GRASP^0 manual

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January 24, 2002

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Contents

1 Introduction **1**

2 I/O files **3**

3 Input data **4**

3.1 CARDIN routine 4

3.2 Summary of input 5

3.3 Description of input variables 7

3.4 Detailed description of input 9

4 File description **21**

4.1 MCT dump 21

4.2 MCP dump 21

4.3 MCDF dump 23

4.4 BENA dump 26

5 References **27**

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1 Introduction

GRASP is an acronym for the General-purpose Relativistic Atomic Structure Package developed by Ian Grant and co-workers at Oxford University.

Three versions of the package have been published in Computer Physics Communications.

1. **Version 0**

   This was published in 1980 (Grant et al (1980), McKenzie et al (1980)). The package was divided into two parts, known as MCDF and BENA. These parts could be easily merged. A major omission from Version 0 was a section to calculate transition probabilities.

2. **Version 1**

   This was published in 1989 (Dyall et al (1989)). Features added to Version 0 include a section to calculate transition probabilities, transformation of the configuration basis from jj to LS-coupling, preprocessing for dimensions and improved handling of angular coefficients.

3. **Version 2/92**

   One of the major drawbacks with the first two versions of GRASP was the failure in many problems to achieve convergence with the SCF equations. The algorithm was not robust. Generally ground-states can be obtained with little difficulty but higher-lying states cause problems. A substantial rewrite of the program was undertaken by Farid Parpia. In particular he adapted many of the algorithms used by Charlotte Fischer in her non-relativistic program HF86 (Fischer (1987)). Version 2 of GRASP has not been published. A related version GRASP92 has been published (Parpia et al (1996)).

Module GRASP^0

This is a version of GRASP developed at Queen's University, Belfast. It is based on Version 0 and contains many of the improvements made in Version 1. However it is not the same as Version 1.

In outline the program is organised as follows.

```
GRASP  AA     CALEN    access date/time at execution
              QUARTZ   timing routine
              DIMSET   set dimensions

              DATAIN   read input data

              MCP      calculate angular integrals
              MCDF     generate orbitals using SCF process
              BENA     add Breit and QED corrections
              OSCL     calculate oscillator strengths

              DIMPRT   final print of dimensions used
```

The major sections of the code are DATAIN, MCP (including MCT and MCBP), MCDF, BENA and OSCL.

Bug

A bug in routine SKINT has been corrected in the latest versions of GRASP (2/92 and GRASP^0). This involved a sign change near the end of the routine. It affects the calculation of full transverse Breit radial integrals. In the low frequency limit the bug does not affect the results. Most results are not greatly affected by this bug.

Module ANGUL

This is a stripped down version of GRASP^0 that only calculates the angular integrals.

NJGRAF/NJSYM package

The angular integrals require the calculation of recoupling coefficients. This is done using either the NJGRAF program of Bar-Shalom & Klapisch (1988) or the NJSYM program of Burke (Scott & Hibbert 1982). The current version of NJGRAF is taken from GRASP92 (Parpia et al 1996).

Slater-type orbitals

Routine INIT has been revised so that Slater-type orbitals (STOs) can be read. This is based on code by Stephen Bailey. Two new routines are STWAVE and STWOPT. Routine STWAVE reads the input from stream IREAD in a format similar to the CIV3 program. This input data is attached to the end of the input file GRASP.INP. A small component is calculated for the orbital and the wavefunction is renormalised. Orthogonality is checked in INIT by a call to PROPG. The routine STWOPT attempts to improve the STO by iterating using the Thomas-Fermi potential.

2 I/O files

These are defined internally. Messages are also written to output stream 6 using the PRINT command.

Whether a particular file is opened can depend on the value of the I/O flag. The I/O flag is an integer variable which may be read as part of the input data. If the input value is greater than 0 then the file is opened.

IREAD, IWRITE and IPUNCH are set internally and the corresponding files are always opened.

In MCDF files IR1 and IP2 are always opened.

In BENA files IO4, IO5 and IO6 are always opened. In OSCL files IO7 and IO8 are always opened.

By default files IO1, IO2 and IO3 are open (flags are 1) while files IR1, IR3 and IP3 are closed (flags are 0).

```
filename         #                                   I/O flag  section
--------         -                                   --------  -------

GRASP.INP  (f)   5 : input data                      IREAD
GRASP.OUT  (f)   7 : output                          IWRITE
GRASP.PUN  (f)   8 : output (summary)                IPUNCH

           (f)   9 : scratch file used for input

GRASP.SH   (f)  29 : orbital output

MCP.DAT    (u)  21 : MCP/MCBP angular coefficients   IO1 >0     MCP
                                                     IO3 >0     MCBP
                                                     IR1        MCDF
                                                     IO4        BENA

MCT.DAT    (u)  22 : MCT angular coefficients        IO2 >0     MCT
                                                     IO7        OSCL

MCDF.DMP   (u)  24 : previous MCDF dump              IR2 >0     MCDF
MCDF.DAT   (u)  25 : present MCDF dump               IP2        MCDF
                                                     IO5        BENA

ORBIN.DAT  (u)  26 : previous orbitals file          IR3 >0     MCDF
ORBOUT.DAT (u)  27 : present orbitals file           IP3 >0     MCDF

BENA.DAT   (u)  30 : present BENA dump               IO6        BENA
                                                     IO8        OSCL
```

```
f = formatted and u = unformatted
```

3 Input data

3.1 CARDIN routine

This routine reads an input record or input records using free format.

NOTE that only the first 72 characters on the input record are read.

The following characters are recognised:
0 1 2 3 4 5 6 7 8 9 - . / * ! + : C c E e D d and BLANK

BLANK is used to separate numbers. BLANKs cannot occur within a number.

'C' or 'c' can be used to continue an input record, another input record will be read by CARDIN. A number cannot be split across two input records. All characters following 'C' or 'c' are ignored.

'/' can be used to input fractions with numerator or denominator being real or integer.

'E' or 'e' or 'D' or 'd' denotes exponent which must be an integer between -99 and 99.

'*' is used to indicate a repeated value as in FORTRAN data statements.

':' specifies a range of numbers.

'!' marks the end of the input record and allows comments to be written.

Some checks on consistency are in the code. An error message will be output if the routine fails.

