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Classic Multiconfiguration-Dirac-Fock And Hartree-Fock-Relativistic Methods Integrated Into A Program Package For The RAL-IBM Mainframe With Automatic Comparative Output

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CLASSIC MULTICONFIGURATION-DIRAC-FOCK AND HARTREE-FOCK-RELATIVISTIC METHODS INTEGRATED INTO A PROGRAM PACKAGE FOR THE RAL-IBM MAINFRAME WITH AUTOMATIC COMPARATIVE OUTPUT.

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ABSTRACT.

A Multi-Configuration-Dirac-Fock (MCDF) computer program written at Oxford University is adapted to interface with the Hartree-Fock-Relativistic (HFR) program written at Los Alamos and translated at RAL for the IBM mainframe computer. The two codes are integrated into a package which includes the Zeeman Laboratory Slater parameter optimisation routines aswell as new RAL routines to further process the HFR and MCDF output. To facilitate usage of this package a description of the adaptions to MCDF and new output extensions is therefore included in this report. In addition more details are given regarding HFR FORTRAN subroutines, and lists of Job Control Language (JCL) files for the complete package are provided. A comprehinsive account of the input and output for the original MCDF program shows its optional capabilities. The instructions as to how to run this suite of programs supplement those in the earlier RAL report on the HFR and Hartree-XR package.

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MASTER JOB A1 *which runs complete set of 3 programs in* HFR *package called* RCN31, RCN2 *and* RCG. SLPM JOB A1 *runs* RCN31 *and* RCN2 *and* SPEC JOB A1 *runs* RCG *and* WVFN JOB A1 RCN31 *only. The JCL is identical to corresponding parts of* MASTER JOB A1 *except for disk file saving.*

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GOP JOB A1 *runs the Zeeman Slater perameter optimisation program.*

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1) INTRODUCTION

Two classic methods for the calculation of atomic structure and atomic data apply the Multi-Configuration-Dirac-Fock (MCDF) and Hartree-Fock-Relativistic (HFR) theoretical models. This Report describes aspects of an integrated program-package for the RAL-IBM mainframe which applies these methods. It is primarily intended to provide the User with the additional necessary information to enable operation of the package. Much of the relevant information is already available. A published[1,2] description of the MCDF program describes operational and theoretical aspects. The HFR program is described in a book[5] which gives an extensive description of the theory of atomic structure and in other publications[5,6]. A guide on how to use the RAL HFR versions is in a previous RAL Report[8]. A Zeeman Laboratory Slater parameter optimisation program, which is also incorporated, is also documented[9]. The following supplementary information will assist the User. Firstly there are instructions on how to run the RAL-adaptions of the MCDF program. Secondly the additional RAL programs which re-format MCDF output and enable automatic MCDF-HFR comparisons are described along with operational details. Next is a catalogue of the FORTRAN files. For the HFR files a brief summary of their contents is included which follows closely an unpublished account by Dr. R. D. Cowan.. A listing follows of the JCL files, which are essential for any User, for the complete program package. A detailed account, written by Dr. I. P. Grant et al., of the input for the unadapted Oxford MCDF version allows the User to delve more deeply into input options. A published description [1] gives further details of the MCDF program.

The integrated atomic structure program package in operation at RAL on the IBM mainframe computer consists of the following four parts (the first two constituting the major items):

a) The MCDF program[1-2] developed at Oxford University by Dr. I. P. Grant. and Co-workers. It, along with another similar one[3],represents the most highly developed MCDF code.It includes Breit and QED corrections. The original version has optional easy to use non-relativistic input which is chosen for the RAL version. It can also be recompiled relatively easily with different array dimensions. The Fortran files, which must be obtained for this purpose, incorporate state of the art programming techniques.

b) The code[4-6] developed by Dr. R. D. Cowan of Los Alamos Scientific Laboratory which incorporates HFR with Blume-Watson[7] for spin-orbit and includes an optional alternative namely the more approximate statistical exchange method (HXR). It has also sections which can compute autoionisation transition probabilities, photoionisation cross-sections and plane-wave-Born collision strengths. It is possibly the most user friendly atomic structure software of its kind in existence. The RAL adaption for the IBM mainframe was described in a previous RAL report[8].

c) A Slater parameter optimisation procedure[9] was originally acquired from the Zeeman Laboratory. Using least squares optimisation procedures it varies Slater parametres so that differences between calculated energy levels and those derived from observations are minimised.

d) A set of programs written at RAL which compute the percentage composition of energy levels from the eigenvector output of the MCDF or HFR packages and gives each level a unique designation. It also arranges for the print out of level compositions and energy levels and of wavelengths, wavenumbers and weighted oscillator strengths in a format suitable for reproduction[10-12]. Furthermore the output of the MCDF and HFR programs are compared automatically[11,12]. The interface of these programs to the MCDF and HFR packages involved minor alterations to both.

Application of the two methods in an integrated computer package has the powerful advantage of permitting direct comparison of results for typical ions.While the MCDF contains the most advanced physics, the HFR produces almost identical results for a wide variety of ions and involves much less computational time and smaller matricies. If no significant difference occurs then the HFR section can be applied to lengthy computations. As HFR involves smaller matricies, more interacting configurations can be included in the computations. Added confidence in the HFR computations can be derived from the assumption that agreement with state of the art *ab initio* computations is a check on validity. The MCDF computations can be chosen where serious differences occur: such as can be expected for high (>40) ionisation stages where Relativistic-Dirac formulation can be expected to have a distinct advantage. It must be emphasised that differences between the best *ab initio* atomic structure computations occur due to restrictions in the number of configuration interactions or correlation effects which can be taken into account in any feasable computation and other possible theoretical limitations. These differences usually account for the largest errors for complex spectra. For this reason optimisation procedures often are necessary, in a non *ab initio* procedure, to minimise reducable errors on such quantities as energy levels, oscillator strengths and computed level composition. Such intrinsic errors may be used to justify more approximate computational methods as were once an asset when computers were slower; however there is now little need to apply faster programs than HFR except in special cases such as those encountered for which convergence is slow.

The more complex theoretical methods offer distinct physical advantages over the more approximate. The MCDF uses the Dirac in place of the Schroedinger one-electron Hamiltonian in the self-consistent Hartree-Fock procedure. It provides a proper treatment of the relativistic effects[14] on total binding energies and radial wavefunctions which become appreciable for Z of about 10 and 30 respectively. Wavefunctions are constructed from central-field Dirac orbitals and each angular state is characterised by a pair of quantum numbers. There are nearly four times as many radial functions involved as in HF with each non-relativistic equation being represented by

several relativistic ones. The DF equations [14] are much more complex than the already highly complicated HF equation . As they contain the most advanced physics, MCDF *ab initio* computations can be used as a standard against which errors in other *ab initio* computations may be estimated. Added to the Oxford MCDF program are routines which compute Breit and QED corrections using the methods of Mc Kenzie et. al. [15] . The transverse Breit interaction is a dynamic correction to the coulomb repulsion between electrons in electrodynamics. The QED includes vacuum polarisation and self energy corrections to the energy level. These effects tend to depress energy levels towards the ground level.

The HF method minimises the correct non-relativistic expression for the energy and treats exchange properly. It leads to complicated equations involving non-homogenious differential equations which present considerable computational problems in their solution[4]. Mass-velocity and Darwin one-electron correcrions are included. The relativistic corrections added in the HFR method and the introduction of the Blume-Watson[7] method for spin orbit compensates for relativistic effects to the extent that comparison with MCDF results may show negligible differences for Z<40. The recent development of faster computers has meant that these equations can be solved in acceptable computing times.

Other computational methods usually assume some form of approximation for the potential-energy function[4] for the field in which the electron moves. Thus the Thomas-Fermi model assumes a statistical potential and the Thomas-Fermi-Dirac elaborates with an exchange contribution to the electron potential energy. The Hartree-Fock-Slater (HFS) treats the direct terms of the electron-electron potential energy properly but approximates for exchange with a statistical free-electron expression. The Cowan Hartree-X (HX) method improves on HFS by applying a statistically based approximation for only the non-self-exchange terms. Using such an approximation in a different form is the Hartree-Slater method. Most of these methods are likely to be less accurate than HFR in most cases and some show very large errors for early ions in an isoelectronic sequence. The Parametric Potential Method applies an assumed analytical potential and this can be chosen to result in best agreement between computed and experimental energy levels: hence it is not in this form an *ab initio* model.

