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SOFTWARE CATALOG

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LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA

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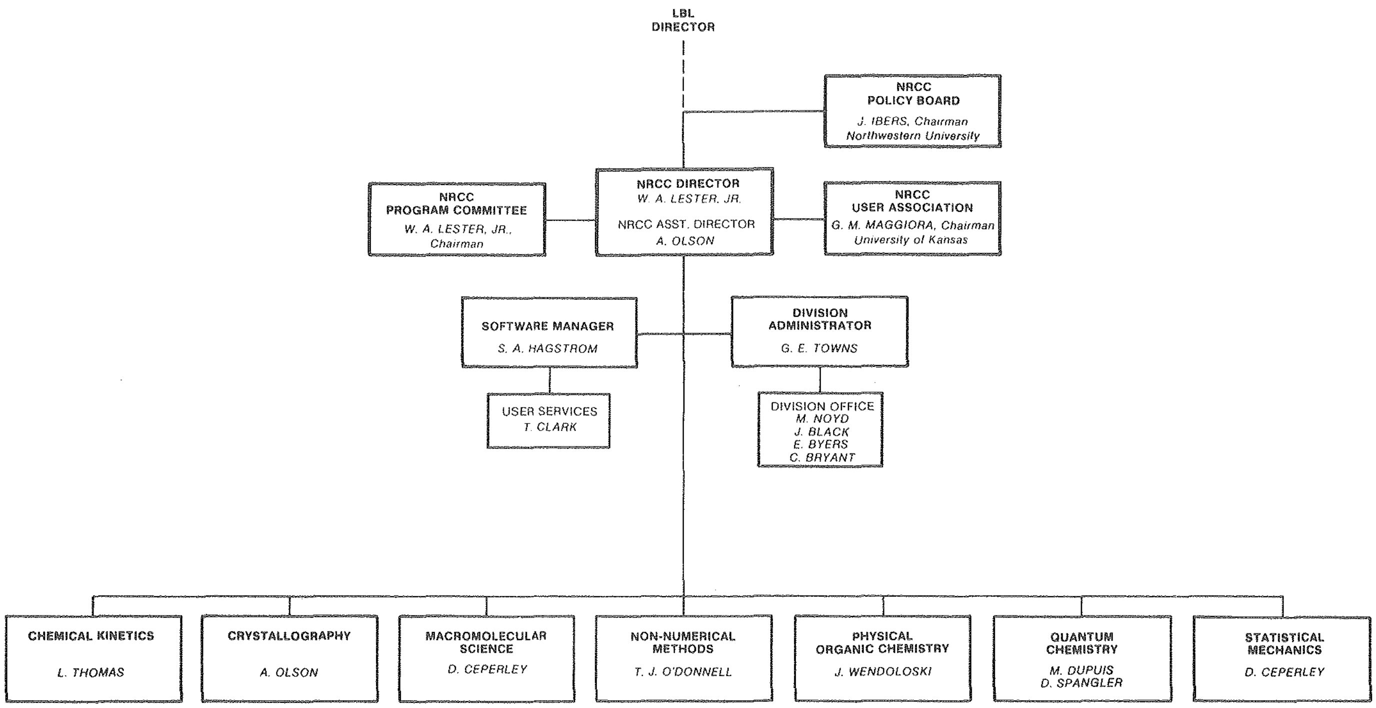

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NRCC SOFTWARE CATALOG

Volume 1

Prepared by the scientific staff of the NRCC

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NRCC SOFTWARE CATALOG

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INTRODUCTION

THE NRCC SOFTWARE LIBRARY

The NRCC software library is a collection of computer programs applicable to problems in chemistry and related sciences. The library was created to make reliable forefront programs available for general use on a timely basis. It is housed at the Lawrence Berkeley Laboratory computer center and can be accessed either on-site or remotely using batch or interactive procedures. The library holdings are distributed upon request. NRCC staff members responsible for maintenance and development of the program library also serve as consultants in the use of the programs.

Library entries are either (1) self-contained applications programs, (2) collections of subroutines that function as a unit intended for use as a module of a self-contained program and (3) individual subroutines and functions. The majority have been written in FORTRAN. Selected subroutines and functions have assembly language replacements where their use leads to significant increase in efficiency. Assembly language routines appear in a few contributed applications programs to provide access to options not available through FORTRAN.

Documentation on how to use the programs is available upon request and includes copies of test input decks and corresponding printed output. For most programs documentation is maintained in machine readable form. Extensive printed documentation is also available for certain programs.

The library came into existence in the Fall 1978. Since that time it has grown considerably in the principal program areas of chemical kinetics, crystallography, macromolecular science, quantum chemistry, physical organic chemistry and statistical mechanics. Although some of the programs in the library were written by NRCC staff, the majority of programs have been made available from elsewhere. Some come from individual research groups that have worked with NRCC staff to make the codes operational at the NRCC. Other programs were made available initially in connection with NRCC-sponsored workshops. In quantum chemistry many have been provided by the Ouantum Chemistry Program Exchange (QCPE) at Indiana University. The NRCC is indebted to the authors of these programs for making them available to the chemistry community at large through the NRCC.

Most computing at the NRCC is carried out on the LBL CDC 7600. This machine is connected to both a CDC 6600 and CDC 6400 for staging jobs for the 7600 and for general interactive use. At present many programs in the library are limited to use on the CDC 7600 in batch mode. Most programs are easily transferable to computers of other manufacture, and where versions for IBM and DEC VAX equipment have been created they are included in the catalog . The NRCC has a DEC VAX 11/780 which has provided the means for generating the existing VAX versions and others under development.

PROGRAM CLASSIFICATION

The software library is organized into the principal scientific program areas listed above (chemical kinetics, crystallography, macromolecular science, etc.) and other computer-related areas (graphics, software tools). A complete listing is found in the table of contents. Besides a program name, each entry has been assigned a unique four character catalog designator. The first character which is always alphabetic identifies the scientific area, the second character (also alphabetic) identifies programs applicable to a common purpose in the scientific area, and the last two characters (numeric) generate unique designators within each subgroup. We illustrate the system with a kinetics program, ABCRRJ - an A + BC classical trajectory program - which has the catalog designation KC02. This designation carries the following meaning: K - chemical kinetics, C - classical method, and 02 - second catalog entry in the section on chemical kinetics.

PROGRAM CONSULTATION SERVICE

Within the catalog format it is not always possible to present sufficient information for the user to decide which program is best suited for a particular application. The NRCC staff can provide guidance on program selection and answer questions about the software library. Potential users are urged to contact the NRCC staff member in the appropriate problem area (see inside front cover) on the toll-free number (800-227-0198) outside of California and on the commercial number provided on the inside front cover within the state. Routine requests for software should be addressed to the Program Librarian.

PROGRAM SUPPORT LEVELS

The following classification scheme has been devised to indicate the level of assistance available from NRCC personnel for programs. It defines three levels of support (complete, partial, none) in each of three areas: programming , consulting and documentation . Of the twenty-seven alternatives , the following four have been adopted:

Classification	Programming	Consulting	Documentation
A	Complete	Complete	Complete
B	Partial	Complete	Complete
C	None	None	Partial
D	None	None	None

A description of the various support levels follows:

Programming
  Complete: Reports of software bugs are acted upon promptly.
  Suggestions for improvement and enhancements
  are explored, and implemented where appropriate.
  Codes written by the NRCC in-house staff are examples

of completely supported programs.

Partial: Reports of software bugs are examined and fixes implemented where feasible. Bugs and deficiencies may be documented rather than remedied and suggested improvements will, in general, not be done. Highly used programs that are written externally will normally fall into this category.

None: No software modifications made by NRCC staff, but codes are available for use.

Consulting

Complete: The NRCC staff is available for advice and help in using the program via personal contact and/or correspondence.

None: No user assistance is guaranteed from the NRCC staff.

Documentation

Complete: On-line documentation is maintained as well as hardcopy manuals. Documentation is geared to a first-time user of the software.

Partial: Documentation is available in hardcopy and on-line form although there is no guarantee that it will be adequate for an inexperienced user of the program.

None: No documentation is available except for a brief abstract of program capability.

Please note that the guidelines for support define the minimal support guaranteed for a program. It could happen that a code is supported beyond the rigid categories. For example, excellent documentation could happen to be available for an obsolete D-category program or a staff member could have developed expertise in a B-category code to implement proposed improvements.

SOURCE CODE DISTRIBUTION POLICY

With one or two exceptions, the source code for NRCC programs is in the public domain and available either from the NRCC or other organizations. The following four categories have been established for source code distribution:

A	Source code is available from NRCC without restrictions.
B	Program is distributed by an organization other than the NRCC. Source code is available at the NRCC for on-site use. Most QCPE programs, but not all, fall in this category. Programs distributed by QCPE have a special BO distribution code.
C	Source code is available for use only at the NRCC and is not available for off-site distribution. This is the situation in a few cases where programs have originated elsewhere and the originators have requested that the source be protected.
D	Program may be run at the NRCC but source code is not accessible to on-site users. Only a very few programs are expected to fall in this catagory.

ACCESSING PROGRAMS AT NRCC

Program documentation and sample input decks and output listings are available for most 7600 programs on GSS tape number 39000 housed in the LBL computer center tape library. They may be retrieved using the file pathnames indicated in the catalog entry and disposed to a printer or examined on-line from a terminal. Source code is similarly available on 39000 (distribution categories A and B only) along with appropriate procedure files to assist in constructing the load module(s) form of the program.

Compiled (load module) versions of most 7600 codes are also found on 39000 (see program write-up for details). Therefore, it is usually not necessary to have access to the source if one wants only to run the program.

OTHER LIBRARIES

A separate chapter describing some 15 other software libraries available to NRCC users is included in the catalog. Some of these are rather specialized (EISPACK,BLAS) while other are of more general interest (IMSL, NAG). Some are relevant only to the VAX.

CATALOG ENTRIES

The text part of each catalog entry consists of a brief summary of the purpose, method and other attributes of the program. Further information is provided in the full program write-up. Literature references are given in some instances.

The names of the authors, and in some cases place of origin of the program are given. Most of the programs coming from outside have undergone some modification for use on the CDC7600 and therefore the NRCC takes partial responsibility for maintaining them. Difficulties encountered in using programs should be brought to the attention of NRCC staff, not the original authors.

A list of available files follows the program origin.. The machine designators CDC, IBM, VAX have been added to distinguish the several machine specific source versions that exist for various programs. Note that all files are in either source (card image) or printed output(line image) format. The NRCC does not distribute object or CDC Update files.

The support level and distribution status are indicated for each program using the classification code described earlier.

OBTAINING PROGRAMS FOR EXTERNAL USE

With only one or two exceptions, library programs are available for external use. For the present, no charge is made for this service . Programs are distributed on 9-track half-inch 800 or 1600 bpi magnetic tape. Card decks and listings are not available. Off-line documentation is also available in a few cases.

Anyone wishing to obtain copies of library materials should fill out one of the program application forms at the back of the catalog and send it along with a magnetic tape (certified at least to 1600bpi and preferably to 6250) to Program Librarian, NRCC, Lawrence Berkeley Laboratory, Building 50D, Berkeley, CA 94720. [Tel. (415)486-6722 or FTS 451-6722 or (800)227-0198 outside California]

RESTRICTIONS ON USE OF LIBRARY MATERIAL

There are no restrictions on the use of library programs either at the NRCC or elsewhere or any prohibitions against third party distributions. Most NRCC programs for which source is available are in the public domain and may be freely distributed, modified, and converted. However, we request that acknowledgment be made in publications and articles resulting from the use of these codes. The recommended form of citation is (e.g., for the program ALIS):

> S.T. Elbert, L.M. Cheung, K. Ruedenberg, Nat. Resour. Comput.
> Chem. Software Cat., Vol.1, Prog. No. QM01 (ALIS), 1980.

In addition, in connection with all codes it should be noted that:

a. The University of California, Lawrence Berkeley Laboratory, and the NRCC make them available on an "as-is", non-exclusive basis and without any warranties whatsoever, including the implied warranties of fitness for a particular purpose and merchantability.

b. The University of California, Lawrence Berkeley Laboratory, and the NRCC shall be under no obligation to maintain, correct, update, change, modify or otherwise support them except as indicated by the support level classification for this software as determined by the NRCC.

c. The University of California, Lawrence Berkeley Laboratory, and the NRCC make no representation and give no warranty as to infringement of patents or copyrights relating to this material.

GRAPHICS

CHEMICAL KINETICS

KC01 ABCRR A + BC Classical Trajectory Program

Computes classical trajectories for rotationally inelastic collisions between an atom, A, and a rigid-rotor diatomic molecule, BC. Data is stored from each trajectory which can be processed into various cross sections by the progam XRR. For a range of angles and j (final angular momentum of BC) selected by the user, XRR will compute differential cross sections vs. j, total differential cross sections (summed over all j), and integral cross sections (integrated over all angles) vs. j.

ORIGIN - L. D. Thomas

AVAILABLE FILES -

ABCRR/DOC	Trajectory documentation
ABCRR/SOURCE	Source code for trajectory calculation
ABCRR/DOC/XRR	Cross section documentation
ABCRR/SOURCE/XRR	Source code for cross section calculations
ABCRR/TESTIN	Test input for trajectories and cross sections
ABCRR/TESTOUT	Printer output of test run

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

KC02 ABCRRJ A + BC Classical Trajectory Program

Computes classical trajectories for atom, A, plus rigid-rotor, BC collisions. This program differs from the program ABCRR in that the total angular momentum, J, is chosen as one of the initial conditions, instead of the usual impact parameter, b.

ORIGIN - L. D. Thomas

AVAILABLE FILES -

ABCRRJ/DOC	Trajectory documentation
ABCRRJ/SOURCE	Source code for trajectory calculation
ABCRRJ/SOURCE/XRRJ	Source code for cross section calulations
ABCRRJ/TESTIN	Test input for trajectories and cross sections
ABCRRJ/TESTOUT	Printer output of test run

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

KC04 CLASTR <u>Reactive A + BC Classical Trajectory Program</u>

Monte carlo quasi-classical trajectory program written by J. T. Muckerman. Revised version of QCPE No. 229. Based on formulation of D. G. Truhlar and J. T. Muckerman, chapter 8b in "Atom - molecule Collision Theory - A Guide for the Experimentalist", edited by R. B. Bernstein, Plenum press, New York (1979), and M. B. Faist, J. T. Muckerman, and F. E. Schubert, J. Chem. Phys. 69, 4087 (1978).