The following are examples of numbers that can be read by CARDIN:

.123 , -.123 , -3.23 , 4.5E6 , 12 , 2E-6 , 2/6 , 2.1/6 , -2./6E-2

3.2 Summary of input

The following is a summary of the input data. A detailed description of the variables is given later. The parameters enclosed in square brackets are optional and if they are not specified then the default values described later are used. The significance of the nested brackets is that for example on input record 11 if you wish to specify CON then it is necessary to give values for H, RNT and ACCY. The optional input records are shown with an asterisk.

Labels are used throughout the input data. In the summary below these labels are enclosed in single quotes and blanks are significant. In the orbital data NH is a 2-character label giving the angular character of the orbital. All other labels are in columns 1 to 4 and are 4-character labels.

Within each section of the code various facilities (e.g. debug printouts) are made available by the use of options. The code can be run in a default mode by not specifying any options.

Input records 1 to 5 and input record 26 (marking the end of the data block) are always required in a block of data. It is possible to have more than one data block e.g. consecutive calculations can be made for H and Hg if required.

The orbital data is defined by non-relativistic configuration state functions (CSFs).

```
  1. IHED                                  - 80-character title
  2. NMAN NWM [IOP [ATW [NCPRIN [CUTOFF ]]]]

     Read NWM input records                - orbital data,

  3. NPX(J) NHX(J) (IQX(J,I),I=1,NMAN)     - repeat for J=1,NWM

  4. 'ANG ' options
  5. 1 or 3 or NMAN numbers

  6. 'MCP ' [IO1 [IEXC]]                   - call MCP, I/O flag

  7. 'MCT ' KA [IOPAR [IO2 ]]              - call MCT, tensor rank,
                                             parity, I/O flag

  8. 'MCBP' [IO3]                          - call MCBP, I/O flag

  9. 'MCDF' options                        - call MCDF
 10. [IR2 [IR3 [IP3 ]]]                    - I/O flags
 11. Z [H [RNT [ACCY [CON [XCAX ]]]]]      - basic data
*12. 'VNUC' NUCTYP [(PARM(I),I=1,NPARM) ] - nuclear potential
*13. 'FIX ' (JFIX(I),I=1,NN)               - fixed orbitals
*14. 'LOAD' (ILO(I),I=1,NW)                - load orbitals
*15. 'ORB ' (IWO(I),I=1,NWO)               - write orbitals
*16. 'SCR ' (SCR(I),I=1,NW)                - orbital screening
*17. 'VPOL' NPOTYP,POLPAR(1),POLPAR(2)     - polarization potential
*18. 'VMOD' NMOTYP, NBPAR, NCBAR,ABAR,     - model potential
     (BPAR(I),I=1,NBPAR),(BBPAR(I),I=1,NBPAR),
     (CPAR(I),I=1,NCPAR),(CCPAR(I),I=1,NCPAR)
 19.  label (other parameters)             -calculation type
                        ... 5 possibilities
                        a  'AL  ' average level
                        b  'EAL ' extended average level
                        c  'OL  ' optimal level
                        d  'EOL ' extended optimal level
                        e  'CI  ' configuration interaction
     'AL  '  [NITIT ]
     'EAL '  CSF weights [NITIT ]
     'OL  '  level [NITIT [CHECK ]]
     'EOL '  number of levels, level numbers [NITIT [CHECK ]]
```

```
     'CI  '

 20. 'BENA' options                        - call BENA
 21.  [WFACT]                              - frequency factor

 22. 'OSCL' options                        - call OSCL
 23.  [LEVELS(I),I=1,NLEV]                 - levels to be included
*24.  [ENLEV(I),I=1,NLEV]                  - if option 17 is set,
                                             level energies
*25.  [GAUGE1, GAUGE2]                     - if option 19 is set,
                                             gauge parameters

 26. 'STOP'                                - no further data
     'END '                                - further data may be
                                             available
```

The input records with labels VPOL and VMOD have not been implemented yet.

Slater-type orbital (STO) input data:

For each orbital J read the following in free-format.

```
A. E(J)
B. M
C. (IRAD(K),K=1,M)
D. (ZE(K),K=1,M)
E. (S(K),K=1,M)
```

The eigenvalue E will be estimated by routine EIGENV if it is zero on input.

3.3 Description of input variables

IHED is the 80-character title

NMAN is the number of non-relativistic CSFs in the input data. NCF is set to the number of relativistic CSFs which are generated.

NWM is the number of non-relativistic orbitals in the input data. NW is set to the number of relativistic orbitals which are generated.

IOP is the data mode.

ATW is the atomic mass. This is used to define units i.e. it modifies the Rydberg. Also it is used to define the nuclear potential for the uniform nucleus case.

NCPRIN is the number of levels output. This reduces the number of eigenvectors and levels printed in routines PROP and SUMMRY. It is useful in large CI calculations.

CUTOFF is the wavefunction cutoff. The wavefunctions are chopped when they become less than CUTOFF in the asymptotic region i.e. far from the nucleus. The default for CUTOFF is 10^{-10} .

NPX(J) is the principal quantum number for non-relativistic orbital J. Array NP is for the generated relativistic orbitals.

NHX(J) is the label which characterises the angular behaviour of non-relativistic orbital J. It is a 2-character label like 'S ' or 'P '. Array NH is for the generated relativistic orbitals.

IQX(J,I) is the occupation number of non-relativistic orbital J in CSF I. Array IQ is for the generated relativistic orbitals.

IO1 is the I/O flag for MCP (Coulomb angular) coefficients. Default is 1, open.

IEXC

KA is the rank of the tensor operator.

IOPAR is the parity of the tensor operator. IOPAR=1 for even parity (M1,E2 transitions), IOPAR=-1 for odd parity (E1,M2 transitions). The default setting is IOPAR=0 which gives both even and odd parity.

IO2 is the I/O flag for MCT (1-electron angular) coefficients. Default is 1, open.

IO3 is the I/O flag for MCBP (Breit angular) coefficients. Default is 1, open.

IR2 is the I/O flag for a previous MCDF dump. Default is 0, closed.

IR3 is the I/O flag for a previous orbitals dump. Default is 0, closed.

IP3 is the I/O flag for the present orbitals dump. Default is 0, closed.

Z is the atomic number.

H is the step-size for radial mesh (default 0.05).