II) HOW TO RUN THE MCDF PROGRAM.

1) To run the main Multi-Configuration-Dirac-Fock Program (MCDF) type:
XPLANT MCDF JOB A1 (SUBMIT

Then the computer will request:

'TYPE IN DTMCDF'

Reply with: **DTMCDF DATA** Where DTMCDF is the main input data file for the MCDF program previously prepared on CMS disk A.

An example of such an input file is now given with an explanation of the main data which must be typed into it. For more complex cases the User is

referred to the original publications[1,2]. In most applications it is only essential to alter some of the data in this file so this data is underlined in the example to aid the User. **Comments are added in this Font** The input is in non-relativistic notation and the program automatically prepares its own file in relativistic notation. For Dirac-relativistic notation input and other options marked with an asterisk* see the Section VI).

The main input file for the MCDF program:

DTMCDF DATA D1

FE XII 3SN3PN3DN (**This is any title Cols 1-72)**
4 6 2 **(4 Configurations,6 orbitals,Always 2 for this input* & LS)**
1S 2 2 2 2 **(Orbital labels (6) for each shell followed by occupation**
2S 2 2 2 2 **numbers for each of the (4) configurations. Here**
2P 6 6 6 6 **the four** $1s^2 2s^2 2p^6 3s^2 3p^3$, $1s^2 2s^2 2p^6 3s 3p^4$,
3S 2 1 2 0 $1s^2 2s^2 2p^6 3s^2 3p^2 3d$ **and** $1s^2 2s^2 2p^6 3p^4 3d$
3P 3 4 2 4 **configurations are represented.)**
3D 0 0 1 1
ANG **(Cols 1-4 = Label. Added numbers give optional* printout)**
-1 **(Negative number ensures all J values)**
MCP 8 **(Label and stream 8. Optional* 1 or 2 for coeffs)**
MCDF **(Label. Many extra numbers can provide extra options*)**
8 0 10 **(Data set streams)**
26.0 **(Atomic number Four optional* numbers define accuracy)**
55.85 **(Atomic weight.Optional numbers can scale exchange)**
EAL **(Asks for extended average level calculations see options*)**
MCT 12 1 -1 **(Label. Output stream 12. Tensor order 1 parity odd -1)**
MCBP 11 **(Label. 11 is MCBP DS file)**
BENA **(Label. Can be followed by many print out options)**
11 10 55.85 1.0 **(File 11 is MCBP coeffs &10 wavefun.At. Weight & c)**
OSCL **(Label. Extra print options* can be added.)**
12 10 **(DS file 12 has MCT coeffs & 10 wavefun., Options available here to limit levels in matrix calcs)**
END

The output form the MCDF JOB, from which printed extracts will be shown in Section VIII, is of three kinds:

i) There is the output form the main MC-Dirac-Fock program which is an abbreviated form of that arranged at Oxford University consisting of the following:

a) A copy of the non-relativistic input.

b) The equivalent relativistic input data.

c) Core and Configuration definitions in JJ and LS coupling.

d) Dimensions needed which must not exceed those frozen in the RAL adaption. For greater dimensions the original Oxford version must be used.

e) Configuration mixing coefficients,eigenvalues and orbital properties.

f) Eigenenergies in A.U.,Rydbergs, cm^{-1} and E.V.

g) A summary of Breit and QED contributions in the same units.

h) Oscillator strengths, energy in A.U, Transition probability and wavelength adapted to Ångstrom units. Both COULOMB [13,14] and BABUSKIN[13,14] gauge oscillator strengths are printed. In the non-relativistic limit the COULOMB gauge becomes the dipole velocity matrix element formulation while the BABUSKIN the dipole length form as computed in the HFR programs. Both COULOMB and BABUSKIN are transmitted to the next section of the suite as added at RAL which converts them into weighted oscillator strengths *gf* in the form usually found in the literature. Also transmitted are eigenvectors (no matrix is printed in the RAL version), wavenumbers in cm^{-1}, wavelengths in Å and in LS notation the designations and configuration specification as optionally used in the HFR program.

ii) In the default option MCDF JOB calls two RAL routines which are adaptations of those added to the HFR program[8]. These are identical to those called by DIRSORT JOB. The extra input files requested by both these routines are explained under section III which deals with DIRSORT. The first routine takes the eigenvector output from MCDF and computes and prints out the percentage composition of each level in LS term designation. The program also automatically selects a unique designation for each level. It names the first level according to the term linked with the largest eigenvector component in the matrix. The corresponding row and column of the matrix are then excluded and the selection procedure repeated until all the levels are named. Energy levels and wavenumbers (in cm^{-1}), wavelengths in Ångstroms and weighted oscillator strengths *gf* are printed both with and without Breit and QED corrections.

iii) The second RAL routine orders the transitions into multipets in a format suitable for reproduction. Wavenumbers (in cm^{-1}), wavelengths in Ångstroms designations and *gf's* are printed.

III) HOW TO OBTAIN COMPARISONS BETWEEN MCDF AND HFR COMPUTED ENERGY LEVELS.

To run the MCDF and HFR programs to obtain comparative output between them requires the following succession of commands:

1) **XPLANT MCDF JOB A1 (SUBMIT GP**
Computer will request:
'TYPE IN NAMY'
Reply with: **YAB** Where AB is varied for each dataset.
'TYPE IN NAMZ'
Reply with: **ZAB** Where AB is varied for each dataset.
'TYPE IN DTMCDF'
Reply with: **DTMCDF DATA** Where DTMCDF is a data file on disk D.
This runs the main MultiConfiguration-Dirac-Fock Program (MCDF). For a discussion of its output see section II i) above.

2) **XPLANT DIRSORT JOB A1 (SUBMIT EL**

(More information on the output from DIRSORT is given in section I) ii) and iii) above.

Computer will request:

'TYPE IN NAMQ'

Reply with: **QAB** Where AB is varied for each dataset.

'TYPE IN NAMZ '

Reply with: **YAB** Where AB is the same as used in 1) above.

'TYPE IN NAMZ'

Reply with: **ZAB** Where AB is the same as used in 1) above.

'TYPE IN ARDATA '

Reply with: **ARDATA DATA** Where ARDATA is a data file on disk D.

TYPE IN CRLFILE'

Reply with: **CRLFILE' DATA** Where CRLFILE is a data file on disk D.

Samples of these two input files are as follows:

CRLFILE DATA D1

SPDFGHIKL0

CALCULATED WL'S AND GF'S OF FE XII EMISSION LINES LEVELS CM-1

0.0100 1 1 1 101001.51

The first line is a title in (1X,9A1) and the second has a FORMAT (1X,F9.4,3I2,I4,5I1,A2,I1). For most purposes only the underlined figures need alteration. The first 0.0100 controls the smallest weighted oscillator strength to be printed in the final ordered printout while .51 is used as shown for J values involving 0.5 and .00 for integer values. Use of the other options is explained in the RAL Report.[8]

ARDATA DATA D1

1 1 0490TABLE XII

001 005 010 011 018 027 038 051 066 179 180 181 182 183 184

002 004 008 013 020 029 040 053 068 194 195 196 197 198 199

003 012 009 015 027 031 042 055 070 209 210 211 212 213 214

etc for a 15X15 array.

The first line has FORMAT(1X,I1,2X,I4,2A8). On this line the underlined figure can be used to restrict the number of transition arrays output. Here it is the first 49 (unlimited in this case). The title in 2A8 can be altered. The 15X15 array in FORMAT (15(1X,I3)) dictates the order of output of the transition arrays. The 15 cols. correspond to the configurations of the first parity input and 15 rows to those of the second. A fuller description is in the RAL Report.[8]

'TYPE IN CFDATA '

Reply with: **CFDATA DATA** Where CFDATA is a data file on disk D.

