the means square radius of gyration, $\langle S^2 \rangle$, have a power law dependence upon $\ell - 1$, the number of bonds, with exponent approximately 1.16 for $\rho = 0.1$ and 1.07 for $\rho = 0.3$ and 0.5. $\langle R^2 \rangle$ and $\langle S^2 \rangle$ scale with density as $\rho^{-\gamma}$ where $\gamma \sim -0.22 \pm 0.02$ for long chains, in reasonable agreement with the scaling prediction of -0.25. The asphericity ratios, the pair correlation functions of the center of masses, and the extent of chain overlaps indicate the nonideal behavior of these systems.

Low Angle Scattering of Li^+ CO, LBL-10040 Rev.

L. D. Thomas, NRCC, Lawrence Berkeley Laboratory
W. P. Kraemer and G. H. F. Diercksen, Max-Planck-Institut für Astrophysik

Abstract: Classical calculations are compared with experiment for the scattering of Li^+ ions by CO at 10° and 4.28 eV. Disagreement between the experimental and classical results is argued to be of quantum mechanical origin. CI calculations are reported for new points on the potential energy surface which demonstrate the need for further points.

On Rainbow Scattering in Inelastic Molecular Collisions, LBL-10921

L. D. Thomas, NRCC, Lawrence Berkeley Laboratory

Abstract: The purpose of this letter is to call attention to a growing misinterpretation in the literature on rainbow scattering in inelastic molecular collisions. The importance of rainbow structures in the angular distributions of elastic scattering cross sections is well established. A few years ago it was suggested that similar structure may also be experimentally observable in the distribution of inelastic scattering cross sections vs. the discrete final molecular rotational angular momentum. Since then a number of experiments have clearly demonstrated the existence of such structure, and the work of Schepper et.al., leaves little doubt that the rainbow explanation of it is correct. Several recent experiments have also reported rainbow structures in the angular distributions of rotationally inelastic cross sections. The importance of these developments lies in the possibility that with sufficient theoretical development and experimental resolution, they may lead to direct experimental measurement of certain anisotropic features in the intermolecular potential energy surfaces.

On the Use of Pressure Broadening Data to Assess the Accuracy of CO-He Interaction Potentials, LBL-11075

S. Green, NASA Goddard Institute for Space Studies
L. D. Thomas, NRCC, Lawrence Berkeley Laboratory

Abstract: Rate constants for rotational excitation of CO by collisions with low energy He atoms are of some importance for interpreting radioastronomical data. Extensive theoretical calculations for this system have been done. The major source of error in these previous studies undoubtedly came from inaccuracies in the intermolecular potential which was obtained from the Gordon-Kim electron gas model.

Recently, Kraemer and Diercksen have obtained the CO-He potential from extensive self-consistent field and configuration interaction (SCF-CI) calculations. Integral cross sections from this potential have been computed and compared with values from the electron gas potential. These comparisons revealed qualitative differences in the energy dependence of the elastic cross sections and quantitative differences (in the range 39-200%) in inelastic cross sections.

This work considers the agreement of the more accurate, SCF-CI surface with pressure broadening data which has traditionally been used to obtain information about intermolecular forces.

Close Coupling Theory: A Survey and Comparison of the Methods, presented at the New York meeting of the American Physical Society, March 24-28 1980, Bulletin of the American Physical Society 25, 3, March 1980.

L. D. Thomas, NRCC, Lawrence Berkeley Laboratory

Abstract: The degree of complexity in molecular collisions which may be studied with close coupling theory, and many other approximate quantum mechanical methods, is limited in practice by the number of coupled second-order differential equations which may be solved in an acceptable amount of time on today's generation of computers.

A novel, two-part workshop, co-chaired by John C. Light, University of Chicago, and myself was organized for the purpose of identifying which of the existing methods for solving these coupled equations perform most efficiently on a variety of problems and making tested versions of the computer codes available through the NRCC software library.

Twenty active researchers in the field met at the Argonne National Laboratory June 24-27, 1979, and most of the methods in current use were presented and discussed. During the second part of the workshop, a set of three, realistic, three-dimensional test problems were taken from the current literature. These problems were than solved on the Lawrence Berkeley Laboratory's CDC 7600 by eight participants of the Argonne meeting. A second meeting was then held in Berkeley, October 26-27, 1979, to compare and discuss the results of the tests.

Although the application of close coupling theory to inelastic molecular collisions has reached a fair degree of maturity in the past ten years, a surprisingly large amount of new material was presented at the workshop and the test results contained a few surprises as well. A brief review of the methods and a presentation of the test results will be given.

NRCC WORKSHOP INFORMATION REQUEST FORM

To receive an application form and additional information for the NRCC workshop on "Biological Software," complete and return the form below.

Please send me additional information and an application form for the NRCC workshop on Biological Software, January 5-8, 1981, Asilomar, California.

Name_____

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Detach and return prior to November 8, 1980 to:

NRCC WORKSHOP INFORMATION
Lawrence Berkeley Laboratory
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Berkeley, California 94720

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Post-Hartree Fock: Configuration Interaction _____

Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Vol. I _____

Stochastic Molecular Dynamics _____

Computational Methods for Molecular Structure Determination: Theory and Technique _____

The Problem of Long-Range Forces in the Computer Simulation of Condensed Media _____

Other Publications

Programmer's Manual for the XTAL System of Crystallographic Programs _____

Attached Scientific Processors for Chemical Computations: A Report to the Chemistry Community _____

Roster of Minicomputer Users _____

Software Catalog _____

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   Yes____ No____

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3. Can you suggest specific codes that should be made a part of the NRCC library at the LBL Computer Center? If so, give the names and as many particulars as possible on a separate sheet. Please comment on quality of documentation, if known.

4. Have you developed codes for your own use which might be of interest to NRCC users? If so, supply detailed information about the code and its level of documentation.

5. Do you have suggestions for workshop topics which the NRCC might sponsor in the next two years? If so, send a brief statement.

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