RNT is the first point in radial mesh (default 10^{-5}).

ACCY is the accuracy (default 10^{-8}).

CON is the factor multiplying the speed of light (default 1). To obtain the non-relativistic limit set CON to be 10^4 . This can be done by setting MCDF option 25.

XCAX is the factor multiplying the exchange potentials (default 1).

NUCTYP

PARM(I)

NPARM

JFIX(I)

ILO(I)

IWO(I)

SCR(I)

NPOTYP

POLPAR(1)

POLPAR(2)

NMOTYP

NBPAR

NCBAR

ABAR

BPAR(I)

BBPAR(I)

CPAR(I)

CCPAR(I)

NITIT

CHECK

WFACT is the factor multiplying the photon frequency. To obtain the low frequency limit use 10^{-3} . This is equivalent to multiplying the speed of light by 10^3 within the matrix elements, thus taking a non-relativistic limit there.

NLEV is the number of levels to be used in the OSCL section. Only transitions between these levels are considered. NLEV is set by the number of integers given on input record 23. If no integers are given then NLEV is set to NCF which is the maximum number of levels available. The integers are the level numbers with 1 being the ground-state, 2 being the first excited state etc.

LEVELS(I)

ENLEV(I)

GAUGE1

GAUGE2

3.4 Detailed description of input

Input record 1 — IHED — title for the calculation

Read an 80-character title for the problem. The title is stored in common block /TITL/. This READ statement uses an END parameter to find the end of data.

The following data defines the configuration state functions (CSFs) that are used to construct the atomic state functions (ASFs). Non-relativistic CSFs are defined and relativistic CSFs are then generated from these. This method is straightforward and requires no knowledge of the internal coupling of the CSFs or seniority.

Routine DATNR reads input record input defining non-relativistic CSFs and uses it to generate all possible relativistic CSFs which produce the required total J-value. NMAN is the number of non-relativistic CSFs and NWM is the number of non-relativistic orbitals. Having defined the non-relativistic CSFs a set of relativistic CSFs is generated from them (by calls to routine MAN4 which in turn calls COUP) and the program prints out the equivalent relativistic input data (from routine MANOUT). This is input data that could be read by other versions of GRASP. The relativistic CSFs can be printed by a call to CFOUT. A restriction on this type of input data is that there can be no more than four open shells in any non-relativistic CSF.

Input record 2

Format: between 2 and 6 numbers
Variables: NMAN, NWM, [IOP, [ATW, [NCPRIN, [CUTOFF]]]]

NMAN — number of non-relativistic CSFs

NWM — number of non-relativistic orbitals

IOP — orbital data mode

- =0 gives the minimal print and LS-jj transformation coefficients are not calculated. (This is the default if IOP is not given i.e. only 2 numbers on the input record)
- =1 calculate the LS-jj transformation coefficients and print the final energy levels using their non-relativistic assignments. MCDF option 30 is set internally.
- =2 as for 1 plus a print of the non-relativistic CSFs
- =3 as for 2 plus a print of the LS-jj transformation and the transformed final eigenvectors. MCDF option 31 is set internally.

ATW — atomic weight of atom to be used to obtain corrections to the Rydberg. If no number or zero is given then an infinite atomic mass is assumed.

NCPRIN — number of levels output. This reduces the number of eigenvectors and levels printed in e.g. PROP and SUMMRY and is useful in large CI calculations.

CUTOFF — wavefunction cutoff. The wavefunctions are chopped when they become less than CUTOFF in the asymptotic region i.e. far from the nucleus. The default for CUTOFF is 1E-10.

Input record 3 — orbital data

Read NWM input records

Format: I2, A2, followed by 0 or 1 or NMAN integers
Variables: NPX(J), NHX(J), (IQX(J,I),I=1,NMAN)

Read NWM input records, one input record for each orbital J, containing the following data:

Label (1S , 2S, 2P , ...); with format I2,A2.

For orbital J, NPX(J) is the principal quantum number and NHX(J) is a 2-character label indicating the kappa-value (S,P,D, etc). The kappa-value corresponding to the label is determined in routine CARDIN.

Note that these are unbarred orbital labels which correspond to j=l+1/2. The letter is the usual spectroscopic notation with S,P,D corresponding to l=0,1,2. The blank in the label of unbarred orbitals is significant. Relativistic orbitals can be barred with a minus following the letter. This corresponds to j=l-1/2. For example the relativistic orbital P- corresponds to l=1, s=1/2 and j=1/2.

Relativistic orbitals are generated from the non-relativistic orbitals. The following arrays refer to the relativistic orbitals. The array NP (principal quantum number) is stored in common block /ORB04/ while NH (orbital label) is in /ORB00/. Associated arrays for orbital J are NAK(J),NKL(J),NKJ(J) which contain the kappa, l and 2j values respectively. Array NAK is stored in /ORB04/ while NKL and NKJ are in /ORB05/.

Orbital occupation numbers for each CSF:

- 0 numbers — subshell is full in each CSF
- 1 number — each CSF has this occupation number
- NMAN numbers — occupation number for each CSF

The generated relativistic orbital occupation numbers are stored in array IQ where IQ(J,I) is the occupation number of orbital J in CSF I. IQ is stored in common block /ORB04/.

The program cannot handle the case of relativistic orbitals with j > 7/2 and occupation number 2 < Q < 2j-1. To handle such a case would require an extension to the tables of fractional parentage coefficients.

Input record 4 — options for the angular momentum calculation

Format: Label 'ANG ' followed by up to 10 options

The label is 'ANG '. This label is followed by up to 10 options. These apply to the sections MCP, MCT and MCBP. Note that no check is made on the label 'ANG ' and therefore any 4-character label can be used.

1 write out the angular coefficients calculated

2 output from RKCO,COR,MUMDAD,VIJOUT (in MCP and MCBP)

3 output from NJSYM or NJGRAF

4 output from VIJOUT (in MCT)

5 output from TMSOUT

6 output from TNSRJJ (in MCT)

7 suppress call to CFOUT. This routine writes out the relativistic CSFs in an easily read form. When there are a large number of CSFs the printing is excessive. This option can then be used when a number of calculations are made on the same problem.

8 suppress calls to all angular momentum packages i.e. MCP, MCT and MCBP.

9 when this option is set there is no rewind of the output files written by MCP, MCT and MCBP.