A sample of this input file is as follows:

CFDATA DATA D1

```
 4
0002P4  1
3S13P4  1
3P23D1  2
3P43D1  3
```

The first line with FORMAT(6X,I2) states the total number of configurations input . That number of lines will follow FORMAT(6X,A6,2X,I2) with each configuration label specified followed by a number corresponding to the order of original input for each parity.

This runs the program for selecting terms and formatting the output in convenient form to show level compositions, wavenumbers in cm^{-1}, wavelengths in Å, and weighted oscillator strengths (gf). It also prepares the output in a dataset RO.FQ**QAB** for input to the program BIRDY (see SEC. 5) which compares MCDF and HFR computations.

3) To obtain Hartree-Fock-Relativistic computations for comparison:

Type: **XPLANT MASTER JOB A1 (SUBMIT GP**

A further option HV must be added after SUBMIT for half integral values of the quantum number 'J'.

Computer will request:

'TYPE IN NAMY'

Reply with: **YZY** Where ZY is varied for each dataset.

'TYPE IN NAMZ'

Reply with: **ZZY** Where ZY is varied for each dataset.

'TYPE IN LCONFG'

Reply with: **LCFG DATA** Where LCFG is a data file on disk A.

. TYPE IN UCONFG'

Reply with: **UCFG DATA** Where UCFG is a data file on disk A.

Samples of these two input files which must match exactly the MCDF input file 'DTMCDF' used in 1) above are as follows:

LFE12 DATA A1

```
 26  12FE  3S23P3      3S2 3P3 3D0
```

UFE12 DATA A1

```
 26  12FE  3S13P4      3S1 3P4 3D0
 26  12FE  3P23D1      3S2 3P2 3D1
 26  12FE  3P43D1      3S2 3P4 3D1
```

The two files have:

FORMAT(I1,I4,I3,I2,3A6,1PF2.1,1PF2.1,8(A3,A2),A2,F6.5) In this example the atomic number 26 is in A4, the degree of ionisation 12 in I2, in the second two A6 lie the configuration label which will later be printed out and should be used identically in the CFDATA and CRDATA files mentioned in the sections 2) and 5). The 8(A3,A2) give the orbital specification and occupation numbers of each shell with inner full shells assumed. To use these input files in different cases a more detailed description must be consulted as contained in the RAL Report RL-83-030 [8] this also provides

details of how to use MASTER and its options and of how to use MASTER divided into two parts SLPM JOB A1 and SPEC JOB A1. The first SLPM computes Slater parameters and Radial dipole matrix elements while the second SPEC uses this data to compute wavelengths, energy levels, oscillator strengths and other atomic data.

4) To convert the HFR output into a form suitable for input for MCDF comparisons and conserve it on a OSDISK file type:

XPLANT SELECT JOB A1 (SUBMIT GP

Computer will request:

'TYPE IN NAMY'

Reply with: **ZZY** Where ZY is the same as used in 3) above.

TYPE IN NAMY

Reply with: **YZY** Where ZY is varied for each dataset.

5) To compare MCDF with HFR computations type:

XPLANT COMPAR JOB A1 (SUBMIT GP

Computer will request:

TYPE IN NAMB

Reply with: **BLA** Where LA is varied for each dataset.

'TYPE IN NAMY'

Reply with: **YZY** Where ZY is the same as used in 4) above.

TYPE IN NAMQ

Reply with: **QAB** Where AB is the same as used in 2) above.

TYPE IN CRDATA

Reply with: **CRDATA DATA** Where CRDATA is a data file on disk D.

A sample of this input file is as follows:

CRDATA DATA A1

```
-1.0 1.0  FE XII
 4
3S13P4
3P43D1
3P23D1
3S23P3
```

In this file the first line must read as above with FORMAT(6X,2F4.1,A8) if the first configuration input in 1) and 3) above has odd parity but the signs on 1.0 should be reversed if even parity appears first. The second line with FORMAT(6X,I2) states the total number of configurations input . That number of lines will follow FORMAT(6X,A6) with each configuration label specified. The order of these configurations is the same as in 1) for even parity first but reversed for odd parity first as in the above example.

The running of the last JOB prepares the output in a dataset RO.FB**BLA** ready for transfer from OSDISK to a CMS 'LISTING' file and subsequent printing on a laser printer or elsewhere.

6) Transfer output to a CMS 'LISTING' file and print on the laser printer.

Once the job has run first find OSDISK number so type: **TESTSOFT** then:

VS2CAT RO Osdatasets will then be listed.

Then type: **OSDISK MVSUnn B** (Substitute OSDISK disk number for nn)

Then: **OSCOPY BLA LISTING D1 B ?? FBBLA (?? is subproject)**
PR6670 BLA LISTING D1 (PRINTER 6670R1A FORM A4D COPY 1
Which takes output, for which an extract is shown in Section IX, to a laser printer destination RAL Bldg. R1.
Remember to erase unwanted OS DATASETS eg. with:
OSUTIL ERASE NAME *??.FBBLA*

IV) CALALOGUE OF THE FORTRAN FILES INCLUDED IN THE PROGRAM-PACKAGE INCLUDING BRIEF COMMENTS ON THE HFR SUBROUTINES.

CONTENTS OF THIS SECTION:

1) LIST OF FORTRAN FILES FOR RCN31 (WVFN JOB) First part of (SLPM JOB) and (MASTER JOB) (Binary RTHBIN)

RCN31 is the main program. It handles all input, some output, controls the self-consistent-field iteration, and portions of the detailed calculation.
SETCFG interprets the configuration-definition input and estimates initial values of the one-electron eigenvalues.
SCHEQ integrates the one-electron radial wave equation, and controls the iteration on the one-electron eigenvalue to give a radial wavefunction which satisfies boundary conditions. It also normalises the function for either a bound or free electron.
C5 a function.
OUTPT handles most of the printed output (in part, via calls to POWER, ZETA1, and SLI1) and the wavefunction output to disk file 2 for input to the next program RCN2.
SUBCOR calculates a modified free-electron correlation energy for a specified electron density.
CROSYM solves a system of linear equations.
POWER computes values of $\langle r^m \rangle$ for each orbital.
ZETA1 computes spin-orbit values from a central-potential formula and also via the Blume-Watson method(the latter more accurate values are used). Also computed and printed are the one electron kinetic-plus-nuclear energy (I) and the relativistic mass-velocity and Darwin corrections.
SLI1 computes and prints all Slater integrals F^k and G^k (in units of rydbergs and cm^{-1}); it also computes overlap integrals and calls RCN3S.
RCN3S prints the overlap integrals, and calculates (from the F^k and G^k , with

the aid of subroutine S3J0SQ) and prints the Coulomb interaction energy between each pair of electrons. It then calculates the correlation-energy corrections (using values of I from ZETA1) calculates and prints one-electron binding energies and the total binding energy of the atom. It prints the single configuration Slater parameters in 1000 cm^{-1} and E_{av} (in Rydbergs).

S3J0SQ is concerned with 3-j symbols.
S6J is concerned with 6-j symbols.
DELSQ Function used by S6J.
FCTRL obtains factorials for S3J0SQ
HFWRTP interpolates the wavefunctions to points on the radial mesh ond obtains other data for useby the Hartree-Fock section
HFPOT calcalates the Hartree-Fock potential (excluding the classical-potential terms, which are calculated in RCN31), written in the form of an effective homogeneous-equation local-potential function.
QUAD5 is a general-purpose 5-interval quadrature routine.
QUAD2 calculates the classical potential via Simpson's rule quadrature.
QUADK is used by HFPOT for the evaluation of Hartree's Y_k function.
CLOCK Calls system CPU-time.
ZETABW evaluates spin-orbit parameters via the Blume Watson method using the following 5 function routines:
SM function routine.
SN function routine.
ZK function routine.
VK function routine.
DYK function routine.