This version of the program is appropriate for reactive scattering of three-atom systems whose potential energy surfaces may be approximated by generalized London-Eyring-Polanyi-Sato functions.

ORIGIN - J. T. Muckerman

AVAILABLE FILES -

CLASTR/DOC	Trajectory documentation
CLASTR/SOURCE	Source code for trajectory calculation
CLASTR/TESTIN	Test input for trajectories calculation
CLASTR/TESTOUT	Printer output of test run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

KC05 ABCD <u>Atom-triatomic Classical Trajectory Program</u>

This program computes state to state energy transfer cross sections for atom - triatomic molecule collisions. the stationary states of the triatomic molecule are determined semiclassically. This program treats nonseparable effects accurately and efficiently enough to enable the determination of state to state cross sections to within a few percent, while requiring only a small fraction of the trajectory computation time to calculate the good action-angle variables. It can be quite easily applied to collisions involving any linear or nonlinear symmetric triatomic molecule for which cubic or quartic force field parameters are available, and it can be used to determine both differential and integral state to state cross sections as well as final translational distributions and moments of the final state distributions.

ORIGIN - G. C. Schatz

AVAILABLE FILES -

ABCD/SOURCE	Source code
ABCD/TESTIN	Test input

ABCD/TESTOUT	Printer output of test run

SUPPORT LEVEL - D

DISTRIBUTION STATUS - A

KE01 RMATOM R-matrix Method for Electron-atom Scattering

The program RMATOM is a suite of three programs - STAGE1, STAGE2 and STAGE3 - for performing atomic electron-atom electron-ion, atomic photo-ionization and atomic frequency dependent polarizability calculations, using the R-matrix method. STAGE1 calculates all one, two and multipole radial integrals involving bound and continuum orbitals. The bound orbitals are specified analytically, while the continuum orbitals are calculated by the program. The integrals are stored on an intermediate file ready for use by STAGE2. STAGE2 reads the atomic integrals generated by STAGE1 and calculates the Hamiltonian matrix elements, the asymptotic potential coefficients and the dipole and velocity matrix elements from a given initial state to the final state specified by L,S and the channel quantum numbers. This information is stored on intermediate files. STAGE3 reads the information generated in STAGE2, diagonalizes the Hamiltonian matrix and calculates the R-matrix and its Buttle correction. Then either the electron-atom or electron-ion cross sections, the photo-ionization cross section and the beta asymmetry parameter or the frequency dependent polarisability are calculated.

ORIGIN - K. A Berrington, P. G. Burke, M. Ledourneuf, W. D. Robb,
K. T. Taylor and Vo Ky Lan

AVAILABLE FILES -

RMATOM/DOC	Documentation
RMATOM/SOURCE/STAGE1	Source code for STAGE1
RMATOM/SOURCE/STAGE2	Source code for STAGE2
RMATOM/SOURCE/STAGE3	Source code for STAGE3
RMATOM/TESTIN/STAGE1	Input for test run of STAGE1
RMATOM/TESTIN/STAGE2	Input for test run of STAGE2
RMATOM/TESTIN/TEST1/STAGE3	Input for test run of STAGE3
RMATOM/TESTIN/TEST2/STAGE3	Input for test run of STAGE3
RMATOM/TESTIN/TEST3/STAGE3	Input for test run of STAGE3
RMATOM/TESTOUT/STAGE1	Output from test run of STAGE1
RMATOM/TESTOUT/STAGE2	Output from test run of STAGE2
RMATOM/TESTOUT/TEST1/STAGE3	Output from TEST1 run of STAGE3
RMATOM/TESTOUT/TEST2/STAGE3	Output from TEST2 run of STAGE3
RMATOM/TESTOUT/TEST3/STAGE3	Output from TEST3 run of STAGE3

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ01 MOLSCAT Molecular Scattering Program

MOLSCAT was designed to facilitate theoretical studies of energy transfer in nonreactive molecular collisions. The coupled equations for the radial wave functions can be solved by two different numerical techniques - the Devogelaere method or the piecewise analytic method of Gordon. The expansion basis functions and angular momentum coupling depend on the type of collision partners. The cases available with MOLSCAT are 1) atom-linear rigid rotor, 2) atom-vibrotor, 3) linear rigid rotor- linear rigid rotor, 4) atom-symmetric top and 5) atom-asymmetric top. In addition the coupled equations may be from any of the following approximate methods: 1) close coupling, 2) effective potential, 3) coupled states, 4) decoupled l-dominant 5) infinite order sudden.

ORIGIN - S. Green

AVAILABLE FILES -

MOLSCAT/DOC	Documentation
MOLSCAT/SOURCE	Source code for MOLSCAT
MOLSCAT/SOURCE/IOS	Additional source code needed for the IOS approximation
MOLSCAT/TESTIN/IOS	Input for test of the IOS approximation
MOLSCAT/TESTIN/TEST1	Input for Gordon algorithm and He-HCl collision
MOLSCAT/TESTIN/TEST2	Input for Devogelaere alg. and He-HCl collision
MOLSCAT/TESTIN/TEST3	Input for test of effective potential approximation
MOLSCAT/TESTIN/TEST4	Input for test of coupled-states approx.
MOLSCAT/TESTIN/TEST5	Input for test of two linear rotors colliding
MOLSCAT/TESTIN/TEST6	Input for test of atom-asymmetric rotor collison
MOLSCAT/TESTOUT/IOS	Printer output from TESTIN/IOS above
MOLSCAT/TESTOUT/TEST1	Printer output from TESTIN/TEST1 above
MOLSCAT/TESTOUT/TEST2	Printer output from TESTIN/TEST2 above
MOLSCAT/TESTOUT/TEST3	Printer output from TESTIN/TEST3 above
MOLSCAT/TESTOUT/TEST4	Printer output from TESTIN/TEST4 above
MOLSCAT/TESTOUT/TEST5	Printer output from TESTIN/TEST5 above
MOLSCAT/TESTOUT/TEST6	Printer output from TESTIN/TEST6 above

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

KQ02 QLEVEL <u>Bound States of 1-D Potentials</u>

Computes bound and quasibound states of one dimensional potentials and matrix elements of powers of x, the independent integration variable, between the wave functions.

ORIGIN - R. J. Le Roy

AVAILABLE FILES -

QLEVEL/DOC	Documentation
QLEVEL/SOURCE	Source code
QLEVEL/TESTIN	Input for test run
QLEVEL/TESTOUT	Printer output from test run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

KQ03 TDELAY <u>Phase Shifts and Time Delays for 1-D Potentials</u>

Computes phase shifts and time delays for scattering by a spherical potential.

ORIGIN - R. J. Le Roy

AVAILABLE FILES -

TDELAY/DOC	Documentation
TDELAY/SOURCE	Source code
TDELAY/TESTIN	Input for test run
TDELAY/TESTOUT	Printer output from test run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

KQ04 VIVAS <u>A-BC (Vib-rotor) Coupled Channel Scattering Program</u>

This program computes the scattering S-matrix and transition probabilities for the collision of an S-state atom, A, with a sigma-state diatomic molecule BC. The S-matrix can be obtained using either the variable-interval, variable-step (VIVS) method or the log derivative method or preferably a combination of both. Both of these methods are fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory there are no coulomb interactions.

The results of the workshop were that in general the log derivative (LOGD) method performed best in the inner integration region, while VIVS performed best in the outer region. Therefore, the two methods have been combined into this hybrid program. It is the recommended program for solving the coupled 2nd order differential equations of quantum scattering theory.

ORIGIN - G. A. Parker, J. V. Lill and J. C. Light

AVAILABLE FILES -

VIVAS/DOC	Documentation
VIVAS/SOURCE	Source code
VIVAS/TESTIN/TEST1	Test input for TEST1
VIVAS/TESTIN/TEST2	Test input for TEST2
VIVAS/TESTOUT/TEST1	Printer output of TEST1 run
VIVAS/TESTOUT/TEST2	Printer output of TEST2 run

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

KQ05 GORDON <u>Inelastic Atom-Diatom Quantum Scattering</u>

This program solves quantum close-coupled equations for rotationally and ro-vibrationally inelastic collisions between an atom (electron) and a diatomic molecule. This is a modification of the GORDON code available as QCPE program No. 187. The basic algorithm is discussed in J. Chem. Phys., 51, 14(1969) and Meth. Comp. Phys. 10, 81 (1971). The most important changes to the original code are - 1) at both the initial and subsequent energies, the zeroth- order method with linear reference potential is used to propagate the solutions. 2) the off-diagonal first-order perturbation corrections are computed using a constant reference potential. These perturbation corrections are used only to determine the step sizes and are not added to the zeroth-order solutions.

ORIGIN - M. H. Alexander

AVAILABLE FILES -

GORDON/DOC	Documentation
GORDON/SOURCE	Source code
GORDON/TESTIN	Test input
GORDON/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ06 LOGD *Coupled Channel Scattering Program*

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the log derivative method. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - B. R. Johnson

AVAILABLE FILES -

LOGD/DOC	Documentation
LOGD/SOURCE	Source code
LOGD/TESTIN	Test input
LOGD/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ07 SAMS *Coupled Channel Scattering Program*

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the integral equations method of Sams and Kouri. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - K. D. Mclenithan and D. Secrest

AVAILABLE FILES -

SAMS/DOC	Documentation
SAMS/SOURCE	Source code
SAMS/TESTIN	Test input
SAMS/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ08 INSCAT Coupled Channel Scattering Program

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using integral equations with reference potentials. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - M. J. Redmon

AVAILABLE FILES -

INSCAT/DOC	Documentation
INSCAT/SOURCE	Source code
INSCAT/TESTIN	Test input
INSCAT/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ09 RMAT Coupled Channel Scattering Program

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the R-matrix propagation method. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - T. G. Schmalz

AVAILABLE FILES -

RMAT/DOC	Documentation
RMAT/SOURCE	Source code
RMAT/TESTIN	Test input
RMAT/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ10 PC Coupled Channel Scattering Program

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the variable-order, variable-step, predictor-corrector program of Shampine and Gordon (L. F. Shampine and M. K. Gordon, "Computer Solution of Ordinary Differential Equations: the Initial Value Problem", W. H. Freeman, San Francisco, 1975) The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - L. D. Thomas.

AVAILABLE FILES -

PC/DOC	Documentation
PC/SOURCE	Source code
PC/TESTIN	Test input
PC/TESTOUT	Printer output of test run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

KQ11 DEVOG Coupled Channel Scattering Program

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the Devogelare algorithm. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - L. D. Thomas

AVAILABLE FILES -

DEVOG/DOC	Documentation
DEVOG/SOURCE	Source code
DEVOG/TESTIN	Test input
DEVOG/TESTOUT	Printer output of test run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

KQ12 MNN <u>Coupled Channel Scattering Program</u>

This is a general and modular close coupling program which integrates the coupled equations of quantum inelastic scattering theory using the Numerov method. Step size selection is automatic.

This is version 79-6 of the Minnesota Numerov (MNN) program. It is an updated and more general version of the program described in, M. A. Brandt, D. G. Truhlar, and F. A. Van-Catledge, J. Chem. Phys., 64, 4957 (1976) and proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Vol. I, pg. 220, Lawrence Berkeley Laboratory Report LBL-9501(1979).

ORIGIN - M. A. Brandt, D. G. Truhlar, and K. Onda and D. Thirumalai

AVAILABLE FILES -

MNN/DOC	Documentation
MNN/SOURCE	Source code
MNN/TESTIN	Test input
MNN/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KQ13 L2RMAT <u>Coupled Channel Scattering Program</u>

This program solves the coupled 2nd order differential equations of quantum inelastic scattering theory using the L-squared approach to the R-matrix propagation method. This method is fully described in the proceedings of the NRCC workshop on "Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory", Lawrence Berkeley Laboratory Report LBL-9501(1979). The S-matrix analysis assumes that there are no coulomb interactions.

ORIGIN - R. B. Walker and B. Schneider

AVAILABLE FILES -

L2RMAT/DOC	Documentation
L2RMAT/SOURCE	Source code
L2RMAT/TESTIN	Test input
L2RMAT/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KS01 KAPPAS Semiclassical 1-D Transmission Probabilities

This program computes semiclassical transmission probabilities for a one - dimensional potential barrier and thermally averages them to obtain transmission coefficients.

ORIGIN - B. C. Garrett and D. G. Truhlar

AVAILABLE FILES -

KAPPAS/DOC	Documentation
KAPPAS/SOURCE	Source code
KAPPAS/TESTIN	Input for test run
KAPPAS/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

KS02 RRKM Unimolecular Rate Constants

QCPE program No. 234. This program calculates unimolecular rate constants as a function of molecular total energy, using the RRKM theory (best description, P. J. Robinson and K. A. Holbrook, "Unimolecular Reactions", Wiley - Interscience, New York, 1972).

ORIGIN - W. L. Hase and D. L. Bunker

AVAILABLE FILES -

RRKM/SOURCE	Source code
RRKM/TESTIN	Test input
RRKM/TESTOUT	Printer output of test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

MACROMOLECULAR SCIENCE

PE01 MMI Molecular Mechanics I

A program for the calculation of conformations and energies of molecules using molecular mechanics. This is the CDC version of QCPE program 358 developed by N. L. Allinger and coworkers.

ORIGIN - N. L. Allinger

AVAILABLE FILES -

MMI/SOURCE	CDC version of MMI
MMI/DOC	User manual for MMI
MMI/TESTIN	Test input for MMI
MMI/TESTOUT	Test output for MMI

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

SS01 CLAMPS Classical Many Particle Simulator

A program package which can use five simulation methods (molecular dynamics, Langevin dynamics, Monte Carlo, polymer reptation or Brownian dynamics) to generate configurations distributed according to the Boltzmann distribution. The potential energy is a sum of spherically symmetric pair potentials and/or bond potentials for polymers. For charged particles the Ewald image potential is used to represent the effect of the system outside the simulation box. The configurations generated by CLAMPS can be stored and then analyzed by other programs.

ORIGIN - D. Ceperley

AVAILABLE FILES -

CLAMPS/SOURCE/CDC	CDC version of CLAMPS
CLAMPS/SOURCE/VAX	VAX version of CLAMPS
CLAMPS/DOC	User manual for CLAMPS
CLAMPS/TESTIN/ARRAH	Test input for CLAMPS. Argon simulation described in A. Rahman, Phys. Rev. 136, A405 (1964).
CLAMPS/TESTOUT/ARRAH	Test output for CLAMPS.
CLAMPS/TESTIN/WATER	Test input for water. Pair potential is taken from A. Rahman, F. Stillinger and H. Lemberg, J. Chem. Phys. 63, 5225(1975). Note that the intial configuration must be obtained from the start routine.
START/SOURCE/WATER	Source to obtain starting configuration

	for water
CLAMPS/TESTOUT/WATER	Test output for TESTIN/WATER above.
RANNUM/SOURCE	Portable random number generator
RANNUM/DOC	Documentation for RANNUM
RANNUM/ASSMBLY/CDC	COMPASS version of RANNUM
RANNUM/ASSMBLY/VAX	MACRO version of RANNUM for VAX
CFS/DOC	Documentation for CFS (time correlation functions)
CFS/SOURCE	Source for time dependant correlation functions
VELCOR/SOURCE	Computes velocity correlation function-uses CFS
VELCOR/TESTIN	VAX test for VELCOR. Uses CLAMPS input.
VELCOR/TESTOUT	Test output for VELCOR and CFS

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

XD02 PROTDAT Protein Data Bank Files

The protein data bank is a computer-based archival file for macromolecular structures. The bank stores in a uniform format atomic co-ordinates and partial bond connectivities, as derived from crystallographic studies. Text included in each data entry gives pertinent information for the structure at hand (e.g. species from which the molecule has been obtained, resolution of diffraction data, literature citations and specifications of secondary structure).

SOURCE - Protein Data Bank, Brookhaven National Laboratories

AVAILABLE FILES -

PROTDAT/SOURCE/BENDER	Paramaters for bent-wire models G. Williams
PROTDAT/SOURCE/CONECT	Generate full connectivity F. Bernstein
PROTDAT/SOURCE/DGPLOT	Diagonal plots on printer E. Swanson, F. Bernstein
PROTDAT/SOURCE/DSTNCE	Calc distns from conect rcrds F. Bernstein
PROTDAT/SOURCE/FISIPL	Phi/psi plots on printer F. Bernstein
PROTDAT/SOURCE/NAMOD	Ball-and-stick model display Y. Beppu
PROTDAT/SOURCE/PHIPSI	Main-chain torsion angles Andrews, Williams, Bernstein
PROTDAT/SOURCE/STEREO	Extract xyz from stereo diagram M. Rossmann
PROTDAT/SOURCE/TOTALS	Validation of master records L. Andrews, F. Bernstein
PROTDAT/DATA/XXXXX	113 protein data files

SUPPORT LEVEL - D

DISTRIBUTION STATUS - B (see comments)

Comments - contact NRCC crystallographic staff for file access at LBL. The files may be obtained from -

Protein Data Bank
Department of Chemistry
Brookhaven National Laboratory
Upton, NY 11937

NUMERICAL METHODS

ND01 GIVENS EIGENVALUES AND EIGENVECTORS BY THE GIVENS METHOD

This routine calculates eigenvalues and eigenvectors of real symmetric matrices stored in packed upper triangular form by a modification of the original Givens technique (Oak Ridge Report Number ORNL 1574 (Physics)), by Wallace Givens, namely, tridiagonalization by the Householder method (see J. H. Wilkinson, Comp. J. 3,23(1960)), root location by the Sturm sequence method, Wilkinson's method for generation of the vectors of the tridiagonal form (Comp. J. 1, 90(1958)), and orthogonalization of vectors for degenerate (or near degenerate) roots by the method of B. Garbow. The Gram-Schmidt process is used for the orthogonalization.

This routine is the same as QCPE 62.4.

ORIGIN - F. Prosser, Indiana University

AVAILABLE FILES -

GIVENS/SOURCE	FORTRAN source (includes documentation)

SUPPORT LEVEL - B

DISTRIBUTION STATUS - BQ

ND02 DIAG Iterative Calculation of a Few of the Lowest Eigenvalues and Eigenvectors of Large Real-symmetric Matrices

This routine solves for the lowest few eigenvalues and eigenvectors (less than 14 in this version) of a large dense real-symmetric matrix stored as a sequential access file on disk or tape. An iterative method which does not modify the original matrix is used (see E. R. Davidson, J. of Comput. Phys. 17, No. 1, Jan. 1975, page 87). Space is required only for the current trial vector and the next iterate so that in practice very large matrices can be handled. Although the present version of the program assumes a dense, row ordered matrix, a sparse encoding using skip counts can also be used with only minor changes to the code. Vectors are obtained one at a time and the entire matrix must be inputted once for each iteration for each root. The code has been vectorized for efficient execution on vector machines such as the CRAY and Cyber 203. The FORTRAN versions of the basic linear algebra routines SDOT and SAXPY have been introduced. These should be replaced by their machine language equivalents where these are available for greater efficiency.

ORIGIN - E. R. Davidson, U. of Washington; CDC 7600 and CRAY adaptations by S. A. Hagstrom, NRCC.

AVAILABLE FILES -

DIAG/SOURCE	FORTRAN IV source for DIAG + driver.
DIAG/DOC	Documentation for DIAG
DIAG/TESTOUT	Test output for test case built into the driver

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

ND03 GIVEIS EISPACK-based Substitute for GIVENS

This collection of subroutines finds all eigenvalues and some eigenvectors of a real symmetric matrix using Householder transformations to convert the matrix to tridiagonal form and inverse iteration to determine the user-specified number of eigenvectors. The EISPACK subroutines TRED3, IMTQLV, TINVIT and TRBAK3 have been modified to increase efficiency and in one version the Basic Linear Algebra Subroutines SDOT and SAXPY have been introduced.

ORIGIN - C. Moler and D. Spangler

AVAILABLE FILES -

GIVEIS/SOURCE	Source of GIVEIS
GIVEIS/SOURCE/BLAS	Source of GIVEIS containing calls to SDOT and SAXPY
GIVEIS/DOC	Documentation for GIVEIS

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

NL01 BIORTH A FORTRAN IV Routine for Matrix Bi-orthogonalization

This routine performs bi-orthogonalization of a real matrix of dimensions N by M. As defined here, bi-orthogonalization involves determining left and right transformation matrices L and R such that

$$L W R = D$$

where L is a lower triangular matrix of dimension N by N with unit diagonal (and zero upper triangular part) and R is a corresponding upper triangular matrix of dimension M by M with unit diagonal (and zero lower triangular part). D is a matrix of all zeros except along the principal diagonal. For further details about the algorithm and its use in the evaluation of matrix elements between non-orthogonal determinental wave functions and the evaluation of cofactors of singular overlap matrices, see F. Prosser and S. Hagstrom, "On the Rapid Computation of Matrix Elements", Int. J. of Quantum Chem. 2, 89-99(1968). Note that if W is a metric (i.e., symmetric and positive definite) bi-orthogonalization reduces to Choleski decomposition. Hence, BIORTH includes Schmidt orthogonalization as a special case.

ORIGIN - F. Prosser and S. A. Hagstrom, Indiana University

AVAILABLE FILES -

BIORTH/DOC	Documentation for BIORTH
BIORTH/SOURCE	FORTRAN IV source for BIORTH + test driver
BIORTH/TESTOUT	Test output for built in test case.

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

NR01 RANNUM *Pseudo-random Number Generator*

RANNUM is a pseudo-random number generator of the congruence type which produces random numbers in the range (0, 1). The base, 2 ** 48, is large enough so that correlations are small and the repeat cycle is very large. A portable FORTRAN version is available for verification of machine independence of programs using random numbers. Two assembly language versions are available for CDC and DEC/VAX machines. Three other subroutines are available to initialize the seed to save the seed and to construct a random seed.

ORIGIN - M. H. Kalos, and D. Ceperley

AVAILABLE FILES -

RANNUM/SOURCE	Portable random number generator
RANNUM/DOC	Documentation for random number generator
RANNUM/ASSMBLY/CDC	Compass version of RANNUM
RANNUM/ASSMBLY/VAX	MACRO version of RANNUM for VAX

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

PHYSICAL ORGANIC CHEMISTRY

PE01 MMI <u>Molecular Mechanics I</u>

A program for the calculation of conformations and energies of molecules using molecular mechanics. This is the CDC version of QCPE program 358 developed by N. L. Allinger and coworkers.

ORIGIN - N. L. Allinger

AVAILABLE FILES -

MMI/SOURCE	CDC version of MMI
MMI/DOC	User manual for MMI
MMI/TESTIN	Test input for MMI
MMI/TESTOUT	Test output for MMI

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QE01 MIEHM <u>Modified Iterative Hueckel Method</u>

A program to perform extended Hueckel method LCAO-MO calculations including elements hydrogen to bromine, with the exception of inert gases and transition metals. One and two center contributions are included in the iterative procedure. This program is also available as QCPE program 246.

ORIGIN - J. Spanget-Larsen

AVAILABLE FILES -

MIEHM/SOURCE	Source for MIEHM
MIEHM/DOC	User manual for MIEHM
MIEHM/TESTIN	Test input for MIEHM
MIEHM/TESTOUT	Test output for MIEHM

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QE02 EHT Extended Hueckel Theory

A program to perform extended Hueckel calculations on molecules containing atoms belonging to the first five rows of the periodic table. The program allows double zeta d orbitals, and calculates bond indices and valencies. This program is also available as QCPE program 358.

ORIGIN - E. I. Toplin

AVAILABLE FILES -

EHT/SOURCE	CDC version of EHT
EHT/SOURCE/PREP	CDC version of EHT preparation program
EHT/DOC	User manual for EHT
EHT/TESTIN	Test input for EHT
EHT/TESTIN/PREP	Test input for EHT preparation program
EHT/TESTOUT	Test output for EHT
EHT/TESTOUT/PREP	Test output for EHT preparation program

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QG01 GAMESS General Atomic and Molecular Electronic Structure System

This program utilizes the Rys polynomial technique of H. F. King and coworkers (J. Chem. Phys. 65, 111(1976)) or the rotation technique of J. A. Pople and coworkers (J. Comp. Phys. 27, 1615(1978)) to evaluate the electron repulsion integrals over s, p and d type cartesian gaussian orbitals. Restricted Hartree-Fock (RHF), unrestricted Hartree-Fock (UHF), restricted open shell Hartree-Fock (ROHF), and perfect pairing generalized valence bond (GVB) wavefunctions can be calculated, along with the analytic energy gradient for each wavefunction. Gradients for s and p gaussians can be done using either the Rys polynomial method or the rotation method. Geometry optimization and force constant matrix calculations, as implemented by A. Komornicki, are provided. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613(1977)). Dipole moments, spin population analysis, and Mulliken and Lowdin poplulation analyses are calculated for each wavefunction. Boys localized orbitals can also be obtained.

ORIGIN - M. Dupuis, D. Spangler, and J. J. Wendoloski

AVAILABLE FILES -

GAMESS/SOURCE/CDC	CDC version of GAMESS
GAMESS/DOC	User manual for GAMESS

GAMESS/TESTIN	Test input for GAMESS
GAMESS/TESTOUT	Test output for GAMESS

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QG02 GVBTWO <u>Generalized Valence Bond Program II</u>

This method uses the generalized valence bond method of W. A. Goddard III and coworkers to calculate restricted Hartree-Fock, restricted open shell Hartree-Fock, and perfect pairing generalized valence bond wavefunctions. Integrals over s, p, d, and f gaussians are generated using the Rys polynomial technique as implemented in HONDO. The standard effective potential method of Goddard can also be used. Dipole moments and Mulliken population analyses are also calculated.

ORIGIN - F. W. Bobrowicz, W. R. Wadt, and W. A. Goddard III

AVAILABLE FILES -

GVBTWO/OBJECT	CDC object code for GVBTWO
GVBTWO/TESTIN	Test input for GVBTWO
GVBTWO/TESTOUT	Test output for GVBTWO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - D

QH02 HONDO Ab Initio Hartree Fock Self-consistent Field Program

This program features a technique developed by H. F. King and coworkers for computation of electron repulsion integrals over s, p, and d-type cartesian gaussian orbitals (J. Chem. Phys. 65, 111(1976)). Algorithms for calculation of closed-shell HF and UHF wave functions are included along with computation of the energy gradient. Geometry optimization and force constant matrix calculations, as implemented by A. Komornicki, are provided. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613(1977)). This program supersedes QCPE program 336.

ORIGIN - H. King, M. Dupuis, and J. Rys

AVAILABLE FILES -

HONDO5/SOURCE/CDC	CDC version of HONDO
HONDO5/SOURCE/IBM	IBM version of HONDO
HONDO5/DOC	User manual for HONDO
HONDO5/TESTIN	Test input for HONDO
HONDO5/TESTOUT	Test output for HONDO

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QH03 GAUSS76 GAUSSIAN 76

GAUSSIAN 76 is a connected system of programs capable of performing ab initio molecular orbital calculations within the linear combination of atomic orbitals framework. The system contains programs for the calculation of the s, p, or d one- and two- electron integrals using gaussian functions. Either restricted Hartree-Fock or unrestricted Hartree-Fock calculations are then performed, followed by Mulliken and a spin density analysis. The energy along specified internal coordinates can be minimized automatically using numerical energy differencing. This program is a development of the GAUSSIAN 70 system. GAUSSIAN 76 is also available from QCPE.

ORIGIN - J. S. Binkley, R. A. Whiteside, P. C. Hariharan, R. Seeger, J. A. Pople, W. J. Hehre, and M. D. Newton

AVAILABLE FILES -

GAUSS76/SOURCE/CDC	CDC version of GAUSS76
GAUSS76/TESTIN	Test input for GAUSS76
GAUSS76/TESTOUT	Test output for GAUSS76

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QH04 GRADSCF Ab Initio Gradient Program System

GRADSCF is a modular set of programs which can perform ab initio SCF molecular orbital calculations. Either the Rys polynomial method of H. F. King and coworkers (J. Chem. Phys. 65, 111(1976)) or the rotation method of J.A.Pople and coworkers (J. Comp. Phys. 27, 161(1978)) can be used to calculate the electron repulsion integrals. Individual restricted Hartree-Fock or unrestricted Hartree-Fock calculations can then be performed, and analytic energy gradients calculated. Automatic geometry optimization, force constant calculation, or stationary point (saddle point) minima location can also be obtained. Dipole moments, spin density analysis, and Mulliken population analyses are also calculated.

ORIGIN - A. Komornicki

AVAILABLE FILES -

GRADSCF/DOC	Documentation for GRADSCF
GRADSCF/SOURCE/FORCX	Source for GRADSCF force calculation (s,p basis)
GRADSCF/TESTIN/FORCX	Test input for GRADSCF FORCX
GRADSCF/TESTOUT/FORCX	Test output for GRADSCF FORCX
GRADSCF/SOURCE/FORCXD	Source for GRADSCF force calcation (s,p,d basis)
GRADSCF/TESTIN/FORCXD	Test input for GRADSCF FORCXD
GRADSCF/TESTOUT/FORCXD	Test output for GRADSCF FORCXD
GRADSCF/SOURCE/OPTX	Source for GRADSCF optimization (s,p basis)
GRADSCF/TESTIN/OPTX	Test input for GRADSCF OPTX
GRADSCF/TESTOUT/OPTX	Test output for GRADSCF OPTX
GRADSCF/SOURCE/OPTXd	Source for GRADSCF optimization (s,p,d basis)
GRADSCF/TESTIN/OPTXD	Test input for GRADSCF OPTXD
GRADSCF/TESTOUT/OPTXD	Test output for GRADSCF OPTXD
GRADSCF/SOURCE/SIGX	Source for GRADSCF transition calculation (s,p basis)
GRADSCF/TESTIN/SIGX	Test input for GRADSCF SIGX
GRADSCF/TESTOUT/SIGX	Test output for GRADSCF SIGX
GRADSCF/SOURCE/SIGXD	Source for GRADSCF transition calculation (s,p,d basis)
GRADSCF/TESTIN/SIGXD	Test input for GRADSCF SIGXD
GRADSCF/TESTOUT/SIGXD	Test output for GRADSCF SIGXD
GRADSCF/SOURCE/LIB	Source for GRADSCF library routines

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QH05 FSGOMF <u>Ab Initio Hartree Fock Self-consistent Field Program Using Floating Spherical Gaussian Orbitals</u>

This program performs ab initio closed shell calculations with floating spherical gaussian orbitals and/or tetrahedral lobe functions. The program handles up to 60 atoms, 120 basis functions, and 180 primitive FSGO's. A Lowdin orbital and total population analysis is provided. This program was made available by R. E. Christoffersen and coworkers.

ORIGIN - R. E. Christoffersen, G. Maggiora, D. Genson, and D. Spangler

AVAILABLE FILES -

FSGOMF/SOURCE/INIT	Source of initial activity of FSGOMF
FSGOMF/SOURCE/EL2	Source of 2 electron activity of FSGOMF
FSGOMF/SOURCE/SCF	Source of SCF activity of FSGOMF
FSGOMF/DOC	Documentation for FSGOMF
FSGOMF/TESTIN/INIT	Test input for FSGOMF (ethylene with tetrahedral lobe functions)
FSGOMF/TESTOUT/INIT	Test output for initial activity of FSGOMF
FSGOMF/TESTOUT/EL2	Test output of 2 ELectron activity of FSGOMF
FSGOMF/TESTOUT/SCF	Test output of SCF activity of FSGOMF

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QH07 SPDFG *Ab Initio Hartree Fock Self-consistent Field Program*

This program features a technique developed by H. F. King and coworkers (J. Chem. Phys. 65, 111(1976)) for computation of electron repulsion integrals over s, p, d, f, and g-type cartesian gaussian orbitals. The algorithm for calculation of closed-shell Hartree-Fock wave functions is included. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613 (1977)). This program is an extension of QCPE program 336.

ORIGIN - H. King, M. Dupuis, and J. Rys

AVAILABLE FILES -

SPDFG/SOURCE/IBM	IBM version of SPDFG, including the user manual.

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QM01 ALIS *Ab Initio MCSCF Program for Atomic and Molecular Electronic Structure Calculations*

A system of programs for performing ab initio quantum mechanical calculations of the electronic structure of atoms and molecules with particular emphasis on the multi-configuration self-consistent-field approach. A novel approach involving the combined use of natural orbitals and the Brillouin-Levy- Berthier theorem is used for optimizing the MCSCF molecular orbitals. In this approach the MCSCF wavefunction is determined through a sequence of eigenvalue problems in the multi-configuration and single excitation space. This leads to an iterative improvement in the natural orbitals which in turn are related, by successively improved "back" transformations, to the MCSCF orbitals. In many applications the method has proven itself a powerful approach to forcing rapid convergence. Adaptation to spin and spatial symmetry is maintained throughout and the procedure is applicable to excited states as well as to ground states.

Included in the program package as part of the over-all MCSCF procedure are: (1) a modified version of the BIGGMOLLI integral program of R. S. Raffenetti for use with non-segmented contracted gaussian bases [J. Chem. Phys. 58, 4452(1973)]; (2) the BIGGMOLLI SCF program by R. C. Raffenetti [Chem. Phys. Lett. 20, 335(1973)]; (3) a program by Salmon and Cheung for construction of Serber-type spin-adapted antisymmetrized orbital products and matrix elements between them [J. Chem. Phys. 57, 2776(1972); J.

Chem. Phys. 57, 2787(1972)]; (4) a reduced four-index transformation program specialized to the requirements of the particular MCSCF formulation used in ALIS.

A detailed description of the method used is given in L. M. Cheung, S. T. Elbert, and K. Ruedenberg, "MCSCF Optimization Through Combined Use of Natural Orbitals and the Brillouin-Levy-Berthier Theorem", Int. J. Quantum Chem. 26, 1069(1979).

Remarks: version 1.5 is available for the CDC 7600 (BKY and SCOPE 2.1 operating systems), IBM 370, VAX 11/780 (VMS) and UNIVAC 1110. A single source file is maintained for all machines and manipulated with an editor to produce machine specific source. Language is FORTRAN IV with extensions mainly in the area of direct access. Size is approximately 25000 statements.

ORIGIN - S. T. Elbert, L. M. Cheung, and K. Ruedenberg, Ames Laboratory, Iowa state university.

AVAILABLE FILES -

ALIS/SOURCE/V15	Source for version 1.5 of ALIS
ALIS/DOC	Implementation and user documentation
ALIS/TESTIN/NH/CDC	NH test input for CDC 7600 (BKY)
ALIS/TESTIN/F2/CDC	F2 test input for CDC 7600 (BKY)
ALIS/TESTIN/H2CO2/CDC	H2CO2 test input for CDC 7600 (BKY)
ALIS/TESTIN/NH/VAX	NH test input for the VAX 11/780
ALIS/TESTIN/F2/VAX	F2 test input for the VAX 11/780
ALIS/TESTIN/H2CO2/VAX	H2CO2 test input for the VAX 11/780
ALIS/TESTOUT/NH	Test output for the NH test run
ALIS/TESTOUT/F2	Test output for F2 test run.
ALIS/TESTOUT/H2CO2	Test output for H2CO2 test run.

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QX01 XASW X(alpha) Scattered Wave Program

This program performs self-consistent x(alpha) scattered wave calculations and is an extensive revision of the MIT programs of K. H. Johnson and F. C. Smith. It uses less memory (especially for large molecules) and is substantially faster than the original programs. New options include, (a) calculation of one-electron properties, (b) generation of the wavefunction on a grid of points, suitable for input to a contour plotting routine, (c) estimation of oscillator strengths and (d) use of quasirelativistic radial functions for heavy atoms. The auxiliary program IPOT may be used to generate starting potentials for input to the SCF procedures.

ORIGIN - M. Cook and D. A. Case

AVAILABLE FILES -

XASW/DOC	Documentation
XASW/DATA/AUXILIARY	Data file used by the auxiliary program
XASW/SOURCE/AUXILIARY	Source code for the auxiliary program
XASW/SOURCE/MAIN	Source code for the X(alpha) program
XASW/TESTIN/AUXILIARY	Input deck for test run of the auxiliary program
XASW/TESTIN/MAIN	Input deck for test run of the X(alpha) program
XASW/TESTOUT/AUXILIARY	Printer output from auxiliary test run
XASW/TESTOUT/MAIN	Printer output from the X(alpha) test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QZ01 CNINDO <u>Complete or Intermediate Neglect of Differential Overlap</u>

This program performs molecular orbital calculations using the CNDO and INDO approximations of Pople, Segal and Beveridge. CNINDO will do CNDO level calculations for molecules containing elements through chlorine and INDO level calculations for elements through fluorine. Valence shell basis functions (up to 3d) are used and up to 35 atoms or 80 basis functions are allowed per molecule. (This is QCPE program 281 - which replaces QCPE 141 and 142.)

ORIGIN - P. Dobosh, and N. S. Ostlund

AVAILABLE FILES -

CNINDO/SOURCE	Source of CNINDO
CNINDO/DOC	User manual for CNINDO
CNINDO/TESTIN	Test input for CNINDO
CNINDO/TESTOUT	Test output for CNINDO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ02 MINDO <u>Modified Intermediate Neglect of Differential Overlap</u>

This program is a modification of MINDO/3 (QCPE #279) to allow dynamic memory allocation. The program performs calculations using the modified intermediate neglect of differential overlap technique on closed-shell and open-shell molecules. The Davidon-Fletcher-Powell geometry minimization procedure is used. Up to 150 atoms and 300 basis functions are allowed if sufficient memory is available.

ORIGIN - M. J. S. Dewar, R. C. Bingham, and D. H. Lo

AVAILABLE FILES -

MINDO/SOURCE	Source of MINDO
MINDO/DOC	User manual for MINDO
MINDO/TESTIN	Test input for MINDO
MINDO/TESTOUT	Test output for MINDO

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QZ03 PCILO *Perturbation Configuration Interaction Using Localized Orbitals*

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order. (This is QCPE program 221.)

ORIGIN - P. C. Laverie, J. P. Daudey, S. Diner, C. L. Giessner-Prettre, M. Gilbert, J. Langlet, J. P. Malrieu, U. Pincelli, and B. Pullman

AVAILABLE FILES -

PCILO/SOURCE	Source of PCILO
PCILO/DOC	User manual for PCILO
PCILO/TESTIN	Test input for PCILO
PCILO/TESTOUT	Test output for PCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ04 GSPCILO *Perturbation Configuration Interaction Using Localized Orbitals*

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order.

The program GSPCILO is a modified version of PCILO by J. Sygusch and A. Goursot, who adapted the conjugate gradient method of Powell to the geometry optimization. (This is QCPE program 272.)

ORIGIN - J. Sygusch, and A. Goursot

AVAILABLE FILES -

GSPCILO/SOURCE	Source of GSPCILO

GSPCILO/DOC	User manual for GSPCILO
GSPCILO/TESTIN	Test input for GSPCILO
GSPCILO/TESTOUT	Test output for GSPCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ05 GLPCILO <u>Perturbation Configuration Interaction Using Localized Orbitals</u>

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order.

The program GLPCILO is a modified version of PCILO by G. Loew and D. Berkowitz which dynamically allocates memory and uses large core memory on the CDC 7600. The program features a modified geometry optimization procedure using a quasi- Newton minimization method Murtaugh and Sargent.

ORIGIN - G. Loew and D. Berkowitz

AVAILABLE FILES -

GLPCILO/SOURCE	Source of GLPCILO
GLPCILO/DOC	User manual for GLPCILO
GLPCILO/TESTIN	Test input for GLPCILO
GLPCILO/TESTOUT	Test output for GLPCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QZ06 MNDO Modified Neglect of Diatomic Overlap

This program (QCPE #353) was developed by M. J. S. Dewar and W. Thiel. The program performs modified neglect of diatomic overlap (MNDO) MO calculations for closed-shell and open-shell molecules containing the elements H, B, C, N, O, and F. Equilibrium geometries on MNDO potential surfaces are located by the Davidon-Fletcher-Powell algorithm. The program handles up to 35 atoms, 75 basis functions, and 99 geometrical variables to be optimized.

ORIGIN - W. Thiel and M. J. S. Dewar

AVAILABLE FILES -

MNDO/SOURCE	Source of MNDO
MNDO/DOC	Documentation for MNDO
MNDO/TESTIN	Test input for MNDO
MNDO/TESTOUT	Test output for MNDO

SUPPORT LEVEL - B

DISTRIBUTION STATUS - BQ

QZ07 INDOCI Neglect of Differential Overlap Configuration Interaction

This program performs INDO/S and CNDO/S configuration interaction closed-shell molecular orbital calculations. The program can handle systems up to 30 centers and 60 orbitals for first row atoms. This program is part of QCPE program 372.

ORIGIN - W. Haque

AVAILABLE FILES -

INDOCI/SOURCE	Source of INDOCI
INDOCI/DOC	User manual for INDOCI
INDOCI/TESTIN	Test input for INDOCI
INDOCI/TESTOUT	Test output for INDOCI

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ08 RINDO Neglect of Differential Overlap for Rydberg States

This program performs MRINDO and RCNDO configuration interaction closed-shell molecular orbital calculations. The program can handle systems up to 17 centers and 96 orbitals for first row atoms. This program is part of QCPE program 372.

ORIGIN - W. Haque

AVAILABLE FILES -

RINDO/SOURCE	Source of RINDO
RINDO/DOC	User manual for RINDO
RINDO/TESTIN	Test input for RINDO
RINDO/TESTOUT	Test output for RINDO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QUANTUM CHEMISTRY

QC02 ATOMCI A Configuration Interaction Program for Atoms

This program carries out iterated natural orbital configuration interaction (INO-CI) calculations on atoms in the non-relativistic Russel-Saunders coupling approximation. A conventional formula tape approach is used in the construction of the Hamiltonian matrix elements. The program can handle up to 100 Slater-type basis orbitals not counting m-degeneracy. Up to i-type Slater orbitals are permitted. All excitations are specified with respect to a single SCF reference configuration. However, the user has almost complete control over the type of coupling used in building up configuration state functions.

A typical energy calculation involves two steps: (1) generation of a sorted formula tape for all elements of the Hamiltonian matrix for a specified set of configuration state functions and (2) a CI calculation with optional natural orbital iteration and orbital exponent optimization. The CI part of the program is essentially that of ALCHEMY adapted to the special case of atoms and the CDC machine environment.

It should be noted that ATOMCI does not include a Hartree-Fock program and the user is responsible for providing appropriate initial occupied orbitals. This version of ATOMCI makes use of small core only.

The capabilities of the program are well illustrated by the first-row atom calculations of F. Sasaki and M. Yoshimine, Phys. Rev. A 9, 17, 26(1974). The method used in constructing matrix elements has been described by F. Sasaki, "Matrix Elements in Configuration Interaction Calculations", Int. J. Quantum Chem. 8, 605-617(1974).

ORIGIN - F. Sasaki, M. Yoshimine, and S. A. Hagstrom

AVAILABLE FILES -

ATOMCI/SOURCE	Source file for system generation
ATOMCI/DOC	User documentaion
ATOMCI/TESTIN/BE1S	Test input for Be singlet S state calculation
ATOMCI/TESTIN/BE3P	Test input for Be triplet P state calculation
ATOMCI/TESTIN/NE1S	Test input for Ne ground state calculation
ATOMCI/TESTIN/AL2P	Test input for Al doublet P state
ATOMCI/TESTIN/AL2D	Test input for Al doublet D state
ATOMCI/TESTOUT/BE1S	Output for Be singlet S state run
ATOMCI/TESTOUT/BE3P	Output for Be triplet P state run
ATOMCI/TESTOUT/NE1S	Output for Ne ground state run
ATOMCI/TESTOUT/AL2P	Output for Al doublet P state
ATOMIC/TESTOUT/AL2D	Output for Al Doublet D state run

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QC03 ALCHEMY Ab Initio Electronic Structure Calculations Package

This is a set of programs designed for molecular structure calculations, in use at the IBM research laboratory in San Jose (U.S.A.). The main component of the package is the open-ended program for configuration interaction calculations, which can handle linear or polyatomic molecules. Self-consistent-field Hartree-Fock, and multi-configuration Hartree-Fock programs are also included. Programs for calculating molecular properties including transition moments are available. Slater-type basis functions may be used for linear molecule wave functions.

The ALCHEMY program was written by M. Yoshimine, A. D. Mclean, B. Liu, M. Dupuis, and P. S. Bagus.

The -MOLECULE- program was written by J. Almlof and adapted by P. S. Bagus.

The -MCSCF- program was written by J. Hinze and adapted by B. Liu.

The -ALCHONDO- program was written by King, Rys, Dupuis and adapted by M. Dupuis.

When using the programs -MOLECULE-, or -MCSCF-, or -ALCHONDO-, proper reference to the writers of the programs should be made, as indicated above.

Because of its complex nature, and machine dependencies, special handling of the program is required for each request.

ORIGIN - M. Yoshimine, A. D. Mclean, B. Liu, M. Dupuis, and P. S. Bagus

AVAILABLE FILES -

ALCHEMY/SOURCE

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QC04 MELD Ab Initio SCF-CI System of Programs

This program was developed by E. R. Davidson and coworkers at the university of Washington in Seattle to calculate restricted HF and CI wavefunctions of molecular systems. It combines their (1) integral computation technique for s, p, d, f, and g-type cartesian gaussian functions; (2) general restricted open-shell formalism; (3) double-coset method to generate integrals over symmetry adapted basis functions for abelian point groups. For a CI wavefunctions, the configurations can be selected by partitioning the molecular orbital space, or on the basis of perturbation energy contribution. Many molecular properties can be calculated from the wavefunction, including transition moments.

ORIGIN - L. McMurchie, S. T. Elbert, S. R. Langhoff, and E. R. Davidson

AVAILABLE FILES -

MELD/SOURCE	Source for all MELD modules
MELD/DOC	User manual for MELD
MELD/TESTIN/CIDIAG	Test input for CIDIAG module of MELD
MELD/TESTIN/CISTAR	Test input for CISTAR module of MELD
MELD/TESTIN/MOLINTL	Test input for MOLINTL module of MELD
MELD/TESTIN/OCCUP	Test input for OCCUP module of MELD
MELD/TESTIN/SINT	Test input for SINT module of MELD
MELD/TESTIN/SSCFEQ	Test input for SSCFEQ module of MELD
MELD/TESTIN/TMOM	Test input for TMOM module of MELD
MELD/TESTIN/TRAIN	Test input for TRAIN module of MELD
MELD/TESTIN/USORT	Test input for USORT module of MELD
MELD/TESTOUT/CIDIAG	Test output for CIDIAG module of MELD
MELD/TESTOUT/CISTAR	Test output for CISTAR module of MELD
MELD/TESTOUT/MOLINTL	Test output for MOLINTL module of MELD
MELD/TESTOUT/OCCUP	Test output for OCCUP module of MELD
MELD/TESTOUT/SINT	Test output for SINT module of MELD
MELD/TESTOUT/SSCFEQ	Test output for SSCFEQ module of MELD
MELD/TESTOUT/TMOM	Test output for TMOM module of MELD
MELD/TESTOUT/TRAIN	Test output for TRAIN module of MELD
MELD/TESTOUT/USORT	Test output for USORT module of MELD

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QC05 SCEP *Self-consistent Electron Pairs Program*

This program carries out an iterative technique to obtain a fully variational wave function in the complete interacting space of a closed-shell reference configuration and associated singly and doubly excited configurations. This is the QCPE program 346.

ORIGIN - C. E. Dykstra

AVAILABLE FILES -

SCEP/SOURCE/CDC	Source for SCEP

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QC06 SPLICE *Software Program Library for the Investigation of Correlation Effects*

SPLICE consists of a number of programs for performing configuration interaction (CI) studies of molecular electronic structure. The system is designed to interface with the ATMOL3 SCF package which supplies basic integrals and starting Hartree-Fock orbitals. The programs currently available are: (1) a file conversion program that acts as an interface between ATMOL3 and SPLICE, (2) an integral transformation program, (3) a general purpose conventional CI program (bonded function formulation of Sutcliffe), (4) a CI matrix diagonalization program providing both the Shavitt and Davidson methods, and (5) the MOLECULE-CI program of Roos and Siegbahn for direct CI calculations from a closed shell ground state (singles and doubles only).

SPLICE runs on the IBM 360/370 or equivalent hardware. It was originally implemented on the 360/195 at Rutherford Laboratory.

ORIGIN - Daresbury Laboratory, England

AVAILABLE FILES -

SPLICE/SOURCE	Source code for SPLICE

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QE01 MIEHM <u>Modified Iterative Hueckel Method</u>

A program to perform extended Hueckel method LCAO-MO calculations including elements hydrogen to bromine, with the exception of inert gases and transition metals. One and two center contributions are included in the iterative procedure. This program is also available as QCPE program 246.

ORIGIN - J. Spanget-Larsen

AVAILABLE FILES -

MIEHM/SOURCE	Source for MIEHM
MIEHM/DOC	User manual for MIEHM
MIEHM/TESTIN	Test input for MIEHM
MIEHM/TESTOUT	Test output for MIEHM

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QE02 EHT <u>Extended Hueckel Theory</u>

A program to perform extended Hueckel calculations on molecules containing atoms belonging to the first five rows of the periodic table. The program allows double zeta d orbitals, and calculates bond indices and valencies. This program is also available as QCPE program 358.

ORIGIN - E. I. Toplin

AVAILABLE FILES -

EHT/SOURCE	CDC version of EHT
EHT/SOURCE/PREP	CDC version of EHT preparation program
EHT/DOC	User manual for EHT
EHT/TESTIN	Test input for EHT
EHT/TESTIN/PREP	Test input for EHT preparation program
EHT/TESTOUT	Test output for EHT
EHT/TESTOUT/PREP	Test output for EHT preparation program

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QG01 GAMESS General Atomic and Molecular Electronic Structure System

This program utilizes the Rys polynomial technique of H. F. King and coworkers (J. Chem. Phys. 65, 111(1976)) or the rotation technique of J. A. Pople and coworkers (J. Comp. Phys. 27, 1615(1978)) to evaluate the electron repulsion integrals over s, p and d type cartesian gaussian orbitals. Restricted Hartree-Fock (RHF), unrestricted Hartree-Fock (UHF), restricted open shell Hartree-Fock (ROHF), and perfect pairing generalized valence bond (GVB) wavefunctions can be calculated, along with the analytic energy gradient for each wavefunction. Gradients for s and p gaussians can be done using either the Rys polynomial method or the rotation method. Geometry optimization and force constant matrix calculations, as implemented by A. Komornicki, are provided. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613(1977)). Dipole moments, spin population analysis, and Mulliken and Lowdin poplulation analyses are calculated for each wavefunction. Boys localized orbitals can also be obtained.

ORIGIN - M. Dupuis, D. Spangler, and J. J. Wendoloski

AVAILABLE FILES -

GAMESS/SOURCE/CDC	CDC version of GAMESS
GAMESS/DOC	User manual for GAMESS
GAMESS/TESTIN	Test input for GAMESS
GAMESS/TESTOUT	Test output for GAMESS

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QG02 GVBTWO <u>Generalized Valence Bond Program II</u>

This method uses the generalized valence bond method of W. A. Goddard III and coworkers to calculate restricted Hartree-Fock, restricted open shell Hartree-Fock, and perfect pairing generalized valence bond wavefunctions. Integrals over s, p, d, and f gaussians are generated using the Rys polynomial technique as implemented in HONDO. The standard effective potential method of Goddard can also be used. Dipole moments and Mulliken population analyses are also calculated.

ORIGIN - F. W. Bobrowicz, W. R. Wadt, and W. A. Goddard III

AVAILABLE FILES -

GVBTWO/OBJECT	CDC object code for GVBTWO
GVBTWO/TESTIN	Test input for GVBTWO
GVBTWO/TESTOUT	Test output for GVBTWO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - D

QH02 HONDO <u>Ab Initio Hartree Fock Self-consistent Field Program</u>

This program features a technique developed by H. F. King and coworkers for computation of electron repulsion integrals over s, p, and d-type cartesian gaussian orbitals (J. Chem. Phys. 65, 111(1976)). Algorithms for calculation of closed-shell HF and UHF wave functions are included along with computation of the energy gradient. Geometry optimization and force constant matrix calculations, as implemented by A. Komornicki, are provided. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613(1977)). This program supersedes QCPE program 336.

ORIGIN - H. King, M. Dupuis, and J. Rys

AVAILABLE FILES -

HONDO5/SOURCE/CDC	CDC version of HONDO
HONDO5/SOURCE/IBM	IBM version of HONDO
HONDO5/DOC	User manual for HONDO
HONDO5/TESTIN	Test input for HONDO
HONDO5/TESTOUT	Test output for HONDO

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QH03 GAUSS76 GAUSSIAN 76

GAUSSIAN 76 is a connected system of programs capable of performing ab initio molecular orbital calculations within the linear combination of atomic orbitals framework. The system contains programs for the calculation of the s, p, or d one- and two- electron integrals using gaussian functions. Either restricted Hartree-Fock or unrestricted Hartree-Fock calculations are then performed, followed by Mulliken and a spin density analysis. The energy along specified internal coordinates can be minimized automatically using numerical energy differencing. This program is a development of the GAUSSIAN 70 system. GAUSSIAN 76 is also available from QCPE.

ORIGIN - J. S. Binkley, R. A. Whiteside, P. C. Hariharan, R. Seeger, J. A. Pople, W. J. Hehre, and M. D. Newton

AVAILABLE FILES -

GAUSS76/SOURCE/CDC	CDC version of GAUSS76
GAUSS76/TESTIN	Test input for GAUSS76
GAUSS76/TESTOUT	Test output for GAUSS76

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QH04 GRADSCF Ab Initio Gradient Program System

GRADSCF is a modular set of programs which can perform ab initio SCF molecular orbital calculations. Either the Rys polynomial method of H. F. King and coworkers (J. Comp. Phys. 27, 161 (1978)) or the rotation method of J. A. Pople and coworkers (J. Chem. Phys. 65, 11(1976)) can be used to calculate the electron repulsion integrals. Individual restricted Hartree-Fock or unrestricted Hartree-Fock calculations can then be performed, and analytic energy gradients calculated. Automatic geometry optimization, force constant calculation, or stationary point (saddle point) minima location can also be obtained. Dipole moments, spin density analysis, and Mulliken population analyses are also calculated.

ORIGIN - A. Komornicki

AVAILABLE FILES -

GRADSCF/DOC	Documentation for GRADSCF
GRADSCF/SOURCE/FORCX	Source for GRADSCF force calculation (s,p basis)
GRADSCF/TESTIN/FORCX	Test input for GRADSCF FORCX

GRADSCF/TESTOUT/FORCX	Test output for GRADSCF FORCX
GRADSCF/SOURCE/FORCXD	Source for GRADSCF force calcation (s,p,d basis)
GRADSCF/TESTIN/FORCXD	Test input for GRADSCF FORCXD
GRADSCF/TESTOUT/FORCXD	Test output for GRADSCF FORCXD
GRADSCF/SOURCE/OPTX	Source for GRADSCF optimization (s,p basis)
GRADSCF/TESTIN/OPTX	Test input for GRADSCF OPTX
GRADSCF/TESTOUT/OPTX	Test output for GRADSCF OPTX
GRADSCF/SOURCE/OPTXd	Source for GRADSCF optimization (s,p,d basis)
GRADSCF/TESTIN/OPTXD	Test input for GRADSCF OPTXD
GRADSCF/TESTOUT/OPTXD	Test output for GRADSCF OPTXD
GRADSCF/SOURCE/SIGX	Source for GRADSCF transition calculation (s,p basis)
GRADSCF/TESTIN/SIGX	Test input for GRADSCF SIGX
GRADSCF/TESTOUT/SIGX	Test output for GRADSCF SIGX
GRADSCF/SOURCE/SIGXD	Source for GRADSCF transition calculation (s,p,d basis)
GRADSCF/TESTIN/SIGXD	Test input for GRADSCF SIGXD
GRADSCF/TESTOUT/SIGXD	Test output for GRADSCF SIGXD
GRADSCF/SOURCE/LIB	Source for GRADSCF library routines

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QH05 FSGOMF Ab Initio Hartree Fock Self-consistent Field Program Using Floating Spherical Gaussian Orbitals

This program performs ab initio closed shell calculations with floating spherical gaussian orbitals and/or tetrahedral lobe functions. The program handles up to 60 atoms, 120 basis functions, and 180 primitive FSGO's. A Lowdin orbital and total population analysis is provided. This program was made available by R. E. Christoffersen and coworkers.

ORIGIN - R. E. Christoffersen, G. Maggiora, D. Genson, D. Spangler, and L. Shipman

AVAILABLE FILES -

FSGOMF/SOURCE/INIT	Source of initial activity of FSGOMF
FSGOMF/SOURCE/EL2	Source of 2 electron activity of FSGOMF
FSGOMF/SOURCE/SCF	Source of SCF activity of FSGOMF
FSGOMF/DOC	Documentation for FSGOMF
FSGOMF/TESTIN/INIT	Test input for FSGOMF (ethylene with tetrahedral lobe functions)
FSGOMF/TESTOUT/INIT	Test output for initial activity of FSGOMF
FSGOMF/TESTOUT/EL2	Test output of 2 ELectron activity of

	FSGOMF
FSGOMF/TESTOUT/SCF	Test output of SCF activity of FSGOMF

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QH06 ATMOL3 ATOMIC AND MOLECULAR HARTREE-FOCK PACKAGE

A system of routines for performing electronic structure calculations for atoms and molecules at the closed and open shell restricted and unrestricted Hartree-Fock level. The system consists of (1) a contracted cartesian gaussian orbital integral program (s, p, and d-type functions), (2) a supermatrix generator module, (3) a collection of programs for performing closed and open shell restricted and unrestricted Hartree-Fock calculations, (4) a Boys localization of molecular orbitals program, (5) a properties package, and (6) various utilities including a contracted cartesian gaussian orbital library and a library maintenance routine.

ATMOL3 runs on both the CDC 7600 and IBM 360/370. Direct access file handlers are implemented in machine language rather than at the FORTRAN level.

ORIGIN - R. V. Saunders and M. F. Guest, Daresbury Laboratory, England

AVAILABLE FILES -

ATMOL3/SOURCE/CDC	CDC 7600 source code for ATMOL3
ATMOL3/SOURCE/IBM	IBM source code for ATMOL3
ATMOL3/TESTIN/NH3/CDC	Test input for CDC 7600
ATMOL3/TESTOUT/NH3/CDC	Test output for NH3 test case

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QH07 SPDFG Ab Initio Hartree Fock Self-consistent Field Program

This program features a technique developed by H. F. King and cowokers (J. Chem. Phys. 65, 111(1976)) for computation of electron repulsion integrals over s, p, d, f, and g-type cartesian gaussian orbitals. The algorithm for calculation of closed-shell Hartree-Fock wave functions is included. The program takes advantage of molecular symmetry as described by King (Int. J. Quantum Chem. 11, 613(1977)). This program is an extension of QCPE program 336.

ORIGIN - H. King, M. Dupuis, and J. Rys

AVAILABLE FILES -

SPDFG/SOURCE/IBM	IBM version of SPDFG, including the user manual.

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QI01 DERIC Diatomic Integrals over Slater-Type Orbitals

This routine may be used to compute diatomic molecular integrals over complex Slater type orbitals. The program is organized into two overlays: the first of which computes one-electron integrals (overlap, 1- and 2-center nuclear attraction, and kinetic energy) and the second of which computes two-electron repulsion integrals (atomic, coulomb, hybrid, and exchange). Slater orbitals of s, p, d, and f type may be used up through a principal quantum number of 8.

The two-electron integrals are computed by the charge distribution approach of Ruedenberg except that a double numerical quadrature is used for all except the atomic integrals, which are done analytically. The quadrature scheme is extremely flexible and 8-9 decimal place accuracy can be obtained if required.

This routine is a substantial enhancement over QCPE 252 and should be considered as a replacement for that routine. An LCM oriented version is available for doing large blocks of integrals but performance is achieved at the expense of portability. The standard version of DERIC is highly portable and runs with only slight program modifications on CDC, IBM and VAX 11/780 systems.

ORIGIN - S. A. Hagstrom, Indiana University

AVAILABLE FILES -

DERIC/SOURCE	FORTRAN source for CDC, VAX and IBM versions
DERIC/DOC	User documentation for DERIC (all systems)
DERIC/TESTIN/AU2	Test input for diatomic gold
DERIC/TESTIN/LIH	Test input for lithium hydride
DERIC/TESTOUT/Au2	Output for Au2 test case
DERIC/TESTOUT/LIH	Output for LiH test case.

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

QI02 ERIC Electron Repulsion Integrals over Slater-type Orbitals

This routine computes 3-center hybrid and 3- and 4-center exchange integrals over s- and p-type real, normalized Slater orbitals of arbitrary orientation. Two center coulomb, hybrid and exchange integrals can also be computed but are more efficiently handled by conventional two-center techniques. Principal quantum numbers up to 6 can be accommodated. A special mode is also provided to enable 3-center nuclear attraction integrals to be computed as a special case of the 3-center hybrid integral.

Integrals are computed by an extension of the Bonham, Peacher, and Cox Fourier transform method for integrals over s-orbitals (J. Chem. Phys. 40, 3083(1964)) to integrals over p-orbitals using the method of parametric differentiation with respect to nuclear coordinates and orbital exponents. The calculation is charge distribution based and is computationally quite efficient, especially for large basis sets on relatively few centers.

ERIC does not require that p-orbitals be pure x, y, or z in type. Namely, any normalized linear combination of px, py, and pz orbitals on the same center is permitted provided they have a common radial factor.

ERIC is highly portable and runs on CDC, IBM, and VAX 11/780. It has run on 36-bit machines (UNIVAC and FACOM) but may experience differencing problems in the single precision mode.

ORIGIN - S. A. Hagstrom, Indiana University

AVAILABLE FILES -

ERIC/SOURCE/CDC	FORTRAN IV source and test driver for CDC
ERIC/SOURCE/VAX	FORTRAN IV source and test driver for VAX

ERIC/DOC	User documentation for ERIC
ERIC/TESTIN	Test input for ERIC (formaldehyde)
ERIC/TESTOUT	Test output for the formaldehyde test case.

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QI04 GINT Molecular Integrals over Slater Type Orbitals

A program for computing one- and two-electron 1-, 2-, 3-, and 4-center molecular integrals over Slater type orbitals using the method of finite expansion of STO's in terms of gaussian orbitals. The program provides a built-in set of expansions that is appropriate for most purposes, but the user can also provide his own expansions. The routine is very general (f and g orbitals) but integrals are done one at a time and may be slow if high accuracy is required. The value of the program lies in its generality and it has proved extremely useful in providing check values for testing Slater integral packages as well as providing integral values where alternative methods (programs) do not exist.

ORIGIN - F. Sasaki, Hokkaido University

AVAILABLE FILES -

GINT/SOURCE	FORTRAN IV source plus test driver program
GINT/DOC	User documentation for GINT
GINT/TESTOUT	Test output for s-, p-, d- test case built into the driver.

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QM01 ALIS

Ab Initio MCSCF Program for Atomic and Molecular Electronic Structure Calculations

A system of programs for performing ab initio quantum mechanical calculations of the electronic structure of atoms and molecules with particular emphasis on the multi-configuration self-consistent-field approach. A novel approach involving the combined use of natural orbitals and the Brillouin-Levy- Berthier theorem is used for optimizing the MCSCF molecular orbitals. In this approach the MCSCF wavefunction is determined through a sequence of eigenvalue problems in the multi-configuration and single excitation space. This leads to an iterative improvement in the natural orbitals which in turn are related, by successively improved "back" transformations, to the MCSCF orbitals. In many applications the method has proven itself a powerful approach to forcing rapid convergence. Adaptation to spin and spatial symmetry is maintained throughout and the procedure is applicable to excited states as well as to ground states.

Included in the program package as part of the over-all MCSCF procedure are: (1) a modified version of the BIGGMOLLI integral program of R. S. Raffenetti for use with non-segmented contracted gaussian bases [J. Chem. Phys. 58, 4452(1973)]; (2) the BIGGMOLLI SCF program by R. C. Raffenetti [Chem. Phys. Lett. 20, 335(1973)]; (3) a program by Salmon and Cheung for construction of Serber-type spin-adapted antisymmetrized orbital products and matrix elements between them [J. Chem. Phys. 57, 2776(1972); J. Chem. Phys. 57, 2787(1972)]; (4) a reduced four-index transformation program specialized to the requirements of the particular MCSCF formulation used in ALIS.

A detailed description of the method used is given in L. M. Cheung, S. T. Elbert, and K. Ruedenberg, "MCSCF Optimization Through Combined Use of Natural Orbitals and the Brillouin-Levy-Berthier Theorem", Int. J. Quantum Chem. 26, 1069(1979).

Remarks: version 1.5 is available for the CDC 7600 (BKY and SCOPE 2.1 operating systems), IBM 370, VAX 11/780 (VMS) and UNIVAC 1110. A single source file is maintained for all machines and manipulated with an editor to produce machine specific source. Language is FORTRAN IV with extensions mainly in the area of direct access. Size is approximately 25000 statements.

ORIGIN - S. T. Elbert, L. M. Cheung, and K. Ruedenberg, Ames Laboratory, Iowa State University.

AVAILABLE FILES -

ALIS/SOURCE/V15	Source for version 1.5 of ALIS
ALIS/DOC	Implementation and user documentation

ALIS/TESTIN/NH/CDC	NH test input for CDC 7600 (BKY)
ALIS/TESTIN/F2/CDC	F2 test input for CDC 7600 (BKY)
ALIS/TESTIN/H2CO2/CDC	H2CO2 test input for CDC 7600 (BKY)
ALIS/TESTIN/NH/VAX	NH test input for the VAX 11/780
ALIS/TESTIN/F2/VAX	F2 test input for the VAX 11/780
ALIS/TESTIN/H2CO2/VAX	H2CO2 test input for the VAX 11/780
ALIS/TESTOUT/NH	Test output for the NH test run
ALIS/TESTOUT/F2	Test output for F2 test run.
ALIS/TESTOUT/H2CO2	Test output for H2CO2 test run.

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QX01 XASW X(alpha) Scattered Wave Program

This program performs self-consistent X(alpha) scattered wave calculations and is an extensive revision of the MIT programs of K. H. Johnson and F. C. Smith. It uses less memory (especially for large molecules) and is substantially faster than the original programs. New options include, (a) calculation of one-electron properties, (b) generation of the wavefunction on a grid of points, suitable for input to a contour plotting routine, (c) estimation of oscillator strengths and (d) use of quasirelativistic radial functions for heavy atoms. The auxiliary program IPOT may be used to generate starting potentials for input to the SCF procedures.

ORIGIN - M. Cook and D. A. Case

AVAILABLE FILES -

XASW/DOC	Documentation
XASW/DATA/AUXILIARY	Data file used by the auxiliary program
XASW/SOURCE/AUXILIARY	Source code for the auxiliary program
XASW/SOURCE/MAIN	Source code for the X(alpha) program
XASW/TESTIN/AUXILIARY	Input deck for test run of the auxiliary program
XASW/TESTIN/MAIN	Input deck for test run of the X(alpha) program
XASW/TESTOUT/AUXILIARY	Printer output from auxiliary test run
XASW/TESTOUT/MAIN	Printer output from the X(alpha) test run

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QZ01 CNINDO <u>Complete or Intermediate Neglect of Differential Overlap</u>

This program performs molecular orbital calculations using the CNDO and INDO approximations of Pople, Segal and Beveridge. CNINDO will do CNDO level calculations for molecules containing elements through chlorine and INDO level calculations for elements through fluorine. Valence shell basis functions (up to 3d) are used and up to 35 atoms or 80 basis functions are allowed per molecule. (This is QCPE program 281 - which replaces QCPE 141 and 142.)

ORIGIN - P. Dobosh, and N. S. Ostlund

AVAILABLE FILES -

CNINDO/SOURCE	Source of CNINDO
CNINDO/DOC	User manual for CNINDO
CNINDO/TESTIN	Test input for CNINDO
CNINDO/TESTOUT	Test output for CNINDO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ02 MINDO <u>Modified Intermediate Neglect of Differential Overlap</u>

This program is a modification of MINDO/3 (QCPE #279) to allow dynamic memory allocation. The program performs calculations using the modified intermediate neglect of differential overlap technique on closed-shell and open-shell molecules. The Davidon-Fletcher-Powell geometry minimization procedure is used. Up to 150 atoms and 300 basis functions are allowed if sufficient memory is available.

ORIGIN - M. J. S. Dewar, R. C. Bingham, and D. H. Lo

AVAILABLE FILES -

MINDO/SOURCE	Source of MINDO
MINDO/DOC	User manual for MINDO
MINDO/TESTIN	Test input for MINDO
MINDO/TESTOUT	Test output for MINDO

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

QZ03 PCILO Perturbation Configuration Interaction Using Localized Orbitals

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order. (This is QCPE program 221.)

ORIGIN - P. C. Laverie, J. P. Daudey, S. Diner, C. L. Giessner-Prettre, M. Gilbert, J. Langlet, J. P. Malrieu, U. Pincelli, and B. Pullman

AVAILABLE FILES -

PCILO/SOURCE	Source of PCILO
PCILO/DOC	User manual for PCILO
PCILO/TESTIN	Test input for PCILO
PCILO/TESTOUT	Test output for PCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ04 GSPCILO Perturbation Configuration Interaction Using Localized Orbitals

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order.

The program GSPCILO is a modified version of PCILO by J. Sygusch and A. Goursot, who adapted the conjugate gradient method of Powell to the geometry optimization. (This is QCPE program 272.)

ORIGIN - J. Sygusch and A. Goursot

AVAILABLE FILES -

GSPCILO/SOURCE	Source of GSPCILO

GSPCILO/DOC	User manual for GSPCILO
GSPCILO/TESTIN	Test input for GSPCILO
GSPCILO/TESTOUT	Test output for GSPCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ05 GLPCILO <u>Perturbation Configuration Interaction Using Localized Orbitals</u>

This program uses the perturbation configuration interaction with localized orbitals method developed in the Laboratoire de Chimie Quantique of the Institut de Biologie Physico-chimique. The program calculates the energy, one-particle density matrix, and the dipole moment of closed-shell molecules containing first row atoms in their ground states. The method employs localized orbitals using the CNDO approach and calculates the energy and dipole moment using a perturbative CI approach through third order.

The program GLPCILO is a modified version of PCILO by G. Loew and D. Berkowitz which dynamically allocates memory and uses large core memory on the CDC 7600. The program features a modified geometry optimization procedure using a quasi- Newton minimization method Murtaugh and Sargent.

ORIGIN - G. Loew and D. Berkowitz

AVAILABLE FILES -

GLPCILO/SOURCE	Source of GLPCILO
GLPCILO/DOC	User manual for GLPCILO
GLPCILO/TESTIN	Test input for GLPCILO
GLPCILO/TESTOUT	Test output for GLPCILO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

QZ06 MNDO Modified Neglect of Diatomic Overlap

This program (QCPE #353) was developed by M. J. S. Dewar and W. Thiel. The program performs modified neglect of diatomic overlap (MNDO) MO calculations for closed-shell and open-shell molecules containing the elements H, B, C, N, O, and F. Equilibrium geometries on MNDO potential surfaces are located by the Davidon-Fletcher-Powell algorithm. The program handles up to 35 atoms, 75 basis functions, and 99 geometrical variables to be optimized.

ORIGIN - W. Thiel and M. J. S. Dewar

AVAILABLE FILES -

MNDO/SOURCE	Source of MNDO
MNDO/DOC	Documentation for MNDO
MNDO/TESTIN	Test input for MNDO
MNDO/TESTOUT	Test output for MNDO

SUPPORT LEVEL - B

DISTRIBUTION STATUS - BQ

QZ07 INDOCI Neglect of Differential Overlap Configuration Interaction

This program performs INDO/S and CNDO/S configuration interaction closed-shell molecular orbital calculations. The program can handle systems up to 30 centers and 60 orbitals for first row atoms. This program is part of QCPE program 372.

ORIGIN - W. Haque

AVAILABLE FILES -

INDOCI/SOURCE	Source of INDOCI
INDOCI/DOC	User manual for INDOCI
INDOCI/TESTIN	Test input for INDOCI
INDOCI/TESTOUT	Test output for INDOCI

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

QZ08 RINDO <u>Neglect of Differential Overlap for Rydberg States</u>

This program performs MRINDO and RCNDO configuration interaction closed-shell molecular orbital calculations. The program can handle systems up to 17 centers and 96 orbitals for first row atoms. This program is part of QCPF program 372.

ORIGIN - W. Haque

AVAILABLE FILES -

RINDO/SOURCE	Source of RINDO
RINDO/DOC	User manual for RINDO
RINDO/TESTIN	Test input for RINDO
RINDO/TESTOUT	Test output for RINDO

SUPPORT LEVEL - C

DISTRIBUTION STATUS - BQ

STATISTICAL MECHANICS

SS01 CLAMPS Classical Many Particle Simulator

A program package which can use five simulation methods (molecular dynamics, Langevin dynamics, Monte Carlo, polymer reptation or Brownian dynamics) to generate configurations distributed according to the Boltzmann distribution. The potential energy is a sum of spherically symmetric pair potentials and/or bond potentials for polymers. For charged particles the Ewald image potential is used to represent the effect of the system outside the simulation box. The configurations generated by CLAMPS can be stored and then analyzed by other programs.

ORIGIN - D. Ceperley

AVAILABLE FILES -

CLAMPS/SOURCE/CDC	CDC version of CLAMPS
CLAMPS/SOURCE/VAX	VAX version of CLAMPS
CLAMPS/DOC	User manual for CLAMPS
CLAMPS/TESTIN/ARRAH	Test input for CLAMPS. Argon simulation described in A. Rahman, Phys. Rev. 136, A405 (1964).
CLAMPS/TESTOUT/ARRAH	Test output for CLAMPS.
CLAMPS/TESTIN/WATER	Test input for water. Pair potential is taken from A. Rahman, F. Stillinger and H. Lemberg, J. Chem. Phys. 63, 5225(1975). Note that the initial configuration must be obtained from the start routine.
START/SOURCE/WATER	Source to obtain starting configuration for water
CLAMPS/TESTOUT/WATER	Test output for TESTIN/WATER above.
RANNUM/SOURCE	Portable random number generator
RANNUM/DOC	Documentation for RANNUM
RANNUM/ASSMBLY/CDC	COMPASS version of RANNUM
RANNUM/ASSMBLY/VAX	MACRO version of RANNUM for VAX
CFS/DOC	Documentation for CFS (time correlation functions)
CFS/SOURCE	Source for time dependant correlation functions
VELCOR/SOURCE	Computes velocity correlation function-uses CFS
VELCOR/TESTIN	VAX test for VELCOR. Uses CLAMPS input.
VELCOR/TESTOUT	Test output for VELCOR and CFS

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

SOFTWARE TOOLS

TC01 PRETTY Convert FORTRAN to Prettier Format

This program processes syntactically-correct FORTRAN text, altering statement numbers so that they occur in ascending order. Format statements are collected and written immediately preceding the end statement of each subroutine. Do loop text is indented by default, but may be suppressed or the indentation changed by specifying alternate values in the control input. Similarly, constants can be converted to single, double, or quadruple precision and functions can be converted to match user-specified precision. Character strings can be converted to Hollerith strings if desired.

The output FORTRAN text can contain sequencing information in columns 73-80. Any number of FORTRAN routines may be provided for processing. Each routine is processed separately, and a listing is provided of the statement number alterations and the output text.

ORIGIN - N. Beebe

AVAILABLE FILES -

PRETTY/SOURCE	Source of PRETTY
PRETTY/DOC	User manual for PRETTY
PRETTY/TESTIN	Test input for PRETTY
PRETTY/TESTOUT	Test output for PRETTY

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

TI01 NAMLST NAMELIST Input Routine for the VAX 11/780

This routine provides the capability for doing NAMELIST input on the VAX 11/780 minicomputer. VAX FORTRAN does not support NAMELIST I/O and the present routine attempts to provide a NAMELIST capability in as convenient a way as possible. The user is required to provide the usual sort of information automatically provided by the compiler, namely, the group name, the variable names, variable data types, dimensions of arrays, and so on, which are all static attributes and are specified in a named common block. The user must provide via a subroutine call the run time locations of all NAMELIST variables, which is done by providing an argument in the NAMLST procedure call for each of the possible items in the list.

The routine is written in VAX FORTRAN IV and includes its own parser and number conversion routines. User documentation for the routine is provided in the form of comments cards within the program. The present version of the program is specific to the VAX 11/780 but can easily be made portable.

ORIGIN - S. A. Hagstrom, NRCC

AVAILABLE FILES -

NAMLST/SOURCE	FORTRAN IV source for VAX 11/780

SUPPORT LEVEL - A

DISTRIBUTION STATUS - A

TP01 RATMAC <u>The RATMAC Preprocessor</u>

RATMAC is a preprocessor based on two programs, RATFOR and MACRO, described in the book "Software Tools" by B. W. Kernighan and P. J. Plauger (Addison-Wesley publishing Co., Reading, Mass.,1976). The preprocessor translates a program written in the structured FORTRAN dialect "RATMAC" into standard ANSI FORTRAN. RATMAC has a bootstrap that is easy to implement on any machine with a FORTRAN compiler.

RATMAC has all the characteristics of RATFOR, but is augmented by a powerful recursive macro processor which is extremely useful in generating transportable FORTRAN programs. A macro is a collection of programming steps which are associated with a keyword. This keyword uniquely identifies the macro, and whenever it appears in RATMAC program it is replaced by the collection of steps.

ORIGIN - R. Munn and J. Stewart

AVAILABLE FILES -

RATMAC/SOURCE/FOR	RATMAC in portable FORTRAN (bootstrap)
RATMAC/SOURCE/RAT	RATMAC in RATMAC (enhanced)
STDIO/SOURCE/RAT	Standard I/O macros
VAXIO/SOURCE/RAT	VAX specific utility macros
SYSFIL/SOURCE/RAT	General utility macros
TEXT/SOURCE/RAT	Macros to open and close files

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

TV01 PFORTV Portable FORTRAN Verifier

The PFORT verifier is a program which checks a FORTRAN program for adherence to PFORT, a portable subset of American National Standard FORTRAN. Most FORTRAN compilers check only that individual program units conform to the standard, the verifier also checks that inter-program communication through the use of common and argument lists is consistent with the standard.

The verifier provides a number of facilities useful in debugging and documentation. It produces intra-program-unit error diagnostics, symbol tables, and cross references. The inter-program-unit output includes for each program unit, a listing of the arguments, the common blocks, the program units called and the program units which call it. A list of global common definitions is also produced.

ORIGIN - B. G. Ryder - Bell Laboratories

AVAILABLE FILES -

PFORTV/SOURCE	Source of PFORTV
PFORTV/DOC	Documentation for PFORTV

SUPPORT LEVEL - C

DISTRIBUTION STATUS - A

CRYSTALLOGRAPHY

XD01 CAMFILE Cambridge Structural Data Files

The Cambridge database is concerned with the crystal structures of organic and organometallic compounds. Three major criteria determine the database coverage:

(1) Compounds: organic and organometallic excluding polymers and proteins
(2) Techniques: crystal structures determined by x-ray or neutron diffraction.
(3) Structures: for each structure three coordinates determined for non-hydrogen atoms.

The Cambridge files currently contain about 17,000 citations from some 350 journals, theses and proceedings of national and international conferences on x-ray and neutron crystallography. The information contained in the Cambridge database is organized with respect to three major files:

(1) Bibliographic: compound name, formula, class, literature reference, etc.
(2) Connectivity: chemical connectivity in terms of atoms, bond types, etc.
(3) Data: unit cell data, symmetry, atomic coordinates etc.

For each publication of the structure of a compound the relevant information is divided into 3 entries which are located in the files (1) - (3).

The principal modes of search and retrieval are governed by three programs:

- BIBSER: bibliographic search of the file SBIB to yield:
  - listing of bibliographic entries
  - sub-file of bibliographic entries
  - sub-file of reference codes
- CONNSER: connectivity search of the file SCONN to yield:
  - listing of reference codes
  - sub-file of connectivity entries
  - sub-file of reference codes
- RETRIEVE: program which reads a sub-file of reference codes and retrieves the corresponding entries from SBIB, SCON, or RDAT.

ORIGIN - Crystallographic Data Center, Cambridge, England cb2 lew

AVAILABLE FILES -

CAMFILE/DATA/FBIB	Formatted bibliographic file
CAMFILE/DATA/SBIB/CDC	Unformated (CDC) bibliographic file
CAMFILE/DATA/FCONN	Formatted connectivity file
CAMFILE/DATA/SCONN/CDC	Unformated (CDC) connectivity file
CAMFILE/DATA/FDAT	Formated data file
CAMFILE/DATA/RDAT/CDC	unformated (CDC) data file

CAMFILE/SOURCE/BIBSER/CDC	Bibliographic search program
CAMFILE/SOURCE/CONSER/CDC	Connectivity search program
CAMFILE/SOURCE/RETRIEV/CDC	Data retrieval program

SUPPORT LEVEL - C

DISTRIBUTION STATUS - B (see comments)

Comments - contact NRCC crystallographic staff for file access at LBL. Copies of the file for use in the U.S.A. can be obtained from -

Fein-Marquart Associates
7215 York Road
Baltimore, MD 21212

XD02 PROTDAT <u>Protein Data Bank Files</u>

The protein data bank is a computer-based archival file for macromolecular structures. The bank stores in a uniform format atomic co-ordinates and partial bond connectivities, as derived from crystallographic studies. Text included in each data entry gives pertinent information for the structure at hand (e.g. species from which the molecule has been obtained, resolution of diffraction data, literature citations and specifications of secondary structure).

SOURCE - Protein Data Bank, Brookhaven National Laboratories

AVAILABLE FILES -

PROTDAT/SOURCE/BENDER	Paramaters for bent-wire models G. Williams
PROTDAT/SOURCE/CONECT	Generate full connectivity F. Bernstein
PROTDAT/SOURCE/DGPLOT	Diagonal plots on printer E. Swanson, F. Bernstein
PROTDAT/SOURCE/DSTNCE	Calc distns from conect rcrds F. Bernstein
PROTDAT/SOURCE/FISIPL	Phi/psi plots on printer F. Bernstein
PROTDAT/SOURCE/NAMOD	Ball-and-stick model display Y. Beppu
PROTDAT/SOURCE/PHIPSI	Main-chain torsion angles Andrews, Williams, Bernstein
PROTDAT/SOURCE/STEREO	Extract xyz from stereo diagram M. Rossmann
PROTDAT/SOURCE/TOTALS	Validation of master records L. Andrews, F. Bernstein
PROTDAT/DATA/XXXXX	113 protein data files

SUPPORT LEVEL - D

DISTRIBUTION STATUS - B (see comments)

Comments - contact NRCC crystallographic staff for file access at LBL. The files may be obtained from -

Protein Data Bank
Department of Chemistry
Brookhaven National Laboratory
Upton, NY 11973

XS01 MULTAN78 X-ray Diffraction Structure Solving Package

A system of programs which can solve crystal structures in a single job. This version of MULTAN includes the ability to use knowledge of molecular structure (for instance, an oriented molecular fragment) to help in the structure determination. In addition, an improved "magic integer" phase permutation is used. The system is made up of the following programs:

NORMAL -- Computes normalized structure amplitudes
MULTAN -- Determines phases using tangent formula
EXFFT -- Computes an e-map from a set of normalized structure factors using fast fourier transform
SEARCH -- Finds the coordinates of the highest peaks in the e-map

The four programs are written on a single file with "*deck" card image used as a separator.

ORIGIN - P. Main

AVAILABLE FILES -

MULTAN78/SOURCE/CDC	CDC version of MULTAN78
MULTAN78/SOURCE/VAX	VAX version of MULTAN78 (suitable for IBM)
MULTAN78/DOC	User manual for MULTAN78

SUPPORT LEVEL - B

DISTRIBUTION STATUS - A

GM01 PLUTO

A Program for Plotting Molecular and Crystal Structures

The program may be used for drawing individual molecules or molecules in a crystalline arrangement. The content of the drawing requires the definition of items such a molecules, atoms within molecules, connections between atoms, labels for atoms, and unit cell representation. The style of the drawing may be like a stick model or a solid ball and spoke model with variable sizes for atoms and bonds. The atoms may be shaded to enhance the solid appearance. Drawings may be made in parallel projection, perspective, or in stereo perspective. The view direction may be chosen with reference to molecular features such as lines and planes defined by atom names or by reference to the cell and orthogonal axial systems. The view direction may be further modified by rotation about the plotting reference axes.

ORIGIN - S. Motherwell

AVAILABLE FILES -

PLUTO/SOURCE/VAX	VAX version of PLUTO

SUPPORT LEVEL - C
DISTRIBUTION STATUS - A

OTHER LIBRARIES

LIBRARIES

This section lists the various software libraries which are available at Lawrence Berkeley Laboratory. In most cases documentation is available from the Computer Center librarian (tel 415-486-5529). Much of the documentation is available online as part of the LBL Computer Center documentation. The LBL Computer Center Newsletter often contains items concerning the software holdings.

1) BLAS Basic Linear Algebra Subroutines

The BLAS are a collection of 38 low level, FORTRAN callable subroutines that perform many of the basic operations of numerical linear algebra such as dot products, vector operations, Given's transformations and vector norms. COMPASS (for the 7600) and FORTRAN versions are available at LBL. To get the current documentation execute the following control card:

```
LIBCOPY,BLAS77,OUTPUT,BLASDOC.
```

The BLAS are an excellent way of maintaining both portablility and machine efficiency. The FORTRAN versions, plus assembly language versions for the IBM 360/370, CDC 6000/7000/CYBER and UNIVAC 1108 and CRAY machines are available from:

International Mathematical and Statistical
 Libraries, INC.
Sixth Floor, GNB Building
7500 Bellaire Boulevard
Houston, TX 77036

(713) 772-1927

The distribution charge of $45 covers the postage and cost of a tape containing documentation and software.

2) CERN

The CERN program library consists of about 350 program packages, nine-tenths of which are in FORTRAN. The documentation consists of a short writeup and a long writeup for each routine. All the short writeups exist in a manual in the computer center library and the long writeups can be ordered from CERN on an individual basis. The source codes can be obtained on the LBL computer as follows:

```
GETTAPE,OLDPL=CERNPL,13214.
UPDATE,Q,8.
COPYSBF,COMPILE,OUTPUT
EOR
*COMPILE <name of routine>
```

3) CPC Computer Physics Communications

The CPC library consists of a set of programs contributed to the journal of that name. The programs are described and indexed in the journal 'Computer Physics Communications.' To retrieve a particular program along with data,corrections and adaptations execute:

```
GETTAPE,catno,24933.
```

where catno is the 4 character CPC catalog number of the program. If the number contains an asterisk, the asterisk must be replaced by the characters 'DATA' in the GETTAPE card.

4) DECUS Digital Equipment Computer Users Society

The DEC Users Society has a program library containing many general purpose programs for use on DEC equipment. Of particular interest are those for doing formatted and unformatted tape and disk I/O, for accounting and various other system services. For further information contact:

DECUS U.S.
One Iron Way
Marlboro, MA 01752

5) EISPACK 2

EISPACK is a set of approximately 70 FORTRAN subprograms for the eigenanalysis of matrices. Short descriptions of these routines are in the 'writeup' LIBRARY of the LBL computer center documentation. Both the object modules and source deck are accessible at BKY. To use an object module with your program use the control cards.

```
GETTAPE,ULIB=EISULIB,13214.
LINK,....,P=ULIB,X.
```

To retrieve a source deck submit:

```
GETTAPE,OLDPL=EIS2XPL,13214.
UPDATE,Q,8.
COPYSBF,COMPILE,OUTPUT.
EOR
*COMPILE <name of routine>
```

To acquire the documentation on microfiche execute:

```
GETTAPE,DOC=EISDOC,13214.
DISPOSE,DOC=MF,T=[EISPACK 2 DOCUMENTATION]
```

EISPACK/2 is available from two sources:

International Mathematical and Statistical
Libraries, Inc.
Sixth Floor, GNB Building
7500 Bellaire Boulevard

Houston, TX 77036

(713) 772-1927

The charge from IMSL is $75.

Principal investigators holding Department of Energy grants can obtain software from The National Energy Software Center without charge at the address:

National Energy Software Center
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

(312) 972-2000

6) FUNPACK

FUNPACK consists of about 15 FORTRAN subroutines to evaluate special functions such as Bessel functions and elliptic integrals. The descriptions are in the writeup 'LIBRARY' of the LBL computer center documentation.

7) GRAFPAC

GRAFPAC is a set of low-level routines to allow device independent graphic display at LBL. These routines can be used by FORTRAN programs on the CDC 6000 and 7600 machines. The package allows the user to clear the screen and plot points, lines and character strings for on-line,off-line or interactive devices. The devices currently implemented in GRAFPAC are CALCOMP,DICOMED (color com),line printers, SC4460, ZETA plotter, TEKTRONIX 4006,4012,4014 and teletypes. For further information consult the LBL computer center WRITEUP, GRAFPAC.

8) IDDS

The integrated data display system is a general purpose, scientific data display graphics package. The system is a collection of FORTRAN callable subroutines that interact with each other to form a comprehensive, high level, device independent data display system. All routines in IDDS are written in portable FORTRAN. All low level device dependent operations are those of GRAFPAC. To obtain the text portion of IDDS documentation execute the control cards at LBL.

```
LIBCOPY,IDDS,OUTPUT,WRITEUP.
DISPOSE,OUTPUT=PR,PA=1F.
```

To obtain the illustrations for the documentation contact the LBL computer center library (415) 486-5529.

9) IMSL

The International Mathematical and Statistical Library consists of approximately 460 subroutines covering the general fields of mathematics and statisics and designed to be used in the development of scientific and engineering application programs. The catalog is available in the computer center library at Berkeley. The sources of the IMSL routines are not available. A compiled user program can be linked with the IMSL routines with the following control cards:

```
FETCHPS,IMSL,IMSL,IMSL7.
LINK,....,P=IMSL.
```

Note that the above control cards are for edition 7.

10) LBL SOURCE

The LBL computer center has either written or acquired about one hundred miscellaneous routines, some in FORTRAN and some in COMPASS exclusively for use at LBL. These routines are described in three different subsets of the LBL computer center documentation.

a) FTNLIB

This subset contains descriptions of routines which are automatically loaded by the FORTRAN Compiler library. They are only useful on other CDC machines and often only at Berkeley. With these routines one can do such non-FORTRAN operations as getting date and time, resetting large and small core memory lengths, packing and unpacking words and performing specialized I/O operations.

b) SOURCE

The PSS subset SOURCE contains sources for about 100 FORTRAN subroutines in many areas of mathematics. Short descriptions are in the WRITEUP LIBRARY. Longer documentation may be obtained from the computer center librarian.

c) UTILITY

The Handbook UTILITY of the LBL computer center documentation contains descriptions of 18 programs available at LBL. The most useful ones CODE9 and ENCODE can convert an ASCII or EBCIDIC tape to internal CDC display code and vice-versa.

11) LINPACK

LINPACK is a collection of FORTRAN subroutines which analyze and solve various systems of simultaneous linear algebr ic equations, including those over- or under-determined systems encountered in least-squares problems and other statistical calculations. For details about the problems which LINPACK can solve and writeups of individual routines, please see the 1979 SIAM publication, LINPACK USER'S GUIDE by Dongarra, Moler, Bunch and Stewart, in the LBL Computer Center library. The part of LINPACK available at LBL is that which performs single-precision operations on real or complex matrices. To access LINPACK routines use the control cards:

```
FETCHGS,LINPACK/ULIB,13214.
LINK,....,P=ULIB.
```

It is available for distribution from the same sources as EISPACK/2 for the same costs.

12) NCAR National Center for Atmospheric Reasearch

The NCAR partial differential equation package contains seven programs along with documentation and an object library. See the Writeup LIBRARY of the LBL computer center documentation for a short description of these routines as well as instructions for their use and for obtaining further documentation and sources.

13) NPL National Physical Laboratory

The NPL optimization library package, from the National Physical Laboratory in England, consists of 35 subroutine packages for finding minima of functions of N variables with varying types of constraints, with and without the availability of first and second derivatives, using modified and quasi-Newton methods. The source code is proprietary and cannot be released. Short descriptions of the routines are in the writeup LIBRARY of the computer center documentation and longer writeups may be obtained from the computer center librarian. To link these subroutines with your own compiled FORTRAN modules use the control cards:

```
FETCHPS,NPLA,ULIB,ULIB.
LINK,...,P=ULIB.
```

14) QCPE Quantum Chemical Program Exchange

The Quantum Chemistry Program Exchange collects maintains and distributes programs useful to computational chemistry. The NRCC only has those QCPE programs which have an entry in this catalog. All QCPE programs should be obtained directly from QCPE. The toll-free number to order programs is 800-457-4022. The mailing address is:

The Quantum Chemistry Program Exchange
Department of Chemistry, Room 204
Indiana University
Bloomingtom, Indiana, 47405 U.S.A.

15) SANDIA

The Sandia Mathematical Program library is a collecton of general purpose mathematical routines written and maintained by the Sandia mathematical program library project at Livermore,California. Outstanding features of this library include an o.d.e. solver with a global error estimate (GERK), a set of Bessel functions, and an adaptive Gauss-Legendre quadrature routine (GAUS8). A catalog describing the SANDIA routines in detail may be obtained form the LBL computer center librarian; short descriptions are contained in the writeup 'LIBRARY' of the LBL computer center documentation. Both object modules and source are available on-line at Berkeley. To link the Sandia routines to your compiled FORTRAN program use the control cards:

```
GETTAPE,SAND=SANULIB,13214.
LINK,X,....,P=SAND.
```

To get a source listing of a routine submit:

```
GETTAPE,OLDPL=SANDIPL,13214.
UPDATE,Q.
COPYSBF,COMPILE,OUTPUT.
EOR
*COMPILE <routine name>
```

16) Software tools

The software tools programs are an outgrowth of concepts and programs discussed in the book "Software Tools" by B.W. Kernighan and P.J. Plauger (Addison-Wesley,1976). The programs are implemented on many machines. Outstanding features of these programs are a machine independant text editor, the RATFOR preprocessor, the ROFF document preparer and numerous other text oriented programs. A users group has been formed and a newsletter is now being produced. The editor is:

Debbie Scherer
Computer Science and Mathematics Department
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

(415) 486-5881

17) STACKLIBE A Vector Function Library for the CDC 7600

STACKLIBE is a library of vector or streaming operations implemented in optimal machine code for the CDC 7600. The routines can be characterized as monadic (e.g. A(i)=B(i)) dyadic (A(i)=B(i)+C(i)) or triadic (A(i)=(B(i)+C(i))*D(i)). The documentation may be obtained from the LBL computer center librarian. The routines themselves can be linked to a users program with the card:

```
FETCHGS,STAKLIB/ULIB,13214.
LINK,...,P=ULIB.
```

The COMPASS versions of the STACKLIBE routines can be obtained by submitting:

```
FETCHGS,STAKLIB/OLDPL,13214.
UPDATE,Q.
REWIND,COMPILE.
COPYSBF,COMPILE,OUTPUT.
EOR
*COMPILE <names of routines>
```

NRCC SOFTWARE LIBRARY ORDER FORMS

NRCC SOFTWARE REQUEST FORM

Recipient ____________________

Address ____________________

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Date ____________

Requestor ____________

Preparer ____________

Tape No. ____________

Date Sent ____________

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Tape Options

No. of Tracks 7 9 Density 800 1600

Character Set ASCII EBCDIC Computer CDC VAX IBM ________ (Other)

Programs Desired

	Program	All	No Assembly	No Test Output	Comments
1.					
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Tape Options

No. of Tracks 7 9 Density 800 1600

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Programs Desired

	Program	All	No Assembly	No Test Output	Comments
1.					
2.					
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Comments ______________________________________

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*  Preparer   ____________    *
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*  Tape No.   ____________    *
*                             *
*  Date Sent  ____________    *
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Tape Options

No. of Tracks 7 9 Density 800 1600

Character Set ASCII EBCDIC Computer CDC VAX IBM ________ (Other)

Programs Desired

	Program	All	No Assembly	No Test Output	Comments
1.					
2.					
3.					
4.					
5.					
6.					
7.					
8.					
9.					
10.					

Comments ______________________

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NRCC SOFTWARE REQUEST FORM

Recipient ______________________________

Address ______________________________

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* * * * * NRCC USE * * * * *

* Date ________________ *

* Requestor ________________ *

* Preparer ________________ *

* Tape No. ________________ *

* Date Sent ________________ *

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Tape Options

No. of Tracks 7 9

Density 800 1600

Character Set ASCII EBCDIC

Computer CDC VAX IBM __________ (Other)

Programs Desired

	Program	All	No Assembly	No Test Output	Comments
1.					
2.					
3.					
4.					
5.					
6.					
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9.					
10.					

Comments ____

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NRCC SOFTWARE REQUEST FORM

Recipient ______________________________

Address ______________________________

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* * * * * NRCC USE * * * * *

Date ________________

Requestor ________________

Preparer ________________

Tape No. ________________

Date Sent ________________

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Tape Options

No. of Tracks 7 9 Density 800 1600

Character Set ASCII EBCDIC Computer CDC VAX IBM __________ (Other)

Programs Desired

	Program	All	No Assembly	No Test Output	Comments
1.					
2.					
3.					
4.					
5.					
6.					
7.					
8.					
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10.					

Comments ____

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