10 The relativistic CSF input data is only written out if this option is set.

Input record 5 — non-relativistic CSF total J values

Read 1 input record containing 1 or 3 or NMAN numbers.

This input record specifies the total J-values of the non-relativistic CSFs as defined above.

- one non-negative number —
  only CSFs with this J-value are included.
- one negative number —
  = -1 all possible CSFs are to be generated i.e. all possible J-values.
  = -2 this input record is followed by NMAN input records, one for each non-relativistic CSF, which contain 2 numbers, JMIN and JMAX. These specify limits for the allowed J-values for the particular CSF i.e. only J-values satisfying JMIN < =J < =JMAX are included.
- 3 numbers with the first < 0 —
  the second and third numbers are JMIN and JMAX. These specify limits for the allowed J-values for all the CSFs i.e. only J-values satisfying JMIN < =J < =JMAX are included.
- NMAN numbers —
  these are the J-values of the CSFs in the order described above.

Input record 6 — calculate MCP coefficients

Format: Label 'MCP ' followed by 0 to 2 integers
Variables: [IO1, [IEXC]]

When this 4-character label is encountered in the input data a call is made to the MCP section of the program. This evaluates the Coulomb angular coefficients required to form the Dirac Hamiltonian. These are usually stored on disc. The options described above with label ANG can be used in the MCP section. In particular option 8 over-rides the label MCP and prevents a call to the MCP section of the program.

IO1 is the I/O dataset flag (> 0 if file is to be written) for output of the MCP coefficients. It is set to zero if no MCP file is required. The default setting is 1.

IEXC controls the calculation of 2-electron integrals
= 1 — only direct 2-electron integrals are evaluated
= -1 — only exchange 2-electron integrals are evaluated
= 0 — both are calculated (default)

IEXC applies to angular coefficients calculated by routine COR. The exchange coefficients involving full shells for diagonal matrix elements will always be calculated.

Input record 7 — calculate MCT coefficients

Format: Label 'MCT ' followed by 1 to 3 integers
Variables: KA, [IOPAR, [IO2]]

KA is the order of the tensor operator (=1 for dipole, =2 for quadrupole).

IOPAR is the parity of the tensor operator :

- = 1 — for even parity (M1,E2, ...)
- = -1 — for odd parity (E1,M2, ...)
- = 0 — for both parities (default setting)

IO2 is the dataset I/O dataset flag (> 0 if file is to be written) for output of the MCT (one electron operator) angular coefficients. Set it to zero if no output file is required. The default setting is 1.

Input record 8 — calculate MCBP coefficients

Format: Label 'MCBP' followed by 0 or 1 integer
Variables: [IO3]

IO3 is the dataset I/O dataset flag (> 0 if file is to be written) for output of the MCBP (Breit) angular coefficients. Set it to zero if no output file is required. The default setting is 1.

Input record 9 — MCDF call and options

Format: Label 'MCDF' followed by up to 50 options

When this label is found then a call will be made to the MCDF section. Up to 50 options can be specified. These options are stored in array ITC in common block /OPT01/.

1 Use Coulomb wavefunctions as initial estimates rather than Thomas-Fermi ones. The default procedure to obtain initial wavefunction estimates is to use any available on the restart dump. If a restart dump is not available (IR2=0) or the particular orbital is not on the dump then a Thomas-Fermi estimate is used. When this option is set then a Coulomb estimate is used instead of Thomas-Fermi.

2 Set all Lagrange multipliers to zero.

3 Set Lagrange multipliers between orbitals of the same generalised occupation number to zero.

4 Use the Mann and Cowan modification to the potentials. See reference given in routine HPOT. The purpose of this modification is to replace the exchange potentials by a direct potential which it is hoped will be better behaved. It has been used with variable success.

5 Write out the Hamiltonian matrix whenever it is calculated i.e. at each call to MATRIX.

6 Write out the eigenvalues and eigenvectors of the Hamiltonian matrix whenever it is diagonalised i.e. at each call to MATRIX.

7 Write out the MCP (angular momentum) coefficients.

Options 8 and 9 use a call to routine PRWF and write on stream 29 to the formatted file GRASP.SH.

8 Write out wavefunctions at convergence.

9 Write out initial wavefunctions as obtained by routine INIT.

12 Stop if the maximum number of iterations in SCF is exceeded.

13 In the case of a failure in SOLV, options 14 to 19 are set and a rerun of SOLV is performed.

Options 14, 15, 16, 17, 18 and 19 provide a debug facility in routines SOLV, OUT and IN.

`DANGER` — These options can produce a lot of output. In particular option 16 prints the wavefunctions at each iteration.

16 This option calls routine PRWF for a printout of the wavefunctions from routine SOLV0/1 and from STWAVE/STWOPT.

20 Suppress call to MCDF routines. Using this option is the same as leaving out the MCDF input data. It is useful in restart situations.

21 When loading a dump, do not rescale the wavefunctions with Z, the atomic number.

22 Do not Schmidt orthogonalise wavefunctions at any stage.

23 When this option is set the MCDF code will use the old value for the speed of light i.e. 137.0373. This is the value set in the CPC-80 version of the codes.

25 When this option is set the input parameter CON is set to 10^4 which gives the non-relativistic limit for the speed of light.

26 When this option is set the radial integrals evaluated in SLATER and RINTI are printed.

30 This option is set automatically if IOP $>$ 0 and allows a call to be made to routine NEWBAS. This will give the energy levels with their LS assignments.

31 This option is set automatically if IOP=3 and allows a printout of the eigenvectors in the LS-basis in routine NEWBAS.

32 Print eigenvectors in jj-basis.

33 Set the screening numbers to zero for the initial wavefunctions. Note this allows the use of Coulomb wavefunctions corresponding to Z, the atomic number, given below. Note that this option will be over-ridden by the input record with label SCR.

41 Copy old orbitals file into new orbitals file.

42 Routine YPOTX is called at the end of the MCDF section and provides some information on the static potential and in particular its asymptotic behaviour. When this option is set the static and nuclear potentials and radial grid are printed.

43 When this option is set the higher order corrections to the deferred correction method are not included in SOLV.

Input record 10 — dataset flags

Format: 0 to 3 integers
Variables: [IR2, [IR3, [IP3]]]

IR2 is the dataset flag that indicates a previous MCDF dump. This dataset is read in the MCDF section. Note that setting IR2 to zero implies that there is no file available. Wavefunctions are read from the dump. These are used as initial estimates in preference to either Thomas-Fermi or Coulomb wavefunctions.

IR3, IP3: The dataset flags IR3 and IP3 are optional input data and are associated with datasets containing orbitals. IR3 is the load file from a previous calculation while IP3 is the dump file from the present calculation. IR3 is only read from while IP3 is only written to. The dataset flags default to zero which implies that the load dataset is not available and a dump dataset is not to be written.
See input records 14 and 15 below.

Input record 11 — basic data

Format: Between 1 and 6 numbers.
Variables: Z, [H, [RNT, [ACCY, [CON, [XCAX]]]]]

Z is the atomic number

H is the step size for the radial grid (default is 0.05)

RNT is the first grid point (default is 10^{-5})

The grid is logarithmic and defined as :

R(I)=RNT*EXP((I-1)*H) for (I=1 .... N)

The number of grid points N is determined during the SCF process. It is chosen so that the asymptotic size of the wavefunctions is small. This is determined using the input parameter CUTOFF.

ACCY is the accuracy to which the wavefunctions and mixing coefficients are to be converged (default is 10^{-8}).

CON is the factor multiplying the speed of light. If this is set to 10^4 then the non-relativistic limit is approached (default is 1).

XCAX is the maximum factor multiplying the exchange potentials (default 1).

Note that a zero or negative value for H, RNT, ACCY or CON also gives the default setting.

Input record 12 — OPTIONAL — nuclear type

Format: label 'VNUC' followed by 1 integer and 1 to 4 numbers.
Variables: NUCTYP, [(PARM(I),I=1,NPARM)]

The default setting (input record not used) is the point nucleus. If the input record is input then the type of charge distribution depends on the parameter NUCTYP. Some of the default parameters used depend on the atomic mass which is read on input record 2.

NUCTYP=1 — uniform charge distribution.

Optionally input one further number which replaces the atomic mass in determining the nuclear radius. If P is the input parameter then the nuclear radius is
$r_{nuc} = kP^{1/3}$ where k is a constant of proportionality.

NUCTYP=2 — Fermi charge distribution.

Optionally input two further numbers giving the nuclear radius r_{nuc} and the skin thickness t_{skin} .
Default values are given by:
$r_{nuc} = (2.2291 A_{mass}^{1/3} - 0.90676) \times 10^{-5}$
$t_{skin} = 1.039 \times 10^{-5}$
where A_{mass} is the atomic mass.

NUCTYP > 2 — another charge distribution

The user must supply his own routine NCHARG which evaluates r^2 times the nuclear charge distribution.

Input record 13 — OPTIONAL — fixed orbitals

Format: label 'FIX ' followed by up to NW-1 integers
Variables: (JFIX(I),I=1,NN)

These are the orbitals to be held fixed during the SCF process. They usually represent a fixed core. The default setting (input record not used) is no fixed orbitals (i.e. all orbitals can be varied in the SCF process).

Input record 14 — OPTIONAL — source of orbitals.

Format: label 'LOAD' followed by NW integers

0 — load from dump file
1 — load from orbitals file
2 — use Thomas-Fermi wavefunctions
3 — use Coulomb wavefunctions
4 — use Slater-type orbitals
5 — use Clementi-type orbitals

If the orbital cannot be obtained in the prescribed manner, the next option is taken. This sets the ILO array.

Options 4 and 5 require data to be input after the 'STOP'/'END ' input record.

Input record 15 — OPTIONAL — orbitals to be dumped

Format: label 'ORB ' followed by up to NW integers

Input the orbital numbers that are to be dumped to the orbitals file (dataset flag IP3). Any fixed orbitals will not be dumped. This sets the IWO array and NWO is the number of orbitals to be dumped.

Input record 16 — OPTIONAL — orbital screening

Format: label 'SCR ' followed by NW numbers
Variables: (SCR(J),J=1,NW)

These are positive screening numbers which are used for the Coulomb estimates for the wavefunctions. The Coulomb function is evaluated for atomic number (Z-SCR(J)). The screening numbers are also used to provide initial estimates for the eigenvalues for Thomas-Fermi estimates. See also MCDF option 33.

Input record 17 — OPTIONAL — polarization potential

Format: label 'VPOL' followed by 1 integer and 2 reals
Variables: NPOTYP, POLPAR(1), POLPAR(2)

NPOTYP —
There are two possibilities for this parameter. When NPOTYP=0 there is no polarization potential. When NPOTYP=1 it takes the form of Migdalek and Baylis.

POLPAR(1) is read when NPOTYP=1 and is the polarizability.
POLPAR(2) is read when NPOTYP=1 and is a cutoff radius.

Input record 18 — OPTIONAL — model potential

Format: label 'VMOD' followed by 3 integers and a number of reals
Variables: NMOTYP, NBPAR, NCBAR, ABAR,
(BPAR(I),I=1,NBPAR), (BBPAR(I),I=1,NBPAR),
(CPAR(I),I=1,NCPAR), (CCPAR(I),I=1,NCPAR)

NMOTYP —
There are two possibilities for this parameter. When NMOTYP=0 there is no model potential. When NMOTYP=1 it takes the form of Hibbert.

Input record 19 — calculation type

The label in columns 1 to 4 defines the calculation type. Remember that in these labels blanks are significant. The possible labels are: 'AL ', 'EAL ', 'OL ', 'EOL ', 'CI '

'AL ' — average level

This optimises the trace of the Hamiltonian. Follow the label with 0 or 1 integers. The integer, if given, is the maximum number of iterations at the final accuracy. If no number is given the default of 3 is taken.

'EAL ' — extended average level

This optimises a weighted trace of the Hamiltonian. Follow the label with 0 or 1 or NCF or NCF+1 or NMAN or NMAN+1 integers.

0 integers — take CSF weights proportional to 2J+1 and allow 3 iterations at final accuracy.
1 integer — take CSF weights proportional to 2J+1 and allow this number of iterations at final accuracy.
NCF integers — these are the CSF weights. Allow 3 iterations at final accuracy.
NCF+1 integers — these are the CSF weights followed by the number of iterations at final accuracy.
NMAN integers — these are the non-relativistic CSF weights.
NMAN+1 integers — these are the non-relativistic CSF weights followed by the number of iterations at final accuracy.