2) LIST OF FORTRAN FILES FOR RCN2 Second part of (SLPM JOB) and (MASTER JOB) (Binary TWOBIN)

RCN2 reads control information and calls various subroutines accordingly.
OVER computes an overlap integral between two specified radial wavefunctions from the same or different configurations.
ZETA2 Can compute the small, usually negligible configuration-interaction spin-orbit integrals.
DIP computes electric dipole and quadrupole integrals.
SLI2 calculates configuration interaction coulomb integrals R^k.
G5INP is a master program which calls SLI2 and DIP as appropriate, and prepares the input decks for RCG.
S3J0SQ is concerned with 3-j symbols.
S3J is concerned with 3-j symbols.
FCTRL calculates factorials for S3J and S3J0SQ.
SBESS evaluates the spherical Bessel function at a specified point.

NB: There is a small linking programme (Binary PPPBIN) between RCN2 and RCG which re-formats and prints the output of RCN2 for RCG input.

3) LIST OF FORTRAN FILES FOR RCG (SPEC JOB) (Binary RESBIN [BVNBIN for Autoionisation calculations])

NB: THESE ROUTINES ARE INCLUDED IN MASTER JOB.

RCG The main control section which obeys control input and calls subroutines accordingly.

CUVFD Reads disk definitions (set at 42,43 and 44) and coefficients of fractional parentage (cfp) and computes coefficients of fractional grand-parentage (cfgp) placing them on 42 and matrix elements for 43 and angular coefficients for 44.

CIJKF calls S3J0SQ to calculate matrix elements.

LOCDSK locates appropriate records on disks 42,43 and 44.

LNCUV reads subshell input specification and prints matrix elements.

PLEV using LNCUV specifications vectorially adds quantum numbers L_i S_i to set up tables for all possible L_i S_i and J_i.

PFGD sets up, and writes to disk 20, preliminary tables of coefficients of Slater single configuration integrals either obtained from disk 44 or computed with the aid of subroutines CIJKF, RDIJ and REIJ: which use matrix elements from disk 43.

PRK computes, and writes to disk 20, tables of coefficients of Slater configuration-interaction integrals $R^k(ij,i'j')$. computed with the aid of cfp and cfgp from disk 43 and matrix elements from disk 43 and subroutines CLASS1-CLASS11.

RDIJ computes coefficients for Slater direct parameters F^k and $R^k(ij,i'j')$.

REIJ computes coefficients for Slater exchange parameters G^k and $R^k(ij,j'i')$.

CLASS1 to CLASS11 eleven subroutines to compute R^k coefficients.

CALCFC (modified at RAL to re-format coefficients file) For each J value selects quantum numbers found by PLEV, computes transformation matrix. Writes to disks 31,32 and 41 and coefficients file (with option CF) to disk 19 for use with GOP Zeeman parameter optimisation routine. Calls SPRIN and CPL37.

CPL37 calculates quantum numbers as required for transformation matrices and writes to disk 41.

SPRIN (modified at RAL) is a multipurpose matrix-print routine which also transfoms some matrix coupling representations.

SPRN37 called by SPRIN to print eigenvectors.

MUPOLE uses quantum numbers, cfp's and matrix elements from disks 31,32,42 and 43 to compute angular coefficient matricies for line strength calculations.

ENERGY (modified at RAL) reads input Slater parameter data then quantum numbers and transformation and coefficient matrices from 41, computes and diagonalises energy matrix and writes sorted eigenvectors to 31 or 32. Optionally deals with autoionisation transition probabilities. Eigenvectors are saved on disk 36 (with the involvement of SPRIN) for level designation and composition determination by the RAL sorting programs.

CALCV is called by ENERGY to calculate the diagonal elements of the coefficient matricies in the intermediate-coupling representation.
LVDIST called by ENERGY to calculate the statistical distribution of level statistical weight and to plot. **(This plotting is omitted in RAL version)**
SPECTR (modified at RAL) is called by ENERGY. It reads the mupole matrix from disk 41 and eigenvalues and vectors from 31 and/or 32. It computes sorts and prints wavelengths, line strengths, weighted oscillator strengths (gf) and transition probabilities. Information is saved on disk 12 for further arrangement by the RAL sorting programs.
WNDIST A gf plotting routine. Calls to this routine are omitted in the RAL version.
BORN calculates plane-wave-Born collision strengths.
AKNINT interpolation routine used by BORN.
UNCPLA computes uncoupling coefficients.
UNCPLB computes uncoupling coefficients.
RECPSH computes shift recoupling coefficients.
RECPJP computes jump recoupling coefficients.
RECPEX computes exchange recoupling coefficients.
CLOCK calls system CPU-time.
S3J0SQ is concerned with 3-j symbols.
S6J is concerned with 6-j symbols.
S9J is concerned with 9-j symbols.
DELSQ Function used by S6J etc.
FCTRL obtains factorials for S3J0SQ etc.
SORT1 calls ORDER1: together they sort an array of integer numbers into numerically increasing order and correspondingly rearrange up to 12 additional arrays.
ORDER1 called by SORT1. Orders integers.
SORT2 calls ORDER2: together they sort an array of real numbers into numerically increasing order and correspondingly rearrange up to 12 additional arrays. Will then call ORDER2 for integers.
ORDER2 called by SORT2. Orders real numbers. NB: the dimensions on FT must be double that of arrays dealt with in calling routine.
MLEW is called by ENERGY to call:SMEVEV ,SMHHTR, PRODHH, DOTPR1 and DOTPR2 which are five matrix diagonalisation routines.
PLOJB small function.
RCOEFF subroutine of BORN.
E1 computes an exponential integral.
BLKDTA Block standard input data.
CSEVL evaluates Chebyshev series.
RCEINP not used at RAL. For a fitting program.

4a) LIST OF FORTRAN FILES FOR (SELECT JOB) (Binary BSTBIN)
SELECT, SORT2, ORDER1, and ORDER2. NB: adjust FT dimension in ORDER2.

4b) LIST OF FORTRAN FILES FOR RCG (MUSORT JOB) (Binary LAGBIN or LASBIN with option LA)

MULTIP (or with option LA MULTIPL) LA is suitable for A4 Format on a laser printer.

SORT2, ORDER1, and ORDER2. NB: adjust FT dimension in ORDER2.

NOTE THAT SLSORT RUNS SELECT AND MUSORT IN SERIES FURTHERMORE THEY ALSO FOLLOW SPEC AND MASTER IN THE DEFAULT OPTION.

5) LIST OF FORTRAN FILES FOR MCDF (MCDF JOB) (Binary MDFBIN)

MCDF, DATAIN, BENA and MCP These contain all the subroutines for the MCDF program (see Ref.1 and 2 for description) with dimensions set for the RAL version. Some routines have had minor alterations to obtain output fot the RAL sorting and comparison routines. These are:

DFMAIN, MANOUT, MATOUT, MCFIRST, NROUT, PRINTA, OSC and SUMMRY.

A complete undimensioned and unaltered set of the MCDF program files exist in files: CMCDF, CDTIN, CBENA and CMCP.

6) LIST OF FORTRAN FILES FOR (DIRSORT JOB) (Binary SELBIN followed by MAGBIN)

NB: THESE ALSO FOLLOW MCDF JOB IN THE DEFAULT OPTION.

For SELBIN:

DFSELB SORT2, ORDER1, and ORDER2. NB: adjust FT dimension in ORDER2.

For MAGBIN:

MULDRC SORT2, ORDER1, and ORDER2. NB: adjust FT dimension in ORDER2.

7) LIST OF FORTRAN FILES FOR (COMPAR JOB) (Binary BRDBIN)

COMPAB, BIRDY, SORT2, ORDER1, and ORDER2. NB: adjust FT dimension in ORDER2.

8) FORTRAN FILE FOR (GOP JOB) (Binary LSFBIN)

PARFIT

V) JCL JOB FILE LISTINGS FOR MCDF AND HFR PACKAGE.

THIS SECTION CONTAINS THE FOLLOWING JCL FILES:

MCDF JOB A1 *which runs the* MCDF *program.*

DIRSORT JOB A1 *which sorts* MCDF *output with two RAL programs.*

COMPAR JOB A1 *which compares* MCDF *and* HFR *output.*

MASTER JOB A1 *which runs complete set of 5 programs in* HFR *package called* RCN31, RCN2 *and* RCG. SLPM JOB A1 *runs* RCN31 *and* RCN2 *and* SPEC JOB A1 *runs* RCG *and* WVFN JOB A1 RCN31 *only. The JCL is identical to corresponding parts of* MASTER JOB A1 *except for disk file saving.*

SLSORT JOB A1 *which sorts* HFR *output with two RAL programs. It runs* SELECT JOB A1 *and* MUSORT JOB A1 *in series with similar JCL.*

GOP JOB A1 *runs the Zeeman Slater perameter optimisation program.*

MCDF JOB A1

```
//IDDMCDF JOB (ACCT,IDD,5-30),'USERNAM',PASSWORD=(XXXX),PRTY=2,
// TIME=(5,30)
//*MAIN ORG=RLVM370.(LL:SYSTEM|:RLR1EP1) ,LINES=35
//* *FILE SITE=RLR1,USER=IDD,FILE=RL1-F13
//    EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=(BB:DFBBIN|:MDFBIN),
//    REGION.G= (BB:6000K|:2900K)Note option BB calls large array version
//G.FT08F001 DD DSN=&&MCP,UNIT=WORK,DISP=(,PASS),
//       SPACE=(CYL,(2,2)),DCB=(RECFM=VBS,LRECL=400,BLKSIZE=408)
//G.FT10F001 DD DSN=&&MCDF,UNIT=WORK,DISP=(,PASS),
//       SPACE=(CYL,(2,2)),DCB=(RECFM=V,LRECL=400,BLKSIZE=408,BUFNO=1)
//G.FT11F001 DD DSN=&&MCBP,UNIT=WORK,DISP=(,PASS),
//       SPACE=(CYL,(3,3)),DCB=(RECFM=VBS,LRECL=400,BLKSIZE=408)
//G.FT12F001 DD DSN=&&MCT,UNIT=WORK,DISP=(,PASS),
//       SPACE=(CYL,(2,2)),DCB=(RECFM=VBS,LRECL=400,BLKSIZE=408)
//G.FT30F001 DD DUMMY
//G.FT09F001 DD DSN=&&TEMP09,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT42F001 DD DSN=&&TEMP42,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT41F001 DD DCB=LINES,SPACE=(TRK,((GP:15|:10),(GP:12|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
// DSN=(GP:RO.FY($P NAMY % % 'TYPE NAMY')|:&&TEMP41),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
//G.FT35F001 DD DCB=LINES,SPACE=(TRK,((GP:30|:10),(GP:40|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
// DSN=(GP:RO.FZ($P NAMZ % % 'TYPE NAMZ')|:&&TEMP35),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
//*
```

```
//G.SYSIN DD *
($A *FM=D1 ($P DTMCDF % FILE 'TYPE IN DTMCDF'))
/*
(CF $A MASD JOB A1|NS $A MASD JOB A1|GP $A MASD JOB A1|$A DIRV JOB
D1)
/* END OF JOB
```

Note that DIRV **is as** DIRSORT JOB A1 ***without first 4 lines.*** MASD **is a** ***dummy file.***

DIRSORT JOB A1

```
//IDDDIRS JOB (ACCT,IDD,2-59),'USERNAM',PASSWORD=(XXXX),PRTY=8,
// TIME=(2,30)
//*MAIN ORG=(LL:RLVM370.SYSTEM|:RLR1EP1),LINES=35
//* *FILE SITE=RLR1,USER=IDD,FILE=RLR1-F13
//  EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=SEBBIN,REGION.G=2500K
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT42F001 DD DCB=LINES,SPACE=(TRK,((GP:15|:10),(GP:12|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
// DSN=(GP:??.FT($P NAMT % % 'TYPE NAMT')|:&&TEMP42),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
//G.FT38F001 DD DCB=LINES,SPACE=(TRK,((EL:8|:4),(EL:30|:8))),
//    DISP=(NEW,(EL:CATLG|:DELETE)),
// DSN=(EL:??.FQ($P NAMQ % % 'TYPE NAMQ')|:&&TEMP38),
//    (EL:UNIT=STORAGE|:UNIT=WORK)
//G.FT41F001 DD DISP=SHR,
// DSN=??.FY($P NAMY % % 'TYPE NAMY')
/*
//G.FT35F001 DD DISP=SHR,
// DSN=??.FZ($P NAMZ % % 'TYPE NAMZ')
/*
//G.FT37F001 DD DCB=LINES,SPACE=(TRK,((GP:30|:10),(GP:40|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
// DSN=(GP:??.FK($P NAMK % % 'TYPE NAMK')|:&&TEMP37),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
/*
//  EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=(LG:MAGBIN|:MAGBIN),
//  REGION.G=(LG:2000K|:2000K)
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT36F001 DD DSN=&&TEMP36,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT31F001 DD DSN=&&TEMP31,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT10F001 DD *
( $A *FM=D1 ($P ARDATA % FILE 'TYPE IN ARDATA'))
( $A *FM=D1 ($P CRLFILE % FILE 'TYPE IN CRLFILE'))
```

```
/*
//G.FT42F001 DD
DSN=&&TEMP42,UNIT=WORK,DCB=LINES,SPACE=(TRK,(10,15)),
//    DISP=(OLD,(GP:KEEP|:DELETE))
/*
//G.FT37F001 DD
DSN=&&TEMP37,UNIT=WORK,DCB=LINES,SPACE=(TRK,(10,15)),
//    DISP=(OLD,(GP:KEEP|:DELETE))
/*
//G.FT12F001 DD *
( $A *FM=D1 ($P CFDATA % FILE 'TYPE IN CFDATA'))
/*
```

COMPAR JOB A1

```
//IDDCMPR JOB (ACCT,IDD,1-00),'USERNAM',PASSWORD=(XXXX),PRTY=2,
// TIME=(1,00)
//*MAIN ORG=(LL:RLVM370.IBM6670B|:RLR1EP1),LINES=35
//* *FILE SITE=RLR1,USER=IDD,FILE=RL1-F13
//  EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=BRDBIN,REGION.G=200K
(GP $A LASP JOB A1 |: $A LINP JOB A1) Default to printer.
//G.FT37F001 DD DISP=SHR,
// DSN=??.FY($P NAMY % % 'TYPE NAMY')
/*
//G.FT38F001 DD DISP=SHR,
// DSN=??.FQ($P NAMQ % % 'TYPE NAMQ')
/*
//G.FT10F001 DD *
($A *FM=A1 ($P CRDATA % FILE 'TYPE IN CRDATA'))
```

LASP JOB A1 *Called from previous job with GP.*

```
//G.FT09F001 DD DSN=RO.FB($P NAMB % % 'TYPE IN NAMB'),
//    DCB=LINES,SPACE=(TRK,(5,8)),
//    DISP=(NEW,CATLG),UNIT=STORAGE
```

/* MASTER JOB A1

```
//IDDMAST JOB (ACCT,IDD,3-30),'USERNAM',PASSWORD=(XXXX),PRTY=2,
// TIME=(3,30)
//*MAIN ORG=(LL:RLVM370.SYSTEM|:RLR1EP1),LINES=35
//* *FILE SITE=RL1,USER=IDD,FILE=RLR1-F13
//  EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=(B1:RCNBIN2|:RTHBIN),
//  REGION.G=960K
//G.FT07F001 DD DSN=&&TEMP7,UNIT=WORK,DCB=THREEKB,
//  SPACE=(TRK,(10,15)),
//    DISP=(NEW,PASS)
//G.FT02F001 DD DSN=&&TEMP2,UNIT=WORK,DCB=THREEKB,
//  SPACE=(TRK,(10,15)),
//    DISP=(NEW,PASS)
```

```
//G.FT03F001 DD DSN=&&TEMP3,UNIT=WORK,DCB=CARD10,SPACE=(TRK,1),
//    DISP=(NEW,DELETE)
//G.FT04F001 DD DSN=&&TEMP4,UNIT=WORK,DCB=THREEKB,
//   SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE)
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT10F001 DD *
(B1 $A RCNPOT DATA A1)
(BN $A BRNAD DATA A1|AU $A AUXAD DATA A1|B1 $A RCNCCD DATA A1
|HC $A CANAX DATA A1|PI $A PHOAD DATA A1|C1 $A *FM=A1 ($P CNTRL1
% FILE 'TYPE CONTROL1')|$A CANAD
 DATA A1)
($A *FM=A1 ($P LCONFG % FILE 'TYPE IN LCONFG'))
(BN $A BRNAD DATA A1|AU $A AUXAD DATA A1|B1 $A RCNCCD DATA A1
|HC $A CANAX DATA A1|PI $A PHOAD DATA A1|C1 $A *FM=A1 ($P CNTRL1
% FILE 'TYPE CORTROL1')|$A CANAD
 DATA A1)
($A *FM=A1 ($P UCONFG % FILE 'TYPE IN UCONFG'))
  -1
/*
//    EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=(B1:RCN2BIN|:TWOBIN),
//   REGION.G=800K
//G.FT02F001 DD DSN=&&TEMP2,UNIT=WORK,DCB=THREEKB,
//   SPACE=(TRK,(10,15)),
//    DISP=(OLD,DELETE)
//G.FT03F001 DD DSN=&&TEMP3,UNIT=WORK,DCB=CARD10,SPACE=(TRK,1),
//    DISP=(NEW,DELETE)
//G.FT11F001 DD DSN=&&TEMP11,UNIT=WORK,DCB=CARD10,
//   SPACE=(TRK,(5,8)),
//       DISP=(NEW,PASS)
//G.FT31F001 DD DSN=&&TEMP31,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT32F001 DD DSN=&&TEMP32,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT10F001 DD *
 (C2 $A *FM=A1 ($P CTRL2 % FILE 'TYPE CONTROL2')
|B1 $A RCN2INP DATA A1|BN $A BRINP DATA A1|
PI $A PHOINP DATA A1|AU $A AUTINP DATA A1|
MQ $A MQINP DATA A1|GP $A LINEINP DATA A1|NS $A RCF8INP DATA
A1|$A LINEINP DATA A1)
/*
//  EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=PPPBIN,REGION.G=20K
//G.FT21F001 DD DSN=&&TEMP21,UNIT=WORK,SPACE=(TRK,(10,15)),
//     DISP=(NEW,DELETE),DCB=CARD10
//G.FT11F001 DD DSN=&&TEMP11,UNIT=WORK,SPACE=(TRK,(5,8)),
//     DISP=(OLD,PASS),DCB=CARD10
```

```
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT02F001 DD *
($A RCGCFPX DATA A1)
/*
// EXEC JOBLIB,LIBRARY='RO.BRI',
// MEMBER=(B1:RCGBIN|:(SM:FEBBIN|:(BN:RESBIN|:(AU:BVNBIN|:RESBIN)))),
// REGION.G=(SM:900K|:2900K)
//G.FT10F001 DD DSN=&&&TEMP11,UNIT=WORK,SPACE=(TRK,(5,8)),
//    DCB=CARD10,DISP=(OLD,DELETE)
//G.FT20F001 DD DSN=&&&TEMP20,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT31F001 DD DSN=&&&TEMP31,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT32F001 DD DSN=&&&TEMP32,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT33F001 DD DSN=&&&TEMP33,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT35F001 DD DSN=&&&TEMP35,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT41F001 DD DSN=&&&TEMP41,UNIT=WORK,
// SPACE=(TRK,((CX:200|:10),(CX:40|:15))),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT42F001 DD DSN=&&&TEMP42,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT43F001 DD DSN=&&&TEMP43,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT44F001 DD DSN=&&&TEMP44,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT49F001 DD DSN=&&&TEMP49,DCB=CARD,SPACE=(TRK,(2,8)),
//    DISP=(NEW,DELETE),UNIT=WORK
//G.FT34F001 DD DCB=CARD10,SPACE=(TRK,((PT:8|:4),(PT:30|:8))),
//    DISP=(NEW,(PT:CATLG|:DELETE)),
// DSN=(PT:??.FF($P NAMF % % 'TYPE NAMF')|:&&&TEMP34),
//    (PT:UNIT=STORAGE|:UNIT=WORK)
//G.FT36F001 DD DCB=LINES,SPACE=(TRK,((GP:30|:10),(GP:40|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
// DSN=(GP:??FZ($P NAMZ % % 'TYPE NAMZ')|:&&&TEMP36),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
//G.FT19F001 DD DCB=CARD10,SPACE=(TRK,(4,8)),
//    DISP=(NEW,DELETE),DSN=&&&TEMP19,UNIT=WORK
//G.FT11F001 DD DCB=CARD10,SPACE=(TRK,(5,10)),
//    DISP=(NEW,DELETE),DSN=&&&TEMP21,UNIT=WORK
//G.FT02F001 DD DCB=CARD10,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DSN=&&&TEMP02,UNIT=WORK
//G.FT12F001 DD DCB=(GP:LINES|:LINES),
//    SPACE=(TRK,((GP:8|:10),(GP:30|:15))),
//    DISP=(NEW,(GP:CATLG|:(NS:DELETE|:PASS))),
```

```
// DSN=(GP:??.FG($P NAMG % % 'TYPE NAMG')|:&&TEMP12),
//    (GP:UNIT=STORAGE|:UNIT=WORK)
//G.FT09F001 DD SYSOUT=(MF:M|:A),DCB=PRINTER
/*
(NS $A MASD JOB A1|GP $A MASD JOB A1|$A (LA:MASX3|:MASX2) JOB A1)
```

Note that MASX3 **and** MASX2 **are as** SLSORT JOB A1 ***without first 4 lines.***

SLSORT JOB A1 SELECT JOB **is first part of** SLSORT.

```
//IDDSORL JOB (ACCT,IDD,1-00),'USERNAM',PASSWORD=(XXXX),PRTY=2,
// TIME=(1,00)
//*MAIN ORG=(LL:RLVM370.SYSTEM|:RLR1EP1),LINES=35
//* *FILE SITE=RLR1,USER=IDD,FILE=RL1-F13
// EXEC JOBLIB,LIBRARY='RO.BRI',MEMBER=BSTBIN,REGION.G=1600K
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT36F001 DD DISP=SHR,
// DSN=??.FZ($P NAMZ % % 'TYPE NAMZ')
/*
//G.FT37F001 DD DCB=LINES,SPACE=(TRK,((GP:200|:10),(GP:40|:15)),RLSE),
//    DISP=(NEW,(GP:CATLG|:PASS)),
// DSN=(GP:??.FY($P NAMY % % 'TYPE NAMY')|:&&TEMP37),
//    (GP:VOL=SER=MVSU01,UNIT=SYSDA|:UNIT=WORK)
// EXEC
JOBLIB,LIBRARY='RO.BRI',MEMBER=(SG:WATBIN|:(LA:LANBIN|:LAGBIN)),
// REGION.G=(SG:1500K|:1980K)
//G.FT09F001 DD SYSOUT=A,DCB=PRINTER
//G.FT45F001 DD DCB=CARD10,
//    SPACE=(TRK,((LA:8|:4),(LA:15|:8))),
//    DISP=(NEW,(LA:CATLG|:(NS:DELETE|:PASS))),
// DSN=(LA:??.FL($P NAML % % 'TYPE NAML')|:&&TEMP45),
//    (LA:UNIT=STORAGE|:UNIT=WORK)
//G.FT35F001 DD DSN=&&TEMP35,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT31F001 DD DSN=&&TEMP31,UNIT=WORK,SPACE=(TRK,(10,15)),
//    DISP=(NEW,DELETE),DCB=THREEKB
//G.FT10F001 DD *
($A *FM=D1 ($P ARDATA % FILE 'TYPE IN ARDATA'))
($A *FM=D1 ($P CRLFILE % FILE 'TYPE IN CRLFILE'))
/*
//G.FT12F001 DD DISP=SHR,
// DSN=??.FG($P NAMG % % 'TYPE NAMG')
/*
//G.FT37F001 DD DSN=&&TEMP37,
// UNIT=WORK,DCB=LINES,SPACE=(TRK,(10,15)),
//    DISP=(OLD,(GP:KEEP|:DELETE))
/*
```

GOP JOB A1

```
//IDDGOP JOB (ACCT,IDD,1-00),'USERNAM',PASSWORD=(XXXX),PRTY=2,
// TIME=(1,00)
//*MAIN ORG=(LL:RLVM370.SYSTEMI:RLR1EP1),LINES=35
//* *FILE SITE=RL1,USER=IDD,FILE=RLR1-F13
//  EXEC JOBLIB,LIBRARY='RO.BR1',MEMBER=LSFBIN,REGION.G=900K
//G.FT05F001 DD DSN=&&TEMP5,
//  DSN=&&TEMP5,UNIT=WORK,DCB=THREEKB,SPACE=(TRK,(10,15)),
//     DISP=(NEW,DELETE)
//G.FT09F001 DD DSN=&&TEMP9,
//  UNIT=WORK,DCB=THREEKB,SPACE=(TRK,(10,15)),
//     DISP=(NEW,DELETE)
//G.FT04F001 DD DSN=&&TEMP4,
// UNIT=WORK,DCB=THREEKB,SPACE=(TRK,(10,15)),
//     DISP=(NEW,DELETE)
//G.FT11F001 DD DSN=&&TEMP3,UNIT=WORK,DCB=CARD10,SPACE=(TRK,1),
//     DISP=(NEW,DELETE)
//G.FT03F001 DD SYSOUT=A,DCB=PRINTER
//G.FT01F001 DD *
{ $A *FM=D1 {$P DATAPP % FILE 'TYPE IN DATAPP'}}
/*
//G.FT02F001 DD *
{ $A *FM=D1 {$P DATAPC % FILE 'TYPE IN DATAPC'}}
/*
```

VI) DESCRIPTION OF THE INPUT DATA FOR THE MCDF PACKAGE IN ITS ORIGINAL FORM. (*Written previously by Dr I. P. Grant et al.*)

==========

Numerical data may take any of a number of forms. These forms are: integer, e.g. 35; fixed point number, e.g. 73.2; floating point number, e.g. 8.9E-4; fraction N1/N2, where N1 and N2 can be any of athe previous three forms, e.g. 3/2, 5.9/1.113, 1/5.E2.

Note that 6D-5 is illegal even if double precision is being used in the program. The card reading routine (CARDIN) will construct a floating point number to the full precision given, so the form 6E-5 should always be used.
Two further constructions may be used: N1 - N2, which is an nabbreviation for N1 N1+1 N1+2 .... N2; and N1*N2, which is an abbreviation for N2 N2 N2 N2 .... N2, the number of times N2 appears being determined by N1. For example,

1 - 5 = 1 2 3 4 5
3*-4 = -4 -4 -4

In the first construction, the minus sign must be isolated, i.e. have a blank on either side, whereas in the second, embedded blanks are not significant. The second construction is the same as in FORTRAN DATA statements.

```
*********************************************
***** READ A TITLE AND ORBITAL DATA ********
*********************************************
```

CARD 1 TITLE (COL. 1-72)

There are two forms of input for the orbital data :

(1) This form requires the definition of each relativistic configuration as in the CPC write-up.

(2) Alternatively non-relativistic configurations may be defined. Relativistic configurations are then generated from these.

CARD 2

READ TWO OR THREE INTEGERS

NMAN - number of configurations (NCF or MCF)
NWM - number of orbitals (NW or MW)
IOP - 0 if relativistic data
- 1 if nonrelativistic data, minimal print
- 2 if nonrelativistic data, print nonrelativistic configurations and transformation coefficients, and give the final eigenvectors in the LS basis.
> 2 as for 2 but do not print transformation coefficients

DEFAULT - IOP = 0

RELATIVISTIC CONFIGURATIONS DEFINED

NCF - number of configurations
NW - number of orbitals

CARDS 3 TO NW+2

ORBITAL DATA

Read NW cards which contain the following data -
one card for each orbital J
(1) Label (1S , 2P-, 2P , ...)
(2) Optional screening numbers for initial estimates of wavefunctions
(3) Orbital occupation numbers for each configuration

FORMAT : I2 , A2 , optional real , 0 or 1 or NCF integers

NP(J) - principal quantum number
NH(J) - label indicating kappa value (S ,P-,P ,D-,D , ...)

CXP(J) - screening number. must be negative so that the effective charge Z is given by Z+SC . Default CXP(J) = 0
Orbital occupation numbers for each configuration
(a) 0 numbers - subshell is full in each configuration
(b) 1 number - each configuration has this occupation number
(c) NCF numbers - occupation number for each configuration

****
*** ANG ***
****

FORMAT : LABEL (COL. 1-4) , 0 - 8 INTEGERS

The label 'ANG ' is followed by up to 8 options

1 - write out the angular coefficients calculated
2 - output from RKCO,COR,MUMDAD,VIJOUT (called by RKCO)
3 - output from NJSYM
4 - output from VIJOUT (called by TNSRJJ)
5 - output from TMSOUT
6 - output from TNSRJJ
7 - suppress call to CFOUT
8 - suppress calls to all angular momentum packages

CARDS 2 TO NCONF+1

READ NCONF CARDS

NCONF is the number of configurations requiring
j , seniority and / or coupling information.
Each card has the following format :

I - number of the configuration being defined (in the sense of going left to right in the occupation cards)

J,V - pairs of J & seniority values.
J values are required for those orbitals whose occupation in the configuration under consideration is not zero, one, full or full - one .
Seniority is only used for J=7/2 orbitals (f ,g-) with occupation 4 and J=2 or 4. The program cannot handle the case of J > 7/2 & 2 < occupation no. < 2J-1.

J is given as an integer or half-integer (1/2, 3/2, etc)
Seniority is given as an integer.

JCUP(K),K=1,NOPEN-1 - the coupling information is given only if there is more than one open shell in the configuration. Note that exactly nopen-1 numbers must be given - the program does not know that J and 0 always couple to give J ! (NOPEN is the number of open shells in the configuration I). The J values should be given in the format described above.

==========

NONRELATIVISTIC CONFIGURATIONS DEFINED

The following input data is for non-relativistic configurations :

The occupation numbers are defined as for the relativistic case - see above
N.B. Screening can only be given for each non-relativistic orbital - thus the screening for np and np- will be the same, for example.

MCF - number of non-relativistic configurations
MW - number of non-relativistic orbitals

CARDS 3 TO MW+2

ORBITAL DATA

Read MW cards which contain the following data -
one card for each orbital J
(1) Label (1s , 3d , 2p , ...)
(2) Optional screening numbers for initial estimates of wavefunctions
(3) Orbital occupation numbers for each configuration

FORMAT : I2 , A2 , optional real , 0 or 1 or MCF integers

NP(J) - principal quantum number
NH(J) - label indicating l value (s ,p ,d , ...)
CXP(J) - screening number - must be negative so that the effective charge Z is given by Z+SC . Default CXP(J)=0
Orbital occupation numbers for each configuration
(a) 0 numbers - subshell is full in each configuration
(b) 1 number - each configuration has this occupation number
(c) MCF numbers - occupation number for each configuration

****
*** ANG ***
****

FORMAT : Label (col. 1-4) , 0 - 8 integers

The label 'ANG' is followed by up to 8 options

1 - write out the angular coefficients calculated
2 - output from RKCO,COR,MUMDAD,VIJOUT (called by RKCO)
3 - output from NJSYM
4 - output from VIJOUT (called by TNSRJJ)
5 - output from TMSOUT
6 - output from TNSRJJ
7 - suppress call to CFOUT
8 - suppress calls to all angular momentum packages

READ ONE CARD CONTAINING ONE OR NMAN NUMBERS

These are the total J-values of the nonrelativistic configurations
as defined above

(1) one positive number - each configuration has this J-value
(2) one negative number - take all possible J-values
(3) MCF numbers - these are the J-values of the configurations
in the order described above

==========

****
*** MCP ***
****

FORMAT : Label "MCP " , 1 - 3 integers

DATA :

(1) stream number for MCP coefficients - this is normally 8.
set to zero if no MCP file is required.
(2) options - 1 - include core - peel coefficients
2 - do not include coefficients of i(a,b) integrals
(t-coefficients)

==========

****
*** MCDF ***
****

CARD 1 FORMAT : Label "MCDF" , 1 - 50 options (integers)

Option 1 - use coulomb wavefunctions as initial estimates
rather than Thomas-fermi functions. This only applies
if no dump is read in, or for those orbitals in the present
problem that are not included in the dump.

2 - set lagrange multipliers to zero

3 - set lagrange multipliers between orbitals of the
same generalised occupation number to zero

4 - use the Mann & Cowan modification to the potentials

5 - write out the hamiltonian matrix whenever it is calculated

6 - write out the eigenvalues and eigenvectors of the hamiltonian
matrix whenever it is diagonalised

7 - write out the MCP coefficients used

8 - write out the grid and wave-functions at convergence

9 -) these are used when

10 -) loading from a dump -

11 -) see below for details

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

14 -)

15 -)

16 -) print options - see program listing for details

17 -) DANGER - THESE CAN PRODUCE A LOT OF PAPER

18 -)

19 -)

20 - suppress call to MCDF routines

21 - when loading a dump, do not rescale with Z

22 - do not Schmidt orthogonalise wave-functions at any stage

23 - print only the first 8 vectors in MATOUT

30 - print eigenvectors in LS basis (set automatically if IOP>1)

32 - do not print eigenvectors in jj coupled basis

41 - copy old orbitals file into new orbitals file

STARTING FROM A DUMP :

(a) default - options 9, 10 & 11 not set
Read wave functions, MCP coefficients, generalised occupation numbers,
and mixing coefficients. Skip the low accuracy runs through SCF.
This is best used only when restarting an identical problem,
or possibly when only Z is changed (but it is usually better to
set option 10 in this case)

(b) Option 10 set
Read wave functions and MCP coefficients. Go through the low accuracy

runs. This should be used when the same configurations have been used in both dump and present run, but something else (grid, accuracy, Z, internal limit of integration, calculation type (AL/OL/EOL/EAL)) has been altered.

(c) Option 11 set
Read only wave-functions

(d) Option 9 set
Read only MCP coefficients

CARD 2 DATA SET STREAM NUMBERS

3 - 5 integers

IR1 - load MCP stream - 'MCP' file - normally 8
IR2 - load MCDF stream - 'read from dump' file - normally 9
IP2 - write MCDF stream - 'write to dump' file - normally 10
IR3 - load orbs stream - 'read from orbitals' file - normally 13
- default 0
IP3 - write ORBS stream - 'write to orbitals' file - normally 14
- default 0

Set to zero if there is no corresponding file

CARD 3 BASIC DATA

Between 1 and 5 real numbers

Z - atomic number
H - step size for grid
RNT - first grid point
Grid is defined as :
R(J)=RNT*EXP((J-1)*H) J=1, ... ,N
ACCY - accuracy to which the wave-functions and mixing coefficients are to be converged
CON - factor multiplying the speed of light -
if this is set to 1000 the non-relativistic limit is approached

N.B. If numbers are given in exponential form they must be given using "e" rather than "d" to indicate exponentiation to the power 10

1 number - Z , default H, RNT, ACCY, CON

2 numbers - Z, H , default RNT, ACCY, CON
3 numbers - Z, H, RNT , default ACCY, CON
4 numbers - Z, H, RNT, ACCY , default CON
5 numbers - Z, H, RNT, ACCY, CON

Also, inputing a zero value gives the default.

Default settings

H = 0.05
RNT = 1.0E-05
ACCY = 1.0E-08
CON = 1.0

CARD 4 - ATOMIC WEIGHT AND MAXIMUM FACTOR MULTIPLYING EXCHANGE

FORMAT : 0 - 2 real numbers

Default 0 and 1 respectively

N.B. this card must be included even if it contains no numbers.

OPTIONAL CARD - NUCLEAR TYPE

FORMAT : label "NUC " , 1 integer , 1 - 4 real numbers

Default - point nucleus

NUCTYP=1 uniform charge distribution
Optionally input one further number - the nuclear radius
Default atomic mass is take from card 3

NUCTYP=2 Fermi charge distribution
Optionally input two further numbers - the nuclear radius
- the skin thickness
Default values are given by
RADIUS = 2.2291E-5 * (ATOMIC MASS)**1/3 - 0.90676E-5
SKIN THICKNESS = 1.039E-5

NUCTYP>2 Some other charge distribution : the user must supply his own routine NCHARG which evaluates R**2 times the nuclear charge distribution

---

OPTIONAL CARD - FIXED ORBITALS

Default - no fixed orbitals

FORMAT : "FIX " , 1 - nw-1 integers

These are the orbitals to be held fixed

In the case of a nonrelativistic calculation, these are non-relativistic orbitals that we fix. In this case it is not possible to fix nl without fixing nl- at the same time.

OPTIONAL CARD - SOURCE OF ORBITALS

FORMAT : "LOAD" , NW or MW integers (one for each orbital)

0 : load from dump file
1 : load from orbitals file
2 : use Thomas-Fermi wavefunctions
3 : use coulomb wavefunctions

If the orbital cannot be obtained in the prescribed manner, the next option is taken.

OPTIONAL CARD - ORBITALS TO BE DUMPED

FORMAT : "ORB " , 1 - NWM integers

Input the orbital numbers that are to be dumped to the ORBS file, defined relativisticly or non-relativisticly depending on IOP.
Any fixed orbitals will not be dumped.

CARD 9 CALCULATION TYPE

The label in columns 1 to 4 defines the calculation type.

(1) "AL " - average level
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.

(2) "EAL " - extended average level

Follow the label with 0 or 1 or NCF or NCF+1 or MCF or MCF+1 integers.

0 integers - take configuration weights proportional to 2J+1 and allow 3 iterations at final accuracy

1 integer - take configuration weights proportional to 2J+1 and allow this number of iterations at final accuracy.

NCF integers - these are the configuration weights. Allow 3 iterations at final accuracy.

NCF+1 integers - these are the configuration weights followed by the number of iterations at final accuracy.

MCF integers - these are the nonrelativistic configuration weights.

MCF+1 integers - these are the nonrelativistic configuration weights followed by the number of iterations at final accuracy.

(3) "OL " - optimal level

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

(4) "EOL " - extended optimal level

Optimise on several levels - more than one, but less than NCF.
Input (1) the number of levels to be optimised on
(2) the numbers of the levels to be optimised on

For cases (3) & (4) there are also two optional parameters -

NITIT - the maximum number of iterations at final accuracy - default 6

CHECK - the damping factor for the mixing factors - default 0.15

N.B. It is possible to perform C.I. calculations by setting NITIT = 0 (NITIT = number of iterations) in any of the above types of calculation.
This involves setting up a hamiltonian using orbitals from a previous dump and (usually) new MCP coefficients.
This, in effect, fixes all the orbitals used. no SCF iterations are performed and the wavefunctions are as before.

==========

==========

****

*** MCT ***
****

FORMAT : Label "MCT " , 2 or 3 integers

(1) DS number for output stream - usually 12 -
set it to zero if no file is required.
(2) order of the tensor operator
(3) parity of the tensor operator :
1 for even parity (M1,E2, ...)
-1 for odd parity (E1,M2, ...)
0 for both parities (default)

==========
========

****
*** MCBP ***
****

FORMAT : Label "MCBP" , 1 integer

(1) DS number of the MCBP file - usually 11 -
use zero if no file is required

==========
========

****
*** BENA ***
****

FORMAT : Label "BENA" , 0 - 20 integers

Options : -

1 print out coulomb matrix (no longer functional)
2 print out eigenvalues of coulomb matrix
3 print out eigenvectors of coulomb matrix
4 print out breit matrix
5 print out contributions of breit matrix elements to eigenvalues
6 print out eigenvectors of coulomb+breit matrix
8 print out each contribution to the breit matrix elements
9 print out 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
13 print restart information
15 print breit eigenenergies and eigenvectