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STATIC AND DYNAMIC MUONIC–ATOM CODES – MUON AND RURP *

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PROGRAM SUMMARY

Title of program: MUON

Catalogue number: ABNB

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computers: CDC 6400, 6600, 7600, IBM 370/168 double precision

Installation: Los Alamos Scientific Laboratory

Operating system: Any batch processor

Programming language used: ASA FORTRAN

High speed storage required: 25339 words as supplied, can vary

No. of bits in a word: 60

Overlay structure: none

No. of magnetic tapes required: none

Other peripherals used: line printer, card reader, card punch

No. of cards in combined program, test deck and description: 2382

Card punching code: BCD

Keywords: nuclear physics, spectroscopy, atomic physics, muonic atoms, energy levels, QED corrections

Nature of physical problem
Muonic-atom energy levels and wave functions are calculated. The results are corrected for nearly all important static effects, including finite nuclear size as produced by a user-specified nuclear charge distribution [1].

Method of solution
Fourth-order Runge–Kutta integration of the radial Dirac equations, with the secant method determining the eigenvalues. Corrections are either included as potentials in the Dirac equations or computed as first-order perturbations.

Restrictions on the complexity of the system
The code assumes spherical symmetry, so that effects of nuclear deformation may be treated only as static first-order perturbations. Dynamic muon–electron and muon–nuclear effects are neglected (the latter are calculated by RURP).

Typical running times
The code and test case as supplied are compiled, loaded, and executed in 59 s on a CDC-6600, of which 21 s is compilation time (FTN compiler with optimization level 2).

Unusual features of the program
The main arrays are allocated semi-dynamically in order to keep core requirements to a minimum. Although the code as supplied is set up for CDC computers, previous versions have been run successfully on IBM 370/168 using the H-compiler with the AUTODOUBLE option. Use of the code on low-precision machines is recommended only if extensive double precision is implemented.

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Reference
[1] extensive numerical results from this code are reported by G.A. Rinker and R.M. Steffen, At. Data and Nucl. Data Tables 20 (1977) 143.

PROGRAM SUMMARY

Title of program: RURP

Catalogue number: ABNC

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computers: CDC 6400, 6600, 7600, IBM 370/168 double precision

Installation: Los Alamos Scientific Laboratory

Operating system: Any batch processor

Programming language used: ASA FORTRAN

High speed storage required: 44990 words as supplied, can vary

No. of bits in a word: 60

Overlay structure: none

No. of magnetic tapes required: none

Other peripherals used: line printer, card reader

No. of cards in combined program, test deck and description: 4564

Card punching code: BCD

Keywords: nuclear physics, spectroscopy, atomic physics, muonic atoms, nuclear polarization, dynamic hyperfine structure, energy levels, transition intensities

Nature of physical problem
Coupled muon–nuclear wave functions, energy levels, and transition energies and intensities are calculated. The results are corrected for nearly all effects of nuclear excitation [2–4].

Method of solution
The muon–nuclear Hamiltonian is represented in an angular-momentum basis and diagonalized to all order in a truncated subspace and to second order in the remainder of the infinite Hilbert space. The finite-space diagonalization is accomplished by standard means. The remaining diagonalization is accomplished by the implicit solution of the appropriate inhomogeneous differential equations in the muon radial coordinate using a band-matrix inversion technique.

Restrictions on the complexity of the system
No more than 9 muon levels and 8 nuclear levels may be included at any one time. The only magnetic interaction included is the static M1 HFS interaction.

Typical running times
The code and test cases as supplied are compiled, loaded and executed in 322 s on a CDC-6600, of which 43 s are compilation (FTN compiler with optimization level 2).

Unusual features of the program
The main arrays are allocated semi-dynamically in order to keep core requirements to a minimum. Although the code as supplied is set up for CDC computers, previous versions have been run successfully on IBM 370/168 using the H-compiler with the AUTODOUBLE option. Use of the code on low-precision machines is recommended only if extensive double precision is implemented.

References
[2] G.A. Rinker, Phys. Rev. A14 (1976) 18;
[3] G.A. Rinker and J. Speth, Nucl. Phys. A 306 (1978) 360.
[4] G.A. Rinker and J. Speth, Nucl. Phys. A 306 (1978) 397.

LONG WRITE-UP

1. Introduction

Two computer codes have been written to calculate energy levels and transition intensities of low-lying states in muonic atoms. Low-lying is here defined to include those muon states which do not interact in a significant dynamic way with the atomic electrons present in the system. The primary objectives are (a) to calculate all static corrections to the energy levels which are experimentally significant and (b) to calculate all corrections to the energy levels and transition intensities which arise from the dynamic coupling between muon and nucleus.

Objective (a) is met by the code MUON, which is an extended and improved version of a code originally written by J.G. Wills. MUON calculates muon binding energies by numerical integration of the radial Dirac equations in the field of a static, spherically symmetric nuclear charge distribution. With one minor exception, all further corrections to the energy levels

which are known to be experimentally significant and which do not depend upon the nuclear excitation spectrum are included. Several additional useful expectation values are computed and printed out. MUON also includes a simple fitting routine which can adjust up to two parameters of the nuclear charge distribution to provide a least-squares fit to specified transition energies.

Objective (b) is met by the code RURP. RURP provides a fairly general framework for calculating the effects of nuclear excitation in the muonic spectra. By a combination of perturbation theory and explicit matrix diagonalizations, RURP can calculate changes in transition energies and/or intensities due to any specified nuclear states which are connected by electric multipole transitions of arbitrary multipolarity. RURP was designed with a high degree of flexibility, which enables any desired nuclear model to be incorporated either through the input data or through a combination of the input data and alteration of a single subroutine.

2. MUON

The principal effects calculated by MUON are discussed in detail in ref. [1], where references to the original literature may be found. These effects are

2.1. Finite nuclear size

This is calculated by fourth-order Runge–Kutta integration of the radial Dirac equations in the potential due to a specified spherical nuclear charge distribution. The Runge–Kutta algorithm was compared to an equivalent routine using Hamming's modified predictor–corrector method and found to be somewhat superior in accuracy and speed. The electrostatic potential is stored in an array, and the equations are solved with a state-dependent step size. The final eigenvalues are found by the secant method. In the most accurate computational mode available with default numerical parameters, numerical errors in the calculated eigenvalues are of order 1 eV or less for most nuclei.

2.2. Vacuum polarization

The second-order $\alpha(Z\alpha)$(Uehling) and fourth-order $\alpha^2 Z\alpha$(Källen–Sabry) electron vacuum polarization energies are computed by including the corresponding static potentials in the Dirac equations before solution, so that the resulting eigenvalues and wave functions are corrected for all static iterations of these effects. Higher-order $\alpha(Z\alpha)^{3,5,\cdots}$ vacuum polarization corrections are presently only estimated but may be incorporated more accurately into future versions of the code. Second-order (Uehling) vacuum polarization energy shifts due to virtual muon pairs are calculated as first-order perturbations.

2.3. Vertex corrections

The vertex correction of order $\alpha(Z\alpha)$ is computed as a first-order perturbation. The order $\alpha(Z\alpha)^2$ vertex correction is estimated as a first-order perturbation. The total vertex correction thus obtained is now known to be quite accurate, as compared to some more detailed calculations [5].

2.4. Other corrections

Relativistic nuclear motion (recoil) corrections beyond the non-relativistic reduced mass are calculated as first-order perturbations. Electron screening corrections are calculated as first-order perturbations using a parametrization of electron densities from atomic Dirac–Hartree–Fock calculations.

The perturbation-theory corrections may be calculated with muon wave functions either corrected or uncorrected for $\alpha(Z\alpha)$ and $\alpha^2(Z\alpha)$ electron vacuum polarization. The corrected wave functions yield slightly more accurate results. The subroutine RAD, which calculates the perturbation corrections, is called after each eigenvalue is computed and the wave function stored. This subroutine may easily be altered to compute additional corrections or expectation values of interest.

Numerical accuracy of the calculations is determined primarily by the size of the wave function and potential arrays. These arrays are dimensioned in a small main program which calls the principal subroutine to execute the calculation. One may thus alter these arrays without disturbing the remainder of the code. Instructions for such alterations are given in comment cards in the main program. Numerical parameters can additionally be read as data, but these input values may be altered by the code to prevent

array overflows. Default values of the numerical parameters are generally chosen to maximize accuracy within the constraints imposed by array size.

The fitting routine uses a sequence of one-dimensional secant-method adjustments of one or two nuclear charge distribution parameters. This algorithm is unsophisticated when compared to others currently available, but it has the advantage of requiring very little storage and is reasonably efficient and stable in the present context.

The FORTRAN source for MUON is liberally provided with comment cards, where further information can be obtained. It should be noted that energies are output from MUON as binding energies and binding energy corrections, which is uniformly opposite to the conventions in RURP.

3. RURP

The principal effects calculated by RURP are formulated and discussed in detail in refs. [2–4]. These are

(1) Dynamic hyperfine structure (HFS) effects calculated by numerical diagonalization of the muon–nuclear Hamiltonian in a truncated, coupled muon–nuclear model space. Eigenvalues and mixed-state wave functions resulting from the diagonalization are used in a cascade calculation to compute radiative transition energies and intensities.

(2) Nuclear polarization (NP) corrections to the energy levels and to the HFS, including both overall (diagonal) energy shifts of the coupled states and off-diagonal corrections to the Hamiltonian matrix. If HFS is calculated, these corrections are computed only for the nuclear states included in the HFS calculation. Alternatively, one may simply compute NP energy shifts of the muonic states coupled to a specified nuclear state.

The main part of the calculation has the formalism and validity of almost degenerate perturbation theory with electric multipole interactions. The entire muon–nucleus spectrum is divided into a model space, in which the Hamiltonian is diagonalized (HFS), and its complement, which is treated in perturbation theory (NP), with exact sums over the entire muon spectrum and certain closure approximations for the nuclear spectrum. The result is an approximate diagonalization of the Hamiltonian over the entire, infinite muon–nuclear spectrum. This is carried out in a representation in which muon and nuclear states are coupled to good total angular momentum, and the residual muon–nuclear interaction is expanded in multipoles. Two principal approximations for the NP corrections beyond the use of perturbation theory are made. First, the true perturbation-theory energy denominators are replaced by approximate values. This does not seriously affect the accuracy and reduces the perturbation calculation from an n^2-process to an n-process in CPU time, where n is the dimensionality of a given Hamiltonian sub-matrix. Second, the only magnetic multipole effect included is the static magnetic dipole interaction.

The only correction made to the muonic energies and wave functions beyond those due to nuclear moments and transitions is that due to $\alpha(Z\alpha)$ electron vacuum polarization. When calculated, this is included in the Dirac equations so that the muon energies and wave functions are approriately corrected, and it is also included in the multipole transition potentials in order to correct the off-diagonal matrix elements. Further corrections to the muon energy levels, e.g., as calculated by MUON, may be read as data. These corrections are important only if a diagonalization is carried out and precise values for the energies are required. In these cases one should also first calculate NP energy shifts due to nuclear states (e.g., giant resonances) outside the model space and add them to the corrections from MUON. In principle, one should also correct the off-diagonal matrix elements for the same effects, since we imagine diagonalizing a total Hamiltonian which contains all of them as effective interactions. In practice, the off-diagonal matrix elements are enough smaller that such accuracy is not required. If one is concerned about off-diagonal NP corrections due to high-lying nuclear states, it is a simple matter to include them in the HFS calculation so that such corrections may be calculated.

The cascade calculation is carried out only within the diagonalized (HFS) configuration. Thus as a practical matter it can be necessary to include muon states which are not seriously mixed with nuclear excitations in order to start the cascade reasonably. Electric multipole transitions up to $L = 6$ are allowed. The radiative muon matrix elements are computed in the long-wavelength approximation from the fully-cor-

rected muon wave functions. The radiative nuclear matrix elements are the same as those used for normalization purposes in the HFS diagonalizations. The mixed muon–nuclear eigenvalues and wave functions resulting from the HFS diagonalizations are used in the cascade, so that the resulting transition energies and intensities are corrected for all calculated effects. It should be noted that the finite radiative widths of the states are neglected in the HFS diagonalizations, where the states are treated as infinitely narrow.

The general philosophy adopted in RURP is to maximize flexibility by avoiding the incorporation of specific nuclear models any more than necessary. The nuclear spectrum is read in as data, as is the electric multipole matrix which describes the transitions between the various nuclear states. It is assumed that only one electric multipole contributes to each possible nuclear transition or moment. Charge form factors for the nuclear moments and transitions are provided separately, so that one may specify energy, transition strength, and form factor independently. In addition, one may specify magnetic dipole moments and form factors for each of the nuclear states. The transition and moment form-factors are calculated in subroutine VTRAN, which may easily be modified if different ones are desired. A similar subroutine VZERO provides the spherically-symmetric potential in which the zero-order muon energies and wave functions are calculated.

The zero-order muon wave functions and eigenvalues are calculated with the variable-order, variable-step size Adams method package of routines ODE [6], using the eigenvalue search method described in ref. [2]. One could probably improve computation speed by incorporating a fixed-order, fixed-step size algorithm such as is used in MUON. This would have the disadvantage of significant complication of the control of numerical error. Further problems of array size would also enter if such a routine were incorporated in a reasonably efficient way. As it is, MUON and RURP provide cross-checks of numerical accuracy because they use different methods of computing eigenvalues and wave functions. Furthermore, if a known eigenvalue is read into RURP as an initial guess, the program will integrate the Dirac equations only once because of the nature of the eigenvalue-adjustment algorithm. This alleviates somewhat any problem of relatively slow solution of the Dirac equations.

The inhomogeneous perturbation equations are solved by the second-order band-matrix technique described in ref. [2]. This technique is stable in all known situations, and its accuracy may be investigated with trial calculations. In most situations the default values of the numerical parameters give electron–volt accuracy. Problems can arise in calculating NP corrections to the HFS if two basis states are nearly degenerate, so that the associated perturbation energy shift is very large. In extracting this unwanted contribution from the desired sum, a result of no numerical significance may be obtained. Such spurious results are generally no larger than a few eV and may be investigated numerically by adjusting the associated nuclear transition strength and/or the numerical parameters.

The calculation is divided into two distinct phases. In the first phase, an information base is constructed. A nucleus and some numerical parameters are specified, various basic potentials are calculated and stored, a set of zero-order muon energies and wave functions is calculated and stored, and a set of nuclear states is specified. This phase may be run by itself if only zero-order results are desired.

In the second phase, the NP, HFS, and cascade calculations are carried out using as a data base the results of the first phase. The actual calculation to be done is specified by a configuration card. This card may be repeated for as many different NP/HFS/cascade calculations as are desired, with a blank card signaling a return to the beginning of the first phase.

Considerable attention is given to efficiency with respect to both execution time and storage requirements. Dimensions of many arrays are given in a small main program, so that unneeded storage may be eliminated and possibilities for storage-sharing may be exercised without modifying the working routines. Control variables are also specified in this main program to provide internal checks for overflow of the most important large arrays. These control variables and their associated overflow messages make it possible to determine optimum array sizes for a given problem semi-empirically by merely starting with small arrays, making test runs, and increasing dimensions as directed.

The FORTRAN source for RURP is liberally provided with comment cards, where further information can be obtained. It should be noted that actual ener-

gies are output from RURP, which is uniformly opposite to the conventions in MUON.

4. Use of the codes

Appended to the test data decks are detailed desciptions and explanations of all input parameters. These descriptions should be referred to for more specific instructions than are given here. The test decks themselves are constructed to illustrate a standard sequence of runs which may be used to interpret a given set of data. Such a standardized sequence of calculations seldom occurs in practice, but it serves to illustrate the principal capabilities of the codes. Further capabilities are probably best left to the user to discover upon gaining more experience with the calculations.

Before use, the test data decks should have the sequence identifiers removed from columns 73–80, as the codes read all 80 columns.

The standard runs are divided into three segments. The initial run is with RURP. Its purpose is to compute the overall NP energy shifts due to the giant nuclear resonances. The program default is to replace each giant resonance by a single discrete nuclear state according to the prescription given in ref. [4]. The results of this run are overall energy shifts of the muon levels coupled to the nuclear ground state. These shifts are then read in as data in the second run, in which MUON computes the remaining (static) corrections to the energy levels and makes a preliminary fit of the nuclear charge distribution to specified experimental transition energies. Finally, the corrections and charge distribution parameters output by MUON are read into RURP for a third run which computes the effects of dynamics HFS due to specified low-lying nuclear states. The ultimate results are muon–nuclear transition energies and intensities, which may be compared directly to measured values. The problem of adjusting parameters further in order to improve agreement with experiment is not treated directly by the codes, as it is quite complicated in cases where HFS effects are large and is probably best left to the experience and intuition of the user. Descriptions of the individual test runs follow.

4.1. Run 1: RURP

Lines 1 through 52 of the test deck provide the input data for this run. The first card tells the code that 7 nuclear form factors, 7 muon states and 8 nuclear states are to be read in and calculated. It also turns off the vacuum polarization switch and specifies nuclear charge and mass, as well as the (default) charge distribution parameters. The next card is blank, specifying minimum printout and the default numerical parameters. The next 7 cards specify the nuclear form factors. The multipolarity of each appears in column 2, and since the remaining fields are blank, the default form factor parameters are to be used. The next 7 cards specify the muon non-relativistic quantum numbers n, l, and $2j$. Then come 8 nuclear level cards. The first three fields of each give the spin, parity and energy of the level. Two things should be noted. The first is that the ground state is given as 0^+ rather than the actual value $\frac{1}{2}^-$ appropriate for the nucleus used as a sample. This simplification is possible because the nuclear spin is not observable in the overall NP shifts once the angular momenta are averaged. If one used the correct spin in this phase of the calculation, it would also be necessary to similarly decompose the giant resonances and do the appropriate summing and averaging, resulting only in a more complicated path to the same answer. The second thing to notice is that the parities of the excited states are given as S or V. These tell the code to use the built-in isoscalar or isovector sum rules and formulae to compute the semi-empirical giant resonance energies and/or transition strengths (these formulae are valid only when the ground state is taken to be 0^+). The next 8 cards specify the electric multipole matrix. These cards are divided into 8 fields of 10 columns each. The first column of each field specifies which form factor to use, and the next 9 columns give the corresponding reduced nuclear matrix element (defaulted here). The non-diagonal matrix element RNM(I,J) is defined (except for sign) by (2*SN(I)+1) * B(EL;I→J) = RNM(I,J) ** 2, where SN(I) is the spin of nuclear state I. The sign is determined by other considerations. Diagonal matrix elements are defined with the same operators and normalization. Form factors are specified by the order read in, i.e., a 3 in column 1 means use the third form factor read in for the transition. Normally, a blank

in a reduced nuclear matrix element field is interpreted as zero, but here it will be filled with a nonzero value by the code since the corresponding nuclear-state parities are read as S or V. A more detailed description of the electric multipole matrix is given in conjunction with run 3.

The next card initiates the actual calculation of the NP energy shifts, based upon the states and form factors specified by the previous cards. The first 9 fields of this configuration card specify the muon states to be included, labeled by the order in which they are read in. In this case, all 7 states are included. They need not be given in increasing order. Column 10 contains a blank, and columns 11 through 18 in a similar way specify which nuclear states are to be included. Two blanks follow, and in the remaining fields appear some switches and further parameters. Here we have only a 1 in column 21, which tells the code to compute only NP energy shifts, with no HFS or cascade calculation. Because no HFS is calculated, the NP shifts will be computed only for those muon states coupled to the first nuclear state (the 0^+ state) on the configuration card. This card could be followed by several more, but since it is here followed by a blank, the code returns to the beginning for another initial data card.

The next part of this run is an abbreviated variation of the preceding part. Here, the numbers of form factors and muon states to be read are both zero, so the code will skip those parts of the calculation and use the ones already available in storage. Seven new nuclear states are read in order to carry the NP calculation through $L = 6$ (storage limitations prevent this from being done in a single data set). It may be noted that form factors 1, 2, 3 and 4 were used in the first part of this run, while 5, 6 and 7 will be used in this part. Since none are used in both parts, it would have been just as economical to include only 4 form factors in the first part and to compute the 3 remaining ones in the second part. This was not done in the test case simply to illustrate how one can carry over information, thereby sometimes saving unnecessary computation. The remainder of this run continues as above, ending with the blank as card number 52. This card would normally be followed by another blank terminating the run.

The output for this run should be reasonably self-explanatory. Most of the first page summarizes the input data and computed parameters, energies and reduced matrix elements. The configuration card is then summarized and the NP calculations begun. Next appear the results for the angular momentum-parity block $\frac{1}{2}^+$. In this block appear the muon $1s_{1/2}$ and $2s_{1/2}$ states coupled to the nuclear ground state. In the column labeled EP are the computed NP energy shifts in MeV. The numbers under the heading JN show that nuclear states 1 through 8 are used in the NP calculation. The convention is that the first nuclear state listed is coupled to the muon state and the remaining nuclear states are summed to give the total value listed under EP. If one desires the contributions from the individual nuclear states separately, two options are available. One may print these out using one of the print parameters, or alternatively, one may read in several configuration cards

```
1234567   12    1
1234567   13    1
          :
1234567   18    1
```

instead of

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1234567   12345678  1 .
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With the second alternative, it is necessary to add the individual contributions by hand to get the total shifts. The remaining angular momentum–parity blocks follow in order. The output for the second part of this run follows similarly, but since no new form factors or muon states are computed, the old ones are not summarized again.

4.2. Run 2: MUON

The test deck for MUON contains two data sets which fit the charge distribution to measured transition energies and compute the further corrections required by RURP for the HFS calculation. The first card specifies the type of charge distribution and number of charge distribution parameters, electron screening parameters, number of muon states, vacuum polarization to be computed, number of transitions to be fitted, and gives instructions to print the numerical charge distribution values and possible muon transitions for each multipole as an aid in searching for muon–nuclear resonances. The next card speci-

fies the nuclear mass and charge, the electron screening charge, and the nuclear spin and magnetic and quadrupole moments. These last three quantities are included here only as an illustration, as they are recomputed by RURP in the HFS calculation. Also on the second card are α and several value of k for which equivalent radii will be computed [7]. The third card contains the charge distribution parameters. The first field is blank, signifying that a default value is to be used, while the second field specifies a value of the skin thickness. The remaining fields are not used in this particular run. Card number 4 contains numerical parameters (defaulted). The next 14 cards contain the muon levels. The first 7 of these are the same as for RURP, except that the F in column 8 indicates not to include vacuum polarization for these levels. Seven similar level cards follow, but with T's in column 8 and entries in the next two fields. The first of these contains corrections not computed by MUON, which are here the NP results of run 1 with RURP and the $\alpha(Z\alpha)^{n\geq 3}$ vacuum polarization, labeled in the next field for easy reference. Set up in this way, the total energy corrections beyond finite nuclear size will appear in a separate column in the output.

Next appear the energy-fitting parameters. The next card indicates that the first charge distribution parameter is to be adjusted to a tolerance of better than 10^{-6} to fit the transition energies read on the next cards. Each of these cards contains a muon transition (e.g., 10 8 refers to a transition from the 10th level read in to the 8th level read in), an associated energy (MeV), and an uncertainty (MeV). Since a 4 appeared in column 30 of the first card, the code will read 4 of these transition cards and then carry out the first part of this run.

The second data set in this run is included in order to obtain the most precise possible set of corrections for the final HFS wun with RURP. Because zero (or blank) appears in columns 6–10, no new charge distribution parameters will be read or computed. Rather, the final values in storage remaining from the previous fit will be used to recompute the muon energies. The significance of this will become apparent at the end of the following discussion of the output of these runs.

At the top of the first page of output appears a summary of input data and various parameters. Then come several blocks of 9 lines each, one block for each level. These blocks result from calculations using the initial charge distribution parameters. The first line gives the muon quantum numbers and the range of integration. The second gives the point–nucleus energy, the initial guess used in the eigenvalue search, and the final converged eigenvalue before perturbation corrections are computed. If a T was read in column 8 of the level card, this value includes second and/or fourth-order vacuum polarization corrections; otherwise, it does not. The next line contains expectation values of specified functions of r and $V(r)$, the electro–static potential generated by the nucleus, and the following line contains expectation values of the kinetic energy, square of the momentum, and the nuclear charge distribution $\rho(r)$. Units for these are described in the comment cards in subroutine RAD. Then come vacuum polarization expectation values, which are not added to the computed binding energies. The next two lines contain corrections computed by the code. With the exception of the anomalous moment (which is included in the $\alpha(Z\alpha)$ vertex correction), these are added together with the read-in corrections to give the number labeled TOTAL at the end of line 7 in this block. TOTAL is added to the value BE(FINAL) in line 2 to give BE(TOTAL) in the summary at the end of the output. The next two lines contain M1 and E2 static HFS corrections for the listed values of total angular momentum F. These corrections are rather superfluous here because they are recomputed by RURP with more flexibility in the form factors. These E2 corrections usually differ from those computed by RURP because different form factors are used.

These blocks are repeated for each level, after which appear several lines giving value of χ^2 and the parameters as the charge distribution is adjusted to fit the read-in transition energies. Then comes what is essentially a repeat of the above except with quantities computed using the final fitted charge distribution parameters. Also included are equivalent radii computed as specified on the second data card, and a printout of the numerical charge distribution values. The computation for this data set ends with summaries of the fitted and computed energies. Two particular things should be noted. The first concerns the column labeled TOTAL CORRECTIONS, which is the difference BE(TOTAL) for a state with T in col-

umn 8 minus BE(FINAL) for a state with the same quantum numbers but with an F in column 8. Thus this column contains all specified corrections beyond finite nuclear size for the state in question, and may be used in certain ways as input for HFS calculations with RURP. The second item concerns the blocks labeled TRANSITIONS FOR L = . . . To construct these blocks, the code searches for possible electric multipole transitions between various muon states, subtracts their energies and estimates nuclear excitation matrix elements (MeV) assuming a nuclear excitation strength of 1 single-particle unit. The matrix element estimates are very crude and are intended only as an aid in searching for possible resonances. They should be recalculated more accurately by RURP if a resonance is suspected.

The second data set in this run is a recomputation including only second-order vacuum polarization, so that the TOTAL CORRECTIONS column contains only this correction. The differences between the values in this column for the two data sets thus represent all corrections not computed by RURP in the following HFS calculation.

4.3. Run 3: RURP

The final HFS run with RURP uses the last 24 data cards in the sample deck, plus two blank cards to terminate the run. The first card tells the code to expect 3 form factor cards, 7 muon state cards, and 5 nuclear level cards. It also turns on the second-order vacuum polarization with a 1 in column 4, and gives the nuclear charge and accurate mass (AMU), as well as the charge distribution parameters fitted by MUON. The first 5 columns of the next card specify print options. The 2 in column 4 dictates printout of the Hamiltonian and perturbation matrices. Zeros in the other columns (which could be blanks) turn off the other print options. The remaining fields of this card are blank, indicating that the default numerical parameters are to be used. The next 3 cards specify transition form factors. The value −1 in the first field of the first card signifies an M1 form factor, and the next 2 cards specify E2 and E3, all with default values and formulae. Then come the 7 muon state cards. In columns 7–20 appear the appropriate eigenvalues as computed by MUON. These will be used as initial guesses by RURP, thereby saving several eigenvalue iterations. In columns 21–30 are the corrections computed as above by MUON and RURP, which are not recomputed here and are thus needed to produce accurate energies for the HFS calculation. These will be added to all muon states regardless of which nuclear states are coupled in. This procedure thus assumes that the NP shifts due to the high-lying resonances are the same for all of the (low-lying) states included in the HFS calculation. It should be realized that this is a definite (but probably good) physical approximation, which may become an issue worth considering if extremely delicate resonance effects arise. It can safely be ignored in most applications.

Next come the 5 nuclear level cards. As before, the first 20 columns specify the spin, parity and energy of each level, but these are no longer defaulted. The 1 in column 21 indicates that form factor number 1 is to be used for a static magnetic dipole calculation, for which the magnetic moment follows in columns 22–30. The last 3 states undoubtedly have magnetic moments also, but values of the moments are not read because they are not known. It would be possible to use different form factors and moments for all states, to the extent that the overall limit of 7 different form factors is not exceeded. The next 5 cards give the reduced electric multipole matrix, as partially described above. This matrix is laid out in normal matrix notation, with 10-column fields allocated for each form factor–matrix element pair. The numbers appearing in the second field of the third card thus correspond, for example, to the nuclear matrix element (3,2) between the third and second nuclear states read in. As above, the first column in each field specifies a form factor, and the remaining 9 columns contain the reduced nuclear matrix element. It is necessary to read in only one of a given pair (I,J), (J,I), as the code will fill in any missing matrix elements if the required information is available. Blanks are here interpreted as zeros since the giant resonance formulae are not being used. Finally come the configuration cards. In the first of these, 013 appears in columns 21–23. These numbers tell the code not to compute additional NP perturbation corrections, but to do an HFS calculation and a cascade allowing radiative transitions up through E3. The second configuration is the same except that NP corrections are additionally included in the HFS calculation.

The output for these runs is rather lengthy and is only partially reproduced here. The first page summarizes the basic input information. The second page begins the HFS calculation with an image of the configuration card and a sequence of calculations for each angular momentum–parity block. The first block contains all states in the configuration which can couple to 0^+. Reference numbers for the coupled basis states run down the left side of the output (in the first block there are four basis states), so that the Hamiltonian matrix, for example, shows its (2,1) matrix element (MeV) in line 2, column 1. The eigenvectors are given in columns under their respective eigenvalues, with the amplitude of each basis state appearing on the approriate line.

The results of the cascade calculation appear after the final Hamiltonian block is printed. First appear one or more final states in the cascade, determined by the fact that they have no allowed radiative decays to lower states. In the example, there are two such final states. One can be identified by its energy, angular momentum, and parity as state number 1 in block 4, and the other is state 1 of block 2. Squares of the component amplitudes are given in the column labeled POPULATION. Then come total radiative level widths (MeV) for each state, e.g., the second number after the label BLOCK 3 is the width of the second eigenstate in the third block. The radiative transitions which appear above specified intensity tolerances are given in order of increasing energy in the final EXTERNAL PHOTONS listing. In the first column appears a number which refers to when the particular transition appeared in the cascade, after which follow the transition energy (MeV), intensity, and a label for the transition. The rightmost four digits of the label describe the block and state of the lower member of the transition, and the four digits to the left of that describe the same for the upper member of the transition. To the left of that in the column(s) labeled N is the number of actual transitions which are averaged and summed to give the printed entry. In this example, the first printed transition which appears which is actually composite is number 192 (the 9th printed transition). We can see that this transition has two components, the stronger of which is state 2 of block 6 to state 1 of block 4. The identity of the weaker component has been lost, but it could be retained by reading in a finer resolution for the averaging process. In this listing appear the transitions which are predominantly nuclear as well as those which are predominantly muonic. For example, our transition number 192 is mainly the $\frac{3}{2}^- \rightarrow \frac{1}{2}^-$ nuclear quadrupole transition, with small admixtures of others. One can identify these transitions first by their energies and then by checking the actual eigenvectors involved.

The remainder of this run is a duplication of the above except with the NP corrections added to the Hamiltonian matrices to account for truncation effects, as described in ref. [3]. The output is similar except for the appearance of the perturbation matrices in the output and slight modification of the results. It may be noted that column EP in the output now is non-zero, as it contains the diagonal elements of the perturbation matrix.

In testing RURP for successful implementation, it should be noted that the transition energies and intensities are quantities most sensitive to variation. If these values which appear at the end of run 3 (combined HFS/NP calculation) are reproduced, the code has probably been implemented successfully. MUON is probably implemented successfully if the fitted charge distribution parameters converge to the same values.

Acknowledgements

A number of people have contributed significantly over the past few years to the effort described here. I would like to thank especially K.W. Ford for introducing me to the subject of muonic atoms in the first place, and for teaching me a great deal; J.G. Wills for providing me with his code MUON, from which the present work grew, and for teaching me elegant FORTRAN programming by his excellent example; L. Wilets for patiently explaining to me the facts of nuclear excitation; R.M. Steffen, L. Schaller, L. Schellenberg, Y. Yamazaki, E.B. Shera and H.D. Wohlfahrt for testing my codes and offering many constructive suggestions; and R.B. Perkins for encouraging and stimulating me to develop RURP. In this last context, it should be noted that RURP stands for Roger's Ultimately Realized Program, an acronym taken from a commercial item of similar intent.

References

[1] G.A. Rinker and R.M. Steffen, At. Data and Nucl. Data Tables 20 (1977) 143.
[2] G.A. Rinker, Phys. Rev. A14 (1976) 18.
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[6] L.F. Shampire and M.K. Gordon, Computer solution of ordinary differential equations: the initial value problem (Freeman, San Francisco, 1975).
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TEST DATA FOR MUON

```
    2    2   81   14    1    4    0    1    1    0    0    0    0    0
206.9759  82.  81.  0.5  0.59 0.0  0.17 1.18 1.44 2.02 2.47 2.78 3.73
          0.523

 1 0 1 F
 2 0 1 F
 2 1 1 F
 2 1 3 F
 3 1 3 F
 3 2 3 F
 3 2 5 F
 1 0 1 T  0.003338  NP+VP3..
 2 0 1 T  0.000462  NP+VP3..
 2 1 1 T  0.001148  NP+VP3..
 2 1 3 T  0.001029  NP+VP3..
 3 1 3 T  0.000296  NP+VP3..
 3 2 3 T  -.000059  NP+VP3..
 3 2 5 T  -.000072  NP+VP3..
     1.E-6
   10    8 5.78379  0.00044
   11    8 5.96889  0.00044
   13   10 2.64293  0.00006
   14   11 2.50110  0.00006
    2    0   81   14    2
206.9759  82.  81.

 1 0 1 F
 2 0 1 F
 2 1 1 F
 2 1 3 F
 3 1 3 F
 3 2 3 F
 3 2 5 F
 1 0 1 T
 2 0 1 T
 2 1 1 T
 2 1 3 T
 3 1 3 T
 3 2 3 T
 3 2 5 T
```

MUON TEST RUN OUTPUT (Run 2)

```
                                        M U O N    AUGUST    1 9 7 8

NUCLEAR CHARGE= 82.0     NUCLEAR MASS= 206.9759     ELECTRON CHARGE= 81.0     AN TO 1/3=    5.915252

SPIN=   .5     G-FACTOR=   .5900     QUADRUPOLE MOMENT=     0.00

FPAR=    .1000E-05  0.          0.          0.          0.          0.          0.          0.


INTEGRATION INTERVAL=   .125*(1+ 1.00*(J-1/2)**2)     DR(OUT)/DR(IN)= 3.0     RMAX=   123.250

SCREENING CALCULATED FOR ZE, NSPAR =  81.000   81

ID=  2 FERMI       RM= 16.281250    DR(RMO)= .031250    RMO(TAIL)=  .995E-08    T= 2.30    R(RMS)= 5.50191

BULK PARAMETERS   RADIUS = 6.644743     DIFFUSENESS =  .523000     WINE BOTTLE = 0.000000     EXPONENT = 1.000
TAIL PARAMETERS   HALF-DISTANCE =0.              ATTACHED AT R =20.000000
MISC. PARAMETERS   PAR(7) =0.              PAR(8) =0.

VACUUM POLARIZATION ORDER  SECOND, FOURTH =    T    T

ITERATION FOR N L J K =  1.  0.   .5 -1.     MATCHING RADIUS=     6.375     RMAX=    58.125
BE(POINT)=  20.992521     BE(GUESS)=  10.666667     BE(FINAL)=  10.526458
(V) = -15.745904   (V**2) =  .276815E+03   (R**2*V**5) =  -.169370E-03
(T) =   5.219446   (P**2) =  .115849E+04   (RHO)       =   .251630E-01
(VP1)    =   .067655   (VP3(PT))  =  -.000818   (VP5(PT))       =  -.000100   (VP7(PT)) =  -.000018
ANOM MOM =  -.000444   VERTEX(ZA) =  -.003197   VERTEX(ZA**2)    =  -.000152   MUON VP   =   .000246
RECOIL   =   .000380   SCREENING  =   .000005   READ IN NP+VP3.. =  0.000000   TOTAL     =  -.002718
F =0.   DM1 =   .000310   DE2 =  0.000000   TOTAL = 10.524050
F =1.   DM1 =  -.000103   DE2 =  0.000000   TOTAL = 10.523637

ITERATION FOR N L J K =  2.  0.   .5 -1.     MATCHING RADIUS=    20.750     RMAX=   101.375
BE(POINT)=   5.385454     BE(GUESS)=   3.389418     BE(FINAL)=   3.580839
(V) =  -6.316692   (V**2) =  .626398E+02   (R**2*V**5) =  -.289220E-04
(T) =   2.735853   (P**2) =  .608045E+03   (RHO)       =   .435051E-02
(VP1)    =   .019481   (VP3(PT))  =  -.000302   (VP5(PT))       =  -.000037   (VP7(PT)) =  -.000007
ANOM MOM =  -.000072   VERTEX(ZA) =  -.000691   VERTEX(ZA**2)    =  -.000025   MUON VP   =   .000043
RECOIL   =   .000086   SCREENING  =   .000026   READ IN NP+VP3.. =  0.000000   TOTAL     =  -.000562
F =0.   DM1 =   .000050   DE2 =  0.000000   TOTAL =  3.580326
F =1.   DM1 =  -.000017   DE2 =  0.000000   TOTAL =  3.580259
```

```
ITERATION FOR N L J K =  2.  1.   .5  1.     MATCHING RADIUS=    13.000     RMAX=    78.250
BE(POINT)=   5.385454     BE(GUESS)=   5.385454     BE(FINAL)=   4.782276
(V) =  -9.296034   (V**2) =  .805645E+03   (R**2*V**5) =  -.590699E-04
(T) =   4.513758   (P**2) =  .992923E+03   (RHO)       =   .450734E-02
(VP1)    =   .032536   (VP3(PT))  =  -.000463   (VP5(PT))        =  -.000056   (VP7(PT)) =  -.000010
ANOM MOM =   .000237   VERTEX(ZA) =  -.000341   VERTEX(ZA**2)    =  -.000064   MUON VP   =   .000044
RECOIL   =   .000109   SCREENING  =   .000013   READ IN NP+VP3.. =   0.000000   TOTAL     =  -.000238
F =0.   DM1 =   .000165   DE2 =  0.000000   TOTAL =  4.782203
F =1.   DM1 =  -.000055   DE2 =  0.000000   TOTAL =  4.781982

ITERATION FOR N L J K =  2.  1.  1.5 -2.     MATCHING RADIUS=    12.875     RMAX=    78.125
BE(POINT)=   4.837283     BE(GUESS)=   4.837283     BE(FINAL)=   4.600080
(V) =  -8.802255   (V**2) =  .941690E+02   (R**2*V**5) =  -.513832E-04
(T) =   4.202176   (P**2) =  .921861E+03   (RHO)       =   .337423E-02
(VP1)    =   .029982   (VP3(PT))  =  -.000436   (VP5(PT))        =  -.000053   (VP7(PT)) =  -.000010
ANOM MOM =  -.000202   VERTEX(ZA) =  -.000639   VERTEX(ZA**2)    =  -.000097   MUON VP   =   .000033
RECOIL   =   .000094   SCREENING  =   .000014   READ IN NP+VP3.. =   0.000000   TOTAL     =  -.000555
F =1.   DM1 =   .000094   DE2 =  0.000000   TOTAL =  4.599618
F =2.   DM1 =  -.000056   DE2 =  0.000000   TOTAL =  4.599468

ITERATION FOR N L J K =  3.  1.  1.5 -2.     MATCHING RADIUS=    29.375     RMAX=   123.125
BE(POINT)=   2.166544     BE(GUESS)=   2.166544     BE(FINAL)=   2.091912
(V) =  -4.085831   (V**2) =  .289459E+02   (R**2*V**5) =  -.143807E-04
(T) =   1.993919   (P**2) =  .437350E+03   (RHO)       =   .115239E-02
(VP1)    =   .010355   (VP3(PT))  =  -.000182   (VP5(PT))        =  -.000022   (VP7(PT)) =  -.000004
ANOM MOM =  -.000058   VERTEX(ZA) =  -.000223   VERTEX(ZA**2)    =  -.000039   MUON VP   =   .000011
RECOIL   =   .000026   SCREENING  =   .000054   READ IN NP+VP3.. =   .000296   TOTAL     =   .000145
F =1.   DM1 =   .000027   DE2 =  0.000000   TOTAL =  2.092084
F =2.   DM1 =  -.000016   DE2 =  0.000000   TOTAL =  2.092041

ITERATION FOR N L J K =  3.  2.  1.5  2.     MATCHING RADIUS=    29.375     RMAX=   123.125
BE(POINT)=   2.166544     BE(GUESS)=   2.166544     BE(FINAL)=   2.173032
(V) =  -4.459556   (V**2) =  .241866E+02   (R**2*V**5) =  -.758871E-05
(T) =   2.286524   (P**2) =  .492448E+03   (RHO)       =   .110441E-03
(VP1)    =   .010639   (VP3(PT))  =  -.000201   (VP5(PT))        =  -.000025   (VP7(PT)) =  -.000005
ANOM MOM =   .000062   VERTEX(ZA) =   .000044   VERTEX(ZA**2)    =  -.000008   MUON VP   =   .000001
RECOIL   =   .000015   SCREENING  =   .000037   READ IN NP+VP3.. =  -.000059   TOTAL     =   .000031
F =1.   DM1 =   .000029   DE2 =  0.000000   TOTAL =  2.173092
F =2.   DM1 =  -.000017   DE2 =  0.000000   TOTAL =  2.173045

ITERATION FOR N L J K =  3.  2.  2.5 -3.     MATCHING RADIUS=    29.500     RMAX=   123.250
BE(POINT)=   2.121983     BE(GUESS)=   2.121983     BE(FINAL)=   2.130293
(V) =  -4.292029   (V**2) =  .220970E+02   (R**2*V**5) =  -.649816E-05
(T) =   2.161736   (P**2) =  .464914E+03   (RHO)       =   .615491E-04
(VP1)    =   .009970   (VP3(PT))  =  -.000192   (VP5(PT))        =  -.000023   (VP7(PT)) =  -.000004
ANOM MOM =  -.000040   VERTEX(ZA) =  -.000051   VERTEX(ZA**2)    =  -.000006   MUON VP   =   .000001
RECOIL   =   .000014   SCREENING  =   .000039   READ IN NP+VP3.. =  -.000072   TOTAL     =  -.000075
F =2.   DM1 =   .000017   DE2 =  0.000000   TOTAL =  2.130234
F =3.   DM1 =  -.000012   DE2 =  0.000000   TOTAL =  2.130206
CHISQ, PAR =  .37899E+03  6.544743   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000
CHISQ, PAR =  .48897E+03  6.545743   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000
CHISQ, PAR =  .61613E+03  6.546743   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000
CHISQ, PAR =  .80418E+02  6.538848   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000
CHISQ, PAR =  .80418E+02  6.538852   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000
CHISQ, PAR =  .80418E+02  6.538853   .523000  0.000000  1.000000  0.000000 20.000000  0.000000  0.000000

ID=  2 FERMI       RM= 16.281250    DR(RHO)= .031250    RHO(TAIL)=  .984E-08    T= 2.30    R(RMS)= 5.49764

BULK PARAMETERS   RADIUS = 6.638853     DIFFUSENESS =  .523000     WINE BOTTLE = 0.000000     EXPONENT = 1.000
TAIL PARAMETERS   HALF-DISTANCE =0.              ATTACHED AT K =20.000000
MISC. PARAMETERS   PAR(7) =0.              PAR(8) =0.

ALPHA=   .170          K        (R**K)**(1/K)        RK

                     1.1800        2.36320        6.7857
                     1.4400        2.73424        6.8910
                     2.0200        3.33903        6.9798
                     2.4700        3.67903        7.0219
                     2.7800        3.87206        7.0470
                     3.7300        4.33230        7.1164
                      .2000         .06200         .0908
                      .4000         .54192        1.0421
                      .6000        1.12631        2.8601
                      .8000        1.63360        5.1293
                     1.0000        2.05091        6.5361
                     1.2000        2.39480        6.7987
                     1.4000        2.68228        6.8805
                     1.6000        2.92657        6.9241
                     1.8000        3.13737        6.9541
                     2.0000        3.32182        6.9777
                     2.5000        3.69897        7.0245
                     3.0000        3.99386        7.0638
                     3.5000        4.23480        7.1002
                     4.0000        4.43819        7.1351
                     4.5000        4.61425        7.1695
                     5.0000        4.76971        7.2037
                     5.5000        4.90920        7.2379
                     6.0000        5.03607        7.2723
                     6.5000        5.15276        7.3070
                     7.0000        5.26115        7.3422
```

```
CHARGE DENSITY
  0.000   .06304148    .125   .06304143    .250   .06304136    .375   .06304128    .500   .06304117    .625   .06304103
   .750   .06304086    .875   .06304064   1.000   .06304036   1.125   .06304001   1.250   .06303956   1.375   .06303899
 1.500    .06303826   1.625   .06303735   1.750   .06303618   1.875   .06303469   2.000   .06303281   2.125   .06303042
 2.250    .06302738   2.375   .06302352   2.500   .06301863   2.625   .06301241   2.750   .06300451   2.875   .06299448
 3.000    .06298176   3.125   .06296560   3.250   .06294509   3.375   .06291907   3.500   .06288605   3.625   .06284416
 3.750    .06279105   3.875   .06272373   4.000   .06263843   4.125   .06253045   4.250   .06239384   4.375   .06222122
 4.500    .06200335   4.625   .06172886   4.750   .06138374   4.875   .06095097   5.000   .06041007   5.125   .05973682
 5.250    .05890313   5.375   .05787732   5.500   .05662493   5.625   .05511046   5.750   .05330004   5.875   .05116541
 6.000    .04868900   6.125   .04586951   6.250   .04272724   6.375   .03930750   6.500   .03568072   6.625   .03193827
 6.750    .02818402   6.875   .02452312   7.000   .02105058   7.125   .01784199   7.250   .01494837   7.375   .01239534
 7.500    .01018599   7.625   .00830585   7.750   .00672858   7.875   .00542116   8.000   .00434816   8.125   .00347474
 8.250    .00276849   8.375   .00220048   8.500   .00174563   8.625   .00138267   8.750   .00109383   8.875   .00086448
 9.000    .00068269   9.125   .00053880   9.250   .00042503   9.375   .00033515   9.500   .00026420   9.625   .00020822
 9.750    .00016407   9.875   .00012926  10.000   .00010183  10.125   .00008021  10.250   .00006317  10.375   .00004975
10.500    .00003918  10.625   .00003086  10.750   .00002430  10.875   .00001914  11.000   .00001507  11.125   .00001187
11.250    .00000934  11.375   .00000736  11.500   .00000579  11.625   .00000456  11.750   .00000359  11.875   .00000283
12.000    .00000223  12.125   .00000175  12.250   .00000138  12.375   .00000109  12.500   .00000086  12.625   .00000067
12.750    .00000053  12.875   .00000042  13.000   .00000033  13.125   .00000026  13.250   .00000020  13.375   .00000016
13.500    .00000013  13.625   .00000010  13.750   .00000008  13.875   .00000006  14.000   .00000005  14.125   .00000004
14.250    .00000003  14.375   .00000002  14.500   .00000002  14.625   .00000001  14.750   .00000001  14.875   .00000001
15.000    .00000001  15.125   .00000001  15.250   .00000000  15.375   .00000000  15.500   .00000000  15.625   .00000000
15.750    .00000000  15.875   .00000000  16.000   .00000000  16.125   .00000000  16.250   .00000000

VACUUM POLARIZATION ORDER  SECOND, FOURTH =    T    T

ITERATION FOR N L J K =  1.  0.   .5 -1.     MATCHING RADIUS=     6.500     RMAX=    58.625
BE(POINT)=  20.992521     BE(GUESS)=  10.526458     BE(FINAL)=  10.530758
(V) = -15.754416   (V**2) =  .277138E+03   (R**2*V**5) =  -.169699E-03
(T) =  5.223658   (P**2) =  .115948E+04   (RHO)       =   .252070E-01
(VP1)    =   .067705   (VP3(PT))  =  -.000818   (VP5(PT))       =  -.000100   (VP7(PT)) =  -.000018
ANOM MOM =  -.000444   VERTEX(ZA) =  -.003201   VERTEX(ZA**2)    =  -.000153   MUON VP   =   .000246
RECOIL   =   .000380   SCREENING  =   .000005   READ IN NP+VP3.. =  0.000000   TOTAL     =  -.002722
F =0.   DM1 =   .000310   DE2 =  0.000000   TOTAL = 10.528346
F =1.   DM1 =  -.000103   DE2 =  0.000000   TOTAL = 10.527933

ITERATION FOR N L J K =  2.  0.   .5 -1.     MATCHING RADIUS=    19.625     RMAX=    98.000
BE(POINT)=   5.385454     BE(GUESS)=   3.580839     BE(FINAL)=   3.581671
(V) =  -6.318654   (V**2) =  .626931E+02   (R**2*V**5) =  -.289717E-04
(T) =  2.736982   (P**2) =  .608318E+03   (RHO)       =   .435803E-02
(VP1)    =   .019490   (VP3(PT))  =  -.000302   (VP5(PT))       =  -.000037   (VP7(PT)) =  -.000007
ANOM MOM =  -.000072   VERTEX(ZA) =  -.000692   VERTEX(ZA**2)    =  -.000025   MUON VP   =   .000043
RECOIL   =   .000086   SCREENING  =   .000026   READ IN NP+VP3.. =  0.000000   TOTAL     =  -.000563
F =0.   DM1 =   .000050   DE2 =  0.000000   TOTAL =  3.581158
F =1.   DM1 =  -.000017   DE2 =  0.000000   TOTAL =  3.581091

ITERATION FOR N L J K =  2.  1.   .5  1.     MATCHING RADIUS=    14.750     RMAX=    83.000
BE(POINT)=   5.385454     BE(GUESS)=   4.782276     BE(FINAL)=   4.782873
(V) =  -9.298371   (V**2) =  .105711E+03   (R**2*V**5) =  -.591381E-04
(T) =  4.515498   (P**2) =  .993328E+03   (RHO)       =   .451045E-02
(VP1)    =   .032548   (VP3(PT))  =  -.000463   (VP5(PT))       =  -.000056   (VP7(PT)) =  -.000010
ANOM MOM =   .000237   VERTEX(ZA) =  -.000341   VERTEX(ZA**2)    =  -.000064   MUON VP   =   .000044
RECOIL   =   .000109   SCREENING  =   .000013   READ IN NP+VP3.. =  0.000000   TOTAL     =  -.000238
F =0.   DM1 =   .000165   DE2 =  0.000000   TOTAL =  4.782800
F =1.   DM1 =  -.000055   DE2 =  0.000000   TOTAL =  4.782579

ITERATION FOR N L J K =  3.  1.  1.5 -2.     MATCHING RADIUS=    30.375     RMAX=   122.625
BE(POINT)=   2.166544     BE(GUESS)=   2.091912     BE(FINAL)=   2.092057
(V) =  -4.086412   (V**2) =  .289594E+02   (R**2*V**5) =  -.143957E-04
(T) =  1.994355   (P**2) =  .437452E+03   (RHO)       =   .115280E-02
(VP1)    =   .010357   (VP3(PT))  =  -.000182   (VP5(PT))       =  -.000022   (VP7(PT)) =  -.000004
ANOM MOM =  -.000058   VERTEX(ZA) =  -.000223   VERTEX(ZA**2)    =  -.000019   MUON VP   =   .000011
RECOIL   =   .000026   SCREENING  =   .000054   READ IN NP+VP3.. =   .000296   TOTAL     =   .000145
F =1.   DM1 =   .000027   DE2 =  0.000000   TOTAL =  2.092229
F =2.   DM1 =  -.000016   DE2 =  0.000000   TOTAL =  2.092186

ITERATION FOR N L J K =  3.  2.  1.5  2.     MATCHING RADIUS=    29.375     RMAX=   123.125
BE(POINT)=   2.166544     BE(GUESS)=   2.173043     BE(FINAL)=   2.173043
(V) =  -4.459835   (V**2) =  .241880E+02   (R**2*V**5) =  -.759008E-05
(T) =  2.286592   (P**2) =  .492464E+03   (RHO)       =   .110307E-02
(VP1)    =   .010639   (VP3(PT))  =  -.000201   (VP5(PT))       =  -.000025   (VP7(PT)) =  -.000005
ANOM MOM =   .000062   VERTEX(ZA) =   .000044   VERTEX(ZA**2)    =  -.000008   MUON VP   =   .000001
RECOIL   =   .000015   SCREENING  =   .000037   READ IN NP+VP3.. =  -.000059   TOTAL     =   .000031
F =1.   DM1 =   .000029   DE2 =  0.000000   TOTAL =  2.173103
F =2.   DM1 =  -.000017   DE2 =  0.000000   TOTAL =  2.173057

ITERATION FOR N L J K =  3.  2.  2.5 -3.     MATCHING RADIUS=    28.875     RMAX=   122.625
BE(POINT)=   2.121983     BE(GUESS)=   2.130298     BE(FINAL)=   2.130298
(V) =  -4.292069   (V**2) =  .220977E+02   (R**2*V**5) =  -.649883E-05
(T) =  2.161770   (P**2) =  .464922E+03   (RHO)       =   .614348E-04
(VP1)    =   .009970   (VP3(PT))  =  -.000192   (VP5(PT))       =  -.000023   (VP7(PT)) =  -.000004
ANOM MOM =  -.000040   VERTEX(ZA) =  -.000051   VERTEX(ZA**2)    =  -.000006   MUON VP   =   .000001
RECOIL   =   .000014   SCREENING  =   .000039   READ IN NP+VP3.. =  -.000072   TOTAL     =  -.000075
F =2.   DM1 =   .000017   DE2 =  0.000000   TOTAL =  2.130240
F =3.   DM1 =  -.000012   DE2 =  0.000000   TOTAL =  2.130211

RADIAL PARAMETER= 1.122328     A**4LN3= 2.298297     RMO(0)=    .630415E-01

FITTING DATA          CHISQ=   .8042E+02          ISW= 25
TRANSITION     ENERGY     UNCERTAINTY     CALCULATED
 10 -) 8      5.783790      .000440        5.782736
 11 -) 8      5.968890      .000440        5.968123
 13 -) 10     2.642930      .000060        2.643347
 14 -) 11     2.501100      .000060        2.500810
```

N	QN	L	J	BE(TOTAL)	BE(POINT)	VAC POL	DB(NP+VP3.. + STANDARD)	TOTAL CORRECTIONS
1	1.	0.	.5	10.528036	20.992521	F	-.002722	0.000000
2	2.	0.	.5	3.581108	5.385454	F	-.000563	0.000000
3	2.	1.	.5	4.782635	5.385454	F	-.000238	0.000000
4	2.	1.	1.5	4.599936	4.837283	F	-.000555	0.000000
5	3.	1.	1.5	2.081578	2.166544	F	-.000149	0.000000
6	3.	2.	1.5	2.162629	2.166544	F	.000090	0.000000
7	3.	2.	2.5	2.120356	2.121983	F	-.000002	0.000000
8	1.	0.	.5	10.599157	20.992521	T	.000609	.068398
9	2.	0.	.5	3.503099	5.385454	T	-.000103	.019427
10	2.	1.	.5	4.816421	5.385454	T	.000905	.033548
11	2.	1.	1.5	4.631034	4.837283	T	.000467	.030542
12	3.	1.	1.5	2.092202	2.166544	T	.000145	.010476
13	3.	2.	1.5	2.173074	2.166544	T	.000031	.010635
14	3.	2.	2.5	2.130223	2.121983	T	-.000075	.009865

ENERGY DIFFERENCES

	1.0. .5	2.0. .5	2.1. .5	2.1. 1.5	3.1. 1.5	3.2. 1.5	3.2. 2.5	1.0. .5	2.0. .5	2.1. .5	2.1. 1.5	3.1. 1.5
	3.2. 1.5	3.2. 2.5										
1.0. .5	0.000000	6.946928	5.745401	5.928099	8.446458	8.365507	8.407680	0.000000	6.926937	5.711615	5.897002	8.435834
	8.354962	8.397813										
2.0. .5	0.000000	0.000000	0.000000	0.000000	1.499530	1.418579	1.460752	0.000000	0.000000	0.000000	0.000000	1.488906
	1.408034	1.450885										
2.1. .5	0.000000	1.201527	0.000000	.182698	2.701057	2.620106	2.662279	0.000000	1.181536	0.000000	.151601	2.690432
	2.609561	2.652411										
2.1. 1.5	0.000000	1.018828	0.000000	0.000000	2.518359	2.437408	2.479581	0.000000	.998838	0.000000	0.000000	2.507734
	2.426862	2.469713										
3.1. 1.5	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000										
3.2. 1.5	0.000000	0.000000	0.000000	0.000000	.080951	0.000000	.042173	0.000000	0.000000	0.000000	0.000000	.070326
	0.000000	.032305										
3.2. 2.5	0.000000	0.000000	0.000000	0.000000	.038778	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	.028153
	0.000000	0.000000										
1.0. .5	.071121	7.018049	5.816522	5.999220	8.517579	8.436628	8.478801	0.000000	6.998058	5.782736	5.968123	8.506954
	8.426083	8.468933										
2.0. .5	0.000000	.019990	0.000000	0.000000	1.519521	1.438570	1.480743	0.000000	0.000000	0.000000	0.000000	1.508896
	1.428025	1.470875										
2.1. .5	0.000000	1.235313	.033786	.216485	2.734843	2.653892	2.696065	0.000000	1.215323	0.000000	.185388	2.724219
	2.643347	2.686198										
2.1. 1.5	0.000000	1.049925	0.000000	.031097	2.549456	2.468505	2.510678	0.000000	1.029935	0.000000	0.000000	2.538831
	2.457960	2.500810										
3.1. 1.5	0.000000	0.000000	0.000000	0.000000	.010625	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	0.000000	0.000000										
3.2. 1.5	0.000000	0.000000	0.000000	0.000000	.091496	.010545	.052718	0.000000	0.000000	0.000000	0.000000	.080872
	0.000000	.042851										
3.2. 2.5	0.000000	0.000000	0.000000	0.000000	.048646	0.000000	.009867	0.000000	0.000000	0.000000	0.000000	.038021
	0.000000	0.000000										

TRANSITIONS FOR L = 1

NLJ-NLJ	E	ME									
3130101	8.506954	.005316	2130101	5.968123	.026910	2110101	5.782736	.026910	3230211	2.643347	.005316
3250213	2.500810	.005316	3230213	2.457960	.005316	3130201	1.508896	.005316	2010211	1.215323	.026910
2010213	1.029935	.026910	3130323	.080872	.005316	3130325	.038021	.005316			

TRANSITIONS FOR L = 2

NLJ-NLJ	E	ME									
3250101	8.468933	.001479	3230101	8.426083	.001479	3130211	2.724219	.001479	3130213	2.538831	.001479
3250201	1.470875	.001479	3230201	1.428025	.001479	2130211	.185388	.016851	3250323	.042851	.001479

TRANSITIONS FOR L = 3

NLJ-NLJ	E	ME									
3250211	2.686198	.000393	3250213	2.500810	.000393	3230213	2.457960	.000393	3130323	.080872	.000393
3130325	.038021	.000393									

TRANSITIONS FOR L = 4

NLJ-NLJ	E	ME
3250323	.042851	.000103

TEST DATA FOR RURP

```
7780 82.  207.
 0
 1
 2
 3
 4
 5
 6
 1 0 1
 2 0 1
 2 1 1
 2 1 3
 3 1 3
 3 2 3
 3 2 5
  0+ 0.0
  0S
  0V
  1V
  2S
  2V
  3S
  3V
0
1
1
2
3
3
4
4
1234567   12345678  100
0070 82.  207.
  0+ 0.0
  4S
  4V
  5S
  5V
  6S
  6V
0
5
5
6
6
7
7
1234567   1234567   100
```

```
3751 82.  206.9759  6.638853  0.523
00020
-1
 2
 3
 1 0 1 -10.597995   -.001162
 2 0 1  -3.601052   -.000046
 2 1 1  -4.815264   -.001157
 2 1 3  -4.630336   -.000698
 3 1 3  -2.091980   -.000222
 3 2 3  -2.172967   -.000107
 3 2 5  -2.130227    .000004
0.5- 0.0           1 0.5895
2.5- 0.56967       1 0.65
1.5- 0.8976
2.5+ 2.6241
3.5+ 2.6619
2 0.0
2  .2064  2
2  .1575  2          2
3  .7565  2          2          2 -.189
3 -.8735  2          2          2  .077   2 -.222
1234567   12345      013
1234567   12345      113
```

RURP TEST RUN OUTPUT (Run 1)

```
                                        R U R P    AUGUST    1 9 7 8

Z = 82.0   A = 207.0000   MC = 197.32858   AL =  .00729735348   CM = 105.65948   AM = 931.5016   UM = 105.60161   EM =  .5110034

PC+ RMS =  6.645015   .520000  0.000000  1.000000  5.498178

FORM FACTORS
```

	L	PT(1)	PT(2)	PT(3)	PT(4)
1	0	6.645015	.520000	0.000000	1.000000
2	1	6.645015	.520000	0.000000	3.000000
3	2	6.645015	.520000	0.000000	3.000000
4	3	6.645015	.520000	0.000000	3.000000
5	4	6.645015	.520000	0.000000	3.000000
6	5	6.645015	.520000	0.000000	3.000000
7	6	6.645015	.520000	0.000000	3.000000

MUON STATES

	N	L	J	K	E0	DE	EU
1	1.0	0.0	.5	-1.0	-10.529654	0.000000	-10.529654
2	2.0	0.0	.5	-1.0	-3.581407	0.000000	-3.581407
3	2.0	1.0	.5	1.0	-4.782824	0.000000	-4.782824
4	2.0	1.0	1.5	-2.0	-4.600487	0.000000	-4.600487
5	3.0	1.0	1.5	-2.0	-2.081721	0.000000	-2.081721
6	3.0	2.0	1.5	2.0	-2.162441	0.000000	-2.162441
7	3.0	2.0	2.5	-3.0	-2.120360	0.000000	-2.120360

NUCLEAR STATES

	I P	EN	M1	GN	NMF	RNM													
1	0.0+	0.00000	0	0.00000	1	0.00000	1	.21423	1	.18703	2	.74231	3	.87690	3	.74126	4	.90560	4	.76551
2	0.0+	14.04707	0	0.00000	1	.21423	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
3	0.0+	28.09415	0	0.00000	1	.18703	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
4	1.0-	13.34472	0	0.00000	2	-.74231	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
5	2.0+	10.53531	0	0.00000	3	.87690	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
6	2.0+	22.47532	0	0.00000	3	.74126	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
7	3.0-	10.53531	0	0.00000	4	-.90560	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000
8	3.0-	22.47532	0	0.00000	4	-.76551	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000

CONFIGURATION IS	123456700	12345678	100	.1E-05	.1E-05
0.	0.	0.	0.	0.	0.

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 1
													F P = .5+
1	1.0	0.0	.5	-1.0	0.0+	-10.529654	0.000000	-10.529654	-.003669	1	1	12345678	
2	2.0	0.0	.5	-1.0	0.0+	-3.581407	0.000000	-3.581407	-.000696	2	1	12345678	

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 2
													F P = .5-
1	2.0	1.0	.5	1.0	0.0+	-4.782824	0.000000	-4.782824	-.001421	3	1	12345678	

R U R P AUGUST 1 9 7 8

Z = 82.0 A = 207.0000 MC = 197.32858 AL = .00729735348 CM = 105.65948 AM = 931.5016 UM = 105.60161 EM = .5110034

RC+ RMS = 6.645015 .520000 0.000000 1.000000 5.498178

NUCLEAR STATES

	I P	EN	M1	GN	NMF	RNM													
1	0.0+	0.00000	0	0.00000	1	0.00000	5	.85356	5	.72153	6	.75199	6	.63567	7	.62506	7	.52837	
2	4.0+	10.53531	0	0.00000	5	.85356	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	
3	4.0+	22.47532	0	0.00000	5	.72153	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	
4	5.0-	10.53531	0	0.00000	6	-.75199	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	
5	5.0-	22.47532	0	0.00000	6	-.63567	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	
6	6.0+	10.53531	0	0.00000	7	.62506	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	
7	6.0+	22.47532	0	0.00000	7	.52837	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	1	0.00000	

CONFIGURATION IS	123456700	12345670	100	.1E-05	.1E-05
0.	0.	0.	0.	0.	0.

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 1
													F P = .5+
1	1.0	0.0	.5	-1.0	0.0+	-10.529654	0.000000	-10.529654	-.000173	1	1	1234567	
2	2.0	0.0	.5	-1.0	0.0+	-3.581407	0.000000	-3.581407	-.000016	2	1	1234567	

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 2
													F P = .5-
1	2.0	1.0	.5	1.0	0.0+	-4.782824	0.000000	-4.782824	-.000078	3	1	1234567	

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 3
													F P = 1.5+
1	3.0	2.0	1.5	2.0	0.0+	-2.162441	0.000000	-2.162441	-.000004	6	1	1234567	

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 4
													F P = 1.5-
1	2.0	1.0	1.5	-2.0	0.0+	-4.600487	0.000000	-4.600487	-.000070	4	1	1234567	
2	3.0	1.0	1.5	-2.0	0.0+	-2.081721	0.000000	-2.081721	-.000021	5	1	1234567	

	N	L	J	K	I P	EU	EN	ETOT	EP	IM	IN	JN	BLOCK 5
													F P = 2.5+
1	3.0	2.0	2.5	-3.0	0.0+	-2.120360	0.000000	-2.120360	-.000004	7	1	1234567	

RURP TEST RUN OUTPUT (Run 3)

```
                                                  R U R P     AUGUST     1 9 7 8

Z = 82.0    A = 206.9759    HC = 197.32858    AL =  .00729735348    CM = 105.65948    AM = 931.5016    UM = 105.60161    EM =  .5110034

PC, RMS =  6.638853    .523000  0.000000  1.000000  5.497644

VACUUM POLARIZATION INCLUDED

FORM FACTORS                        L   PT(1)       PT(2)       PT(3)       PT(4)
                                 ------------------------------------------------
                               1   -1  6.638853    .523000   0.000000   3.000000
                               2    2  6.638853    .523000   0.000000   3.000000
                               3    3  6.638853    .523000   0.000000   3.000000

MUON STATES                       N     L     J    K        EO              DE             EU
                                 ---------------------------------------------------------------
                            1   1.0   0.0    .5 -1.0   -10.597991      -.001162   -10.599153
                            2   2.0   0.0    .5 -1.0    -3.601054      -.000046    -3.601100
                            3   2.0   1.0    .5  1.0    -4.815262      -.001157    -4.816419
                            4   2.0   1.0   1.5 -2.0    -4.630336      -.000698    -4.631034
                            5   3.0   1.0   1.5 -2.0    -2.091980      -.000222    -2.092202
                            6   3.0   2.0   1.5  2.0    -2.172967      -.000107    -2.173074
                            7   3.0   2.0   2.5 -3.0    -2.130227       .000004    -2.130223

NUCLEAR STATES

       I P    EN        MI   GN        NMF   RNM
      ---------------------------------------------------------------------------------------------
  1    .5-   0.00000  1    .58950  2  0.00000  2    .20640  2  -.15750  3    .75650  3    .87350
  2   2.5-    .56967  1    .65000  2   .20640  2  0.00000  2  0.00000  2  0.00000  2  0.00000
  3   1.5-    .89760  0  0.00000  2    .15750  2  0.00000  2  0.00000  2  0.00000  2  0.00000
  4   2.5+   2.62410  0  0.00000  3    .75650  2  0.00000  2  0.00000  2  -.18900  2  -.07700
  5   3.5+   2.66190  0  0.00000  3   -.87350  2  0.00000  2  0.00000  2    .07700  2  -.22200

                                                  R U R P     AUGUST     1 9 7 8

Z = 82.0    A = 206.9759    HC = 197.32858    AL =  .00729735348    CM = 105.65948    AM = 931.5016    UM =    .53516    EM =  .5110034

        ==========================================================================================
        *     CONFIGURATION IS      123456700     12345000      013          .1E-05       .1E-05     *
        *   0.         0.         0.         0.         0.         0.         0.         0.         0.        *
        ==========================================================================================

        N     L     J     K     I P      EU            EN            ETOT           EP          IM IN    JN            BLOCK   1
       -------------------------------------------------------------------------------------------------------    F P =   0.0+
  1    2.0   1.0    .5  1.0    .5-    -4.816419     0.000000     -4.816419     0.000000     3  1     12345
  2    2.0   1.0   1.5 -2.0   1.5-    -4.631034      .897600     -3.733434     0.000000     4  3     12345
  3    3.0   1.0   1.5 -2.0   1.5-    -2.092202      .897600     -1.194602     0.000000     5  3     12345
  4    3.0   2.0   2.5 -3.0   2.5+    -2.130223     2.624100       .493877     0.000000     7  4     12345

       HAMILTONIAN MATRIX

  1   -4.816586
  2     .006698    -3.733434
  3     .002979     0.000000    -1.194602
  4    -.005624     0.000000     0.000000      .493174

       EIGENVALUES

      -4.816636    -3.733392    -1.194600      .493180

       EIGENVECTORS

  1     .999980      .006184      .000823     -.001059
  2    -.006184      .999981      .000002     -.000002
  3    -.000823     -.000007     1.000000     -.000002
  4     .001059      .000008      .000003      .999999

        N     L     J     K     I P      EU            EN            ETOT           EP          IM IN    JN            BLOCK   2
       -------------------------------------------------------------------------------------------------------    F P =   0.0-
  1    1.0   0.0    .5 -1.0    .5-   -10.599153     0.000000    -10.599153     0.000000     1  1     12345
  2    2.0   0.0    .5 -1.0    .5-    -3.601100     0.000000     -3.601100     0.000000     2  1     12345
  3    3.0   2.0   2.5 -3.0   2.5-    -2.130223      .569670     -1.560553     0.000000     7  2     12345
  4    3.0   2.0   1.5  2.0   1.5-    -2.173074      .897600     -1.275474     0.000000     6  3     12345

       HAMILTONIAN MATRIX

  1  -10.599466
  2    0.000000    -3.601151
  3    -.002616      .000712    -1.560646
  4     .002014     -.000642     0.000000    -1.275474
```

```
      EIGENVALUES

   -10.599467   -3.601151   -1.560645   -1.275474

      EIGENVECTORS

1    1.000000     .000000    -.000289     .000216
2    -.000000    1.000000     .000349    -.000276
3     .000289    -.000349    1.000000    -.000003
4    -.000216     .000276     .000003    1.000000


       N    L    J    K    I P     EU          EN          ETOT        EP        IM IN   JN          BLOCK  13
                                                                                          F P =  6.0+
1    3.0  2.0  2.5 -3.0  3.5+   -2.130223    2.661900     .531677    0.000000   7  5    12345

      HAMILTONIAN MATRIX

1     .531385

      EIGENVALUES

      .531385

      EIGENVECTORS

1    1.000000

FINAL STATE IN CASCADE     E =  -10.599050     F P =  1.0-

      IM IN    N    L    J    K    I P   POPULATION
      ----------------------------------------------
      1  1    1.0  0.0   .5 -1.0   .5-      .747853
      1  3    1.0  0.0   .5 -1.0  1.5-      .000000
      2  1    2.0  0.0   .5 -1.0   .5-      .000000
      2  3    2.0  0.0   .5 -1.0  1.5-      .000000
      6  1    3.0  2.0  1.5  2.0   .5-      .000000
      4  4    2.0  1.0  1.5 -2.0  2.5+      .000000
      6  2    3.0  2.0  1.5  2.0  2.5-      .000000
      7  2    3.0  2.0  2.5 -3.0  2.5-      .000000
      6  3    3.0  2.0  1.5  2.0  1.5-      .000000
      7  3    3.0  2.0  2.5 -3.0  1.5-      .000000
      5  4    3.0  1.0  1.5 -2.0  2.5+      .000000

FINAL STATE IN CASCADE     E =  -10.599467     F P =  0.0-

      IM IN    N    L    J    K    I P   POPULATION
      ----------------------------------------------
      1  1    1.0  0.0   .5 -1.0   .5-      .252142
      2  1    2.0  0.0   .5 -1.0   .5-      .000000
      7  2    3.0  2.0  2.5 -3.0  2.5-      .000000
      6  3    3.0  2.0  1.5  2.0  1.5-      .000000

      LEVEL WIDTHS

BLOCK   1
        .001147    0.000000    0.000000    0.000000
BLOCK   2
       0.000000     .000073    0.000000    0.000000
BLOCK   3
        .001147     .001334     .001335     .001147     .001335     .000327    0.000000    0.000000    0.000000    0.000000

       0.000000
BLOCK   4
       0.000000     .000000     .000073    0.000000     .000417     .001333    0.000000    0.000000    0.000000    0.000000

       0.000000
BLOCK   5
        .000000     .001334     .001147     .001335    0.000000    0.000000     .000327    0.000000    0.000000    0.000000

       0.000000    0.000000    0.000000    0.000000
BLOCK   6
        .000000     .000000    0.000000    0.000000     .001145     .000417     .000403     .001334     .001333    0.000000

       0.000000    0.000000    0.000000    0.000000    0.000000
BLOCK   7
        .000000     .000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000

       0.000000    0.000000    0.000000
BLOCK   8
        .000000    0.000000     .001147     .001134     .000414     .001336     .001335    0.000000    0.000000    0.000000

       0.000000    0.000000    0.000000
BLOCK   9
        .000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
BLOCK  10
       0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
BLOCK  11
       0.000000    0.000000    0.000000
BLOCK  12
       0.000000    0.000000    0.000000
BLOCK  13
       0.000000
```

EXTERNAL PHOTONS	ENERGY	INTENSITY	N B S B S
36	.037647	.000004	105070805
38	.037903	.000002	103060607
57	.080973	.000004	105070606
58	.080999	.000002	103060405
156	.568762	.000016	106010401
157	.569179	.000025	106010201
164	.570141	.000091	108010401
171	.646033	.000002	104030503
192	.897497	.000019	206020401
196	.897914	.000008	106020201
211	1.030008	.035976	104030502
212	1.030046	.014396	102020302
213	1.030114	.007200	104030302
219	1.215283	.010759	102020301
220	1.215351	.021514	104030301
221	1.215552	.010763	104030101
225	1.427857	.000063	104050403
226	1.427925	.000063	106060403
227	1.427993	.000042	106060202
229	1.470953	.000052	106070403
230	1.471021	.000078	106070202
231	1.471252	.000172	108050403
232	1.508855	.012516	103060403
233	1.508899	.062589	105070403
234	1.508923	.025035	103060202
257	1.603277	.000002	106070305
303	1.788659	.000005	106070304
324	1.888442	.000002	106060504
326	1.888583	.000004	106060303
342	1.931611	.000002	106070303
343	1.931759	.000010	108050504
377	2.073958	.000002	106060503
392	2.116987	.000002	106070503
393	2.117285	.000030	108050503
412	2.457865	.002520	104050502
413	2.457933	.022697	106060502
414	2.457971	.012604	104050302
415	2.458039	.002526	106060302
416	2.476061	.000024	108040502
418	2.500962	.016811	106070502
419	2.501067	.151357	106070302
420	2.501260	.222937	108050502
422	2.538864	.000074	103060502
423	2.538907	.000172	105070502
424	2.538969	.000074	103060302
425	2.539012	.000074	105070302
429	2.623997	.002287	205010401
432	2.624414	.000490	107010201
437	2.643208	.029086	104050301
438	2.643276	.145600	106060301
439	2.643409	.058190	104050101
444	2.661797	.013368	209010401
445	2.662214	.003178	107020201
448	2.686304	.000002	106070301
449	2.686603	.000001	108050301
451	2.724207	.000167	103060301
452	2.724249	.000167	105070301
453	2.724450	.000111	105070101
483	4.884919	.000002	101010402
484	4.885119	.000001	203010402
485	5.070355	.000008	203020602
486	5.070461	.000001	205020602
489	5.213853	.000013	103010601
491	5.397817	.000053	105020801
492	5.399091	.000002	103020601
500	5.764095	.000233	206060702
501	5.781792	.000028	105030801
502	5.782223	.004225	208040901
503	5.782414	.069063	101010401
504	5.782479	.000500	206050701
505	5.782615	.138168	103010401
506	5.782698	.000013	208030501
507	5.782764	.000005	203040602
508	5.783032	.069112	103010201
509	5.783171	.000008	105030601
510	5.801827	.000238	204050501
511	5.801895	.000034	206060501
512	5.807123	.000019	206070702
513	5.807421	.011912	208050901
515	5.844923	.001724	206070501
518	5.845221	.000081	208050501
524	5.964767	.000080	204060501
525	5.965174	.000086	206090702
527	5.967308	.000003	105040801
528	5.967853	.062742	103020401
529	5.967958	.301156	105020401
530	5.968145	.000003	203050402
531	5.968270	.125478	103020201
532	5.968546	.000006	103030601
533	5.968687	.000010	105040601
534	5.968713	.000095	206080501
535	5.969278	.000071	208070702
536	5.970885	.000011	208060701
564	7.609325	.000005	203060802
586	7.936723	.000007	105070801
602	8.425824	.004364	104050401
603	8.425891	.004367	106060401
604	8.426308	.002914	106060201
605	8.444019	.000001	108040401
606	8.468920	.003171	106070401
607	8.469219	.010513	108050401
608	8.469337	.004759	106070201
609	8.506822	.023087	103060401
610	8.506864	.115440	105070401
611	8.507239	.046179	103060201

R U R P AUGUST 1 9 7 8

Z = 82.0 A = 206.9759 HC = 197.32858 AL = .00729735348 CM = 105.65948 AM = 931.5016 UM = .53516 EM = .5110034

```
*****************************************************************************
*     CONFIGURATION IS     123456700     12345000     113        .1E-05      .1E-05     *
*  0.          0.          0.          0.          0.          0.          0.          0.          0.          *
*****************************************************************************
```

	N	L	J	K	I P	EU	EN	ETOT	ER	IM	IN	JN
1	2.0	1.0	.5	1.0	.5-	-4.816419	0.000000	-4.816419	-.000122	3	1	12345
2	2.0	1.0	1.5	-2.0	1.5-	-4.631034	.897600	-3.733434	-.000012	4	3	12345
3	3.0	1.0	1.5	-2.0	1.5-	-2.092202	.897600	-1.194602	-.000079	5	3	12345
4	3.0	2.0	2.5	-3.0	2.5+	-2.130223	2.624100	.493877	-.000105	7	4	12345

BLOCK 1
F P = 0.0+

HAMILTONIAN MATRIX

1	-4.816586			
2	.006698	-3.733434		
3	.002979	0.000000	-1.194602	
4	-.005624	0.000000	0.000000	.493174

PERTURBATION MATRIX

1	-.000122			
2	0.000000	-.000012		
3	0.000000	-.000133	-.000079	
4	-.000008	.000165	.000099	-.000105

EIGENVALUES

-4.816758 -3.733404 -1.194679 .493075

EIGENVECTORS

1	.999980	.006183	.000823	-.001061
2	-.006183	.999981	-.000050	.000037
3	-.000823	.000045	1.000000	.000056
4	.001061	-.000031	-.000056	.999999

```
        N    L    J    K    I P     EU          EN          ETOT        EP        IM IN   JN          BLOCK  12
                                                                                                      F P =  5.0-
1     2.0  1.0  1.5 -2.0  3.5+   -4.631034    2.661900   -1.969134   -.000015   4  5    12345
2     3.0  2.0  2.5 -3.0  2.5-   -2.130223     .569670   -1.560553   -.000000   7  2    12345
3     3.0  1.0  1.5 -2.0  3.5+   -2.092202    2.661900    .569698    -.000005   5  5    12345

      HAMILTONIAN MATRIX

1   -1.970576
2    0.000000   -1.560487
3   -.000645     0.000000     .569312

      PERTURBATION MATRIX

1   -.000015
2    .000001    -.000000
3   -.000009     .000001    -.000005

      EIGENVALUES

     -1.970591   -1.560487     .569308

      EIGENVECTORS

1    1.000000     .000003    -.000257
2   -.000003     1.000000     .000000
3    .000257    -.000000     1.000000

        N    L    J    K    I P     EU          EN          ETOT        EP        IM IN   JN          BLOCK  13
                                                                                                      F P =  6.0+
1     3.0  2.0  2.5 -3.0  3.5+   -2.130223    2.661900    .531677    -.000001   7  5    12345

      HAMILTONIAN MATRIX

1     .531385

      PERTURBATION MATRIX

1    -.000001

      EIGENVALUES

      .531384

      EIGENVECTORS

1    1.000000

FINAL STATE IN CASCADE      E =  -10.599278     F P =  1.0-

      IM IN    N    L    J    K    I P   POPULATION
      1  1    1.0  0.0   .5 -1.0   .5-      .747865
      1  3    1.0  0.0   .5 -1.0  1.5-      .000000
      2  1    2.0  0.0   .5 -1.0   .5-      .000000
      2  3    2.0  0.0   .5 -1.0  1.5-      .000000
      6  1    3.0  2.0  1.5  2.0   .5-      .000000
      4  4    2.0  1.0  1.5 -2.0  2.5+      .000000
      6  2    3.0  2.0  1.5  2.0  2.5-      .000000
      7  2    3.0  2.0  2.5 -3.0  2.5-      .000000
      6  3    3.0  2.0  1.5  2.0  1.5-      .000000
      7  3    3.0  2.0  2.5 -3.0  1.5-      .000000
      5  4    3.0  1.0  1.5 -2.0  2.5+      .000000

FINAL STATE IN CASCADE      E =  -10.599695     F P =  0.0-

      IM IN    N    L    J    K    I P   POPULATION
      1  1    1.0  0.0   .5 -1.0   .5-      .252130
      2  1    2.0  0.0   .5 -1.0   .5-      .000000
      7  2    3.0  2.0  2.5 -3.0  2.5-      .000000
      6  3    3.0  2.0  1.5  2.0  1.5-      .000000

      LEVEL WIDTHS

BLOCK  1
       .001147    0.000000    0.000000    0.000000
BLOCK  2
      0.000000     .000073    0.000000    0.000000
BLOCK  3
       .001147     .001335     .001335     .001147     .001335     .000327    0.000000    0.000000    0.000000    0.000000
      0.000000
BLOCK  4
      0.000000     .000000     .000073    0.000000     .000417     .001333    0.000000    0.000000    0.000000    0.000000
      0.000000
BLOCK  5
       .000000     .001334     .001147     .001335    0.000000    0.000000     .000327    0.000000    0.000000    0.000000
      0.000000    0.000000    0.000000    0.000000
BLOCK  6
       .000000     .000000    0.000000    0.000000     .001145     .000417     .000403     .001334     .001333    0.000000
      0.000000    0.000000    0.000000    0.000000    0.000000
```

```
BLOCK   7
        .000000     .000000     0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
BLOCK   8
        .000000     0.000000    .001147     .001134     .000414     .001336     .001335     0.000000    0.000000    0.000000
        0.000000    0.000000    0.000000
BLOCK   9
        .000000     0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
BLOCK   10
        0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
BLOCK   11
        0.000000    0.000000    0.000000
BLOCK   12
        0.000000    0.000000    0.000000
BLOCK   13
        0.000000
```

EXTERNAL PHOTONS	ENERGY	INTENSITY	N B S B S
36	.037460	.000004	105070805
41	.037850	.000002	103060607
60	.080938	.000004	105070606
61	.080965	.000002	103060405
159	.568984	.000016	106010401
160	.569401	.000025	106010201
167	.570362	.000091	108010401
174	.646014	.000002	104030503
195	.897719	.000019	206020401
199	.898135	.000008	106020201
214	1.030098	.035976	104030502
215	1.030136	.014396	102020302
216	1.030203	.007200	104030302
222	1.215383	.010759	102020301
223	1.215450	.021515	104030301
224	1.215651	.010764	104030101
228	1.427874	.000063	104050403
229	1.427942	.000063	106060403
230	1.428009	.000042	106060202
232	1.470989	.000052	106070403
233	1.471057	.000078	106070202
234	1.471420	.000173	108050403
235	1.508840	.012516	103060403
236	1.508880	.062590	105070403
237	1.508907	.025036	103060202
260	1.603296	.000002	106070305
309	1.788676	.000005	106070304
330	1.888439	.000002	106060504
332	1.888587	.000004	106060303
347	1.931635	.000002	106070303
349	1.931918	.000010	108050504
385	2.073955	.000002	106060503
402	2.117003	.000002	106070503
403	2.117434	.000030	108050503
422	2.457972	.002519	104050502
423	2.458039	.022694	106060502
424	2.458078	.012602	104050302
425	2.458145	.002526	106060302
426	2.476245	.000024	108040502
428	2.501087	.016811	106070502
429	2.501193	.151359	106070302
430	2.501518	.223011	108050502
432	2.538937	.000074	103060502
433	2.538978	.000172	105070502
434	2.539043	.000074	103060302
435	2.539083	.000074	105070302
439	2.624182	.000652	107010401
441	2.624190	.001634	105010401
443	2.624599	.000490	107010201
448	2.643324	.029086	104050301
449	2.643392	.145603	106060301
450	2.643525	.058191	104050101
455	2.661982	.010934	109010401
456	2.661990	.002371	107020401
457	2.662407	.003165	107020201
460	2.686440	.000002	106070301
461	2.686870	.000001	108050301
463	2.724290	.000167	103060301
464	2.724330	.000167	105070301
465	2.724531	.000111	105070101
508	4.884801	.000002	101010402
509	4.885002	.000001	203010402
510	5.070250	.000008	203020602
511	5.070355	.000001	205020602
514	5.213737	.000013	103010601
516	5.397712	.000053	105020801
517	5.398984	.000002	103020601
528	5.764123	.000233	106060702
530	5.781795	.000028	105030801
531	5.782328	.000971	108040702
532	5.782335	.003233	108040901
533	5.782484	.000102	106050501
534	5.782492	.000397	106050701
535	5.782520	.069065	101010401
536	5.782717	.000007	108030501
537	5.782721	.138172	103010401
538	5.782725	.000005	108030701
539	5.782767	.000005	203040602
540	5.783138	.069114	103010201
541	5.783174	.000008	105030601
542	5.801855	.000238	104050501
544	5.801923	.000034	106060501
546	5.807171	.000019	106070702
548	5.807601	.004173	108050702
549	5.807609	.007684	108050901
552	5.844971	.001013	106070501
553	5.844979	.000710	106070701
557	5.845401	.000080	108050501
558	5.845409	.000002	108050701
569	5.964729	.000080	104060501
571	5.965135	.000086	106090702
574	5.967312	.000003	105040801
575	5.967958	.062742	103020401
576	5.968074	.301226	105020401
577	5.968146	.000003	203050402
578	5.968385	.125478	103020201
579	5.968543	.000006	103030601
580	5.968690	.000010	105040601
581	5.968715	.000076	106080501
582	5.968723	.000020	106080701
583	5.969281	.000054	108070702
584	5.969290	.000017	108070901
585	5.970912	.000005	108060501
586	5.970920	.000006	108060701
616	7.609293	.000005	203060602
638	7.936690	.000007	105070801
654	8.426045	.004363	104050401
655	8.426113	.004367	106060401
656	8.426530	.002913	106060201
657	8.444318	.000001	108040401
658	8.469161	.003171	106070401
659	8.469578	.004758	106070201
660	8.469591	.010515	108050401
661	8.507011	.023087	103060401
662	8.507051	.115439	105070401
663	8.507428	.046179	103060201