‘OL ’ — optimal level

Optimise on one level only. Input one integer giving the number of the level to be optimised on.

‘EOL ’ — extended optimal level

Optimise on several levels - more than one, but less than NCF. Input the number of levels to be optimised on and the level numbers.

For cases OL and EOL there are also two further optional parameters :

NITIT is the maximum number of iterations at final accuracy - default 6
CHECK is the damping factor for the mixing factors - default 0.15

‘CI ’ — configuration interaction

When this label is read then a configuration interaction calculation is performed. Note that it is possible to perform CI calculations by setting NITIT=0 (NITIT = number of iterations) in any of the above types of calculation. A CI calculation involves setting up a Hamiltonian using orbitals from a previous dump (but new estimates, Thomas-Fermi or Coulomb, can be used) and (usually) new MCP coefficients. This, in effect, fixes all the orbitals used. No SCF iterations are performed and the wavefunctions are unchanged. The type of calculation specified is not important as no SCF process is carried out.

Input record 20 — call BENA section

Format: Label ‘BENA’ followed by up to 20 integers

If the 4-character label ‘BENA’ is found in the input data then a call is made to the BENA section. The label is followed by up to 20 options. This section of the program will calculate Breit and QED corrections to the energy levels. It requires MCBP (Breit angular) coefficients. The available options are described below. They are stored in array KTC.

1 Print the Coulomb matrix calculated in routine COUMAT.

2 Print the eigenvalues of the Coulomb matrix.

3 Print the eigenvectors of the Coulomb matrix.

4 Print the Breit matrix.

5 Print the contributions of the Breit matrix elements to eigenvalues.

6 Print the eigenvectors of the Coulomb+Breit matrix.

8 Print each contribution to the Breit matrix elements calculated in routine BREMAT. This option also applies to the Coulomb matrix if it is evaluated in routine COUMAT.

9 Print each contribution to the Breit energy levels resulting from the QED corrections

10 Suppress the final summary printing.

11 Give information on the Bessel function evaluation and on the source of the function.

16 The final printout from routine SUMMRY is in Ryd. (default)

17 The final printout from routine SUMMRY is in au.

18 The final printout from routine SUMMRY is in cm^{-1} .

19 The final printout from routine SUMMRY is in eV.

20 Suppress the call to the BENA package.

Options 16, 17, 18 and 19 can be set in various combinations to give a print out with different units.

Input record 21 — BENA data

Format: 1 optional number
Variables: [WFACT]

WFACT is a factor multiplying the photon frequency. Using 10^{-3} will enable the long wavelength (low frequency) limit to be obtained. The default is 1 which calculates the full transverse Breit corrections.

Input record 22 — call OSCL section

Format: Label 'OSCL' followed by up to 20 integers

If the 4-character label 'OSCL' is found in the input data then a call is made to the OSCL section. The label is followed by up to 20 options. The available options are described below. They are stored in array LTC.

This section of the program will calculate transition probabilities and oscillator strengths between the energy levels.

Electric transitions are calculated in two gauges. The Babushkin gauge can be shown to reduce non-relativistically to the length form of the matrix element while the Coulomb gauge reduces to the velocity form. Other gauges can be used by using option 19 described below.

OSCL requires MCT (one-electron angular) coefficients. These must be obtained by calling MCT separately.

5 Print the angular coefficients in routine MCTIN.

6 Print the Bessel functions.

7 Print the radial integrals from routine SPME.

8 Gives a debug print from routine CSFM.

9 Use Coulomb eigenvectors and eigenvalues.

10 Use Coulomb+Breit eigenvectors and eigenvalues.

11 Use Coulomb+Breit eigenvectors and eigenvalues, with QED corrections for eigenvalues.

Options 9, 10 and 11 can all be set in the same run. If options 9, 10 and 11 are not set then the default is 11. If BENA energies are not available (i.e. BENA has not been run) then Coulomb energies are used.

12 Print the level energies and eigenvectors used.

13 Print the integrand of the gauge dependent integrals from routine SPME.

14 Print transition energies in cm^{-1} . (Default Ang)

15 Print transition energies in eV. (Default Ang)

16 Print transition energies in au. (Default Ang)

17 Use the input energy levels in the calculations. When this option is specified it is necessary to include an extra input record 24. See description below.

18 This is a new option which gives the lowest order expansion for the Bessel functions calculated in routine BESSJ. It was included in an attempt to give a non-relativistic limit to the oscillator strengths. It was not totally successful.

19 When this option is set input record 25 which contains gauge parameters is read. This allows other gauges besides Babushkin and Coulomb. The normal form for the matrix element is

$H_{bab} = H_{coul} + \mathrm{sqrt}((L+1)/L) H_{gauge}$

where L is the order of the multipole (L=1 for dipole, L=2 for quadrupole). The gauge parameter is then sqrt(2)=1.41.. for dipole and sqrt(3/2)=1.22.. for quadrupole.

20 Suppress the call to the oscillator strengths routines.

Input record 23 — OSCL data — levels

Format: up to NCF numbers
Variables: [LEVELS(I),I=1,NLEV]

LEVELS is a list of the levels between which matrix elements for transition probabilities are to be calculated. The default is all levels.

Input record 24 — OPTIONAL — level energies

OPTIONAL if OSCL option 17 is set

Format: up to NCF numbers
Variables: [ENLEV(I),I=1,NLEV]

ENLEV contains the level energies in au. Note that as only energy differences are used the energy of the first level can be set to zero and excitation energies relative to this level can be given. This is the form in which experimental data is usually given.

Input record 25 — OPTIONAL — gauge parameters

OPTIONAL if OSCL option 19 is set

Format: 2 numbers
Variables: [GAUGE1, GAUGE2]

These are gauge parameters which allow gauges other than Babushkin and Coulomb to be used. They can be used to test the sensitivity of results to the particular gauge.

Input record 26 — end of input data block

A label 'END ' or 'STOP' marks the end of the input data. This input record must be included. If 'STOP' is read then no further input data is read. If 'END ' is read then the

code will attempt to read further input data and terminates using the END= parameter on input record 1.

Input record 27 — STO input data

For each orbital J read the following in free-format.

```
A. E(J)
B. M
C. (IRAD(K),K=1,M)
D. (ZE(K),K=1,M)
E. (S(K),K=1,M)
```

The eigenvalue E will be estimated by routine EIGENV if it is zero on input.

4 File description

4.1 MCT dump

The following is the format of the dump file written by routine MCT in the MCP section of GRASP. The file is unformatted.

```
 1. IHED,RECORD
 2. NCF,NW
 3. (NH(I),NP(I),NAK(I),NKL(I),NKJ(I),I=1,NW)
 4. ((IQ(I,J),J=1,NCF),I=1,NW)
 5. (ITJPO(J),J=1,NCF)
 6. (ISPAR(J),J=1,NCF)
 7. (((JQS(K,I,J),J=1,NCF),I=1,NW),K=1,3)
 8. ((JCUP(I,J),J=1,NCF),I=1,8)
 9. ((ICHOP(I,J),J=1,NCF),I=1,NW)
10. KA,IOPAR
```

A record is written for each non-zero coefficient with the following form

```
11. JA,JB,IA1,IA2,COEF
```

where JA, JB are CSF labels and IA1, IA2 are orbital labels. COEF is the angular coefficient.

The last record is

```
12. IZ,IZ,IZ,IZ,ZERO
```

where IZ is integer zero.

When routine MCT is called by OSCL then records 1 to 10 are not written. This occurs when one of the options 1, 2, 3 or 4 is set in OSCL.

4.2 MCP dump

The following is the format of the dump file written by routine MCP in the MCP section of GRASP. The file is unformatted.

```
 1. IHED,RECORD
 2. NCF,NW
 3. (NH(I),NP(I),NAK(I),NKL(I),NKJ(I),I=1,NW)
 4. ((IQ(I,J),J=1,NCF),I=1,NW)
 5. (ITJPO(J),J=1,NCF)
 6. (ISPAR(J),J=1,NCF)
 7. (((JQS(K,I,J),J=1,NCF),I=1,NW),K=1,3)
 8. ((JCUP(I,J),J=1,NCF),I=1,8)
 9. ((ICHOP(I,J),J=1,NCF),I=1,NW)
```

For each pair of CSF labels JA and JB record 10 is written followed by record 11 for each non-zero coefficient. Record 12 marks the end of the block with IZ being integer zero.

```
10. JA,JB
11. ISTORE,ITYPE,COEF
12. IZ,IZ,ZERO
```

This is repeated for JA=1,NCF and JB=JA,NCF i.e. JA $\leq$ JB.
Thus there are NCF*(NCF+1) blocks.

ISTORE is a codeword for each coefficient which can be decoded to give the labels K, IA, IB, IC, ID.

```
ISTORE=IC*NWA+ID                                if ABS(ITYPE)=7
ISTORE=(((K*NWA+IA)*NWA+IB)*NWA+IC)*NWA+ID      otherwise
```

IA,IB,IC,ID are orbital labels, K is the order of the 2-electron angular coefficient and NWA=NW+1. This choice of NWA ensures that the coding is unique. The main reason for the coding is to reduce storage.

ISTORE is set negative if the angular coefficient belongs to the core/peel or core/core interactions. This applies only to Coulomb angular coefficients. These coefficients are not required by the MCDF section which generates them automatically. However they are required in the BENA section.

```
ITYPE=1 to 6 for 2-electron Breit angular coefficients
ITYPE=7      for 1-electron Coulomb angular coefficients
ITYPE=8      for direct 2-electron Coulomb angular coefficients
ITYPE=9      for exchange 2-electron Coulomb angular coefficients
```

When ITYPE < 0 this indicates that the coefficient belongs to the core. These coefficients are common to all diagonal matrix elements and are only written in the block with JA=JB=1. This reduces storage and computation. These coefficients only involve orbitals which come from full subshells. COEF is the angular coefficient.

4.3 MCDF dump

The following is the format of the dump file written by routine DUMP in the MCDF section of GRASP. The file is unformatted.

```
 1. IHED,RECORD
 2. NCMIN,NW,NCF,N
 3. ZX,RNT,H,C
```

ZX < 0 if iterations are unconverged.

Records 4 to 6 are repeated for I=1,NW

```
 4. NH(I),NP(I),NAK(I),E(I)
 5. PZ(I),QZ(I)
 6. (P(J),J=1,N),(Q(J),J=1,N)
 7. (COUENG(I),I=1,NCF)
 8. (UCF(I),I=1,NW)
```

Records 9 and 10 are written if NCMIN > 0.

Record 14 is written if NEC > 0.

Record 19 is written if NPARM > 0.

```
 9. (CCR(I),I=1,NCFTT)        where NCFTT=NCF*NCMIN
10. (ICCMIN(I),I=1,NCMIN)
11. ((IQ(I,J),J=1,NCF),I=1,NW)
12. EAV,((COUVEC(I,J),J=1,NCF),I=1,NCF),(BREENG(I),I=1,NCF)
13. NEC
14. (IECC(I),I=1,NEC),(ECV(I),I=1,NEC)
15. NUCTYP
16. (ZZ(I),I=1,N)
17. Z1
18. NPARM
19. (PARM(I),I=1,NPARM)
20. ((ICHOP(I,J),I=1,NW),J=1,NCF)
21. (((JQS(K,I,J),I=1,NW),J=1,NCF),K=1,3)
22. ((JCUP(I,J),I=1,8),J=1,NCF)
23. (ITJPO(J),J=1,NCF)
24. (ISPAR(J),J=1,NCF)
```

In more detail the variables are :

Record 1

IHED is an 80-character title for the calculation.
RECORD is a 20-character record of time and date.
IHED is taken from the input data with RECORD being obtained from system calls in routine CALEN.

Record 2

NCMIN indicates the type of calculation. It is the number of levels used in the optimisation. NCMIN=0 is AL (average level) or EAL (extended average level). NCMIN=1 is OL (optimal level) and NCMIN > 1 is EOL (extended optimal level).
NW is the number of relativistic orbitals.
NCF is the number of relativistic CSFs
N is the number of radial mesh points at which each wavefunction is tabulated.

Record 3

—ZX— is the atomic number of the system being considered. If ZX is negative this indicates that the SCF iteration process did not converge.
RNT is the first radial mesh point.
H is the step-size for the radial mesh. The radial mesh is defined as:
R(I)=RNT*EXP((I-1)*H) for I=1,N
This is a logarithmic mesh which has more points near the origin than further out.
C is the speed of light used in the MCDF calculation. It is possible to multiply the speed of light by a factor (e.g. 1000) to give a non-relativistic calculation.

Record 4, 5, 6

The record block 4, 5, 6 is repeated for each of the NW relativistic orbitals in turn.

NH is a 2-character label which distinguishes the angular character of the orbital e.g. 'S ','P-','P ','D-'
NP is the principal quantum number.
NAK is the kappa quantum number.
E is the orbital eigenvalue in atomic units.
PZ is the leading coefficient in the power series expansion of the large component of the radial wavefunction, denoted by P.
QZ is the leading coefficient in the power series expansion of the small component of the radial wavefunction, denoted by Q.
(PF(J,I),J=1,N) is the large component of the radial wavefunction for orbital J tabulated at the N radial mesh points.
(QF(J,I),J=1,N) is the small component of the radial wavefunction for orbital J tabulated at the N radial mesh points.

Record 7, 8

COUENG are the configuration mixing coefficients.
UCF are the generalised orbital occupation numbers.
These depend on the type of calculation i.e. AL, EAL, OL or EOL.

Record 9, 10

These records are not output if NCMIN=0, i.e. an average level calculation.
CCR are the mixing coefficients of the NCMIN levels being optimised.
ICCMIN are the labels of the levels being optimised.

Record 11

IQ(I,J) is the occupation number of orbital I in CSF J.

Record 12

EAV is the average level energy in atomic units i.e. sum of the diagonal elements of the Hamiltonian divided by NCF.
COUVEC contains the eigenvectors of the Hamiltonian. These are the configuration mixing coefficients for the levels. COUVEC(I,J) is the mixing coefficient of CSF I in level J i.e. column J corresponds to level J. The eigenvectors are normalised and their sign is chosen so that the largest mixing coefficient is positive.
BREENG contains the eigenvalues of the Hamiltonian. These are the level energies in atomic units.

Record 13, 14

NEC is the number of Lagrange multipliers. If NEC=0 then record 14 is skipped.
IECC is a code-word which when decoded gives the orbital numbers for the Lagrange multiplier i.e. IECC=A*NWA+B where A,B are the orbital numbers and NWA=NW+1.
ECV is the Lagrange multiplier.

Record 15, 16, 17, 18, 19

The record block 15, 16, 17, 18, 19 contains information on the nuclear potential, which can be either point or finite.
NUCTYP is a parameter which gives the type of nuclear potential. NUCTYP=0 is a point nucleus; NUCTYP $>$ 0 is a finite nucleus. If NUCTYP=1 there is a uniform charge distribution (one parameter is required) and if NUCTYP=2 there is a Fermi 2-parameter charge distribution.
ZZ is an array containing the nuclear potential tabulated at the radial mesh points. For a point nucleus this array contains the atomic number Z.
Z1 is the leading coefficient in the expansion of the nuclear potential.
NPARM is the number of parameters required to specify the nuclear potential. If NPARM is 0 then record 19 is skipped
PARM is an array containing the parameters for a nuclear potential.

Record 20, 21, 22, 23, 24

```
((ICHOP(I,J),I=1,NW),J=1,NCF)
(((JQS(K,I,J),I=1,NW),J=1,NCF),K=1,3)
((JCUP(I,J),I=1,8),J=1,NCF)
(ITJPO(J),J=1,NCF)
(ISPAR(J),J=1,NCF)
```

This record block contains all the information necessary to uniquely specify the CSFs.
ICHOP(I,J) is a flag indicating the occupancy of subshell I in CSF J; =1 if subshell is empty, =1 if subshell is full, =0 otherwise.
(JCUP(I,J),I=1,NOPEN-1) : This array contains the intermediate coupling information for CSF J. It is only required if there is more than one open shell in the CSF. An open shell is one whose occupation number is neither zero nor full. NOPEN is the number of open shells in the CSF. Exactly NOPEN-1 numbers are given — the program does not know that J and 0 always couple to give J !

Suppose that there are 4 open shells with subshell angular momenta (J_1 ,J_2 ,J_3 ,J_4) . Then the coupling scheme for the CSF is:

$(((J_1 , J_2)X_1 , J_3)X_2 , J_4)X_3$

The intermediate coupling information (X_1 ,X_2 ,X_3) is given in array JCUP with X_3 being the total angular momentum for the CSF. The J-values are stored as 2J+1 .

ITJPO(J) is the 2J+1 value for CSF J.
ISPAR(J) indicates the parity of CSF J; =1 for even, =-1 for odd.

4.4 BENA dump

The following is the format of the dump file written by routine DUMPB in the BENA section of GRASP. The file is unformatted. Some of the records are blank. This dump has similar structure to the MCDF dump except that many of the records contain no information. Records 25 to 27 are extra.

```
 1. IHED,RECORD
 2. NCMIN,NW,NCF,N
 3. Z,RNT,H,C
```

Records 4 to 6 are repeated for I=1,NW

```
 4. NH(I),NP(I),NAK(I),E(I)
 5.
 6. (P(J),J=1,N),(Q(J),J=1,N)
 7.
 8. (UCF(I),I=1,NW)
```

Records 9 and 10 are written if NCMIN > 0

```
 9.
10. (ICCMIN(I),I=1,NCMIN)
11. ((IQ(I,J),J=1,NCF),I=1,NW)
12. EAV,((COUVEC(I,J),J=1,NCF),I=1,NCF),(BREENG(I),I=1,NCF)
```

with EAV=0

```
13. NEC
```

with NEC=0 i.e. record 14 is skipped

Record 19 is written if NPARM > 0

```
15. NUCTYP
16. (ZZ(I),I=1,N)
17. Z1
18. NPARM
19. (PARM(I),I=1,NPARM)
20.
21.
22.
23.
24.
25. ((BREVEC(I,J),J=1,NCF),I=1,NCF)
26. (BREENG(I),I=1,NCF)
27. (COUENG(I),I=1,NCF)
```

BREVEC contains the Breit eigenvectors, BREENG contains the Coulomb+Breit level energies, COUENG contains the Coulomb+Breit+QED level energies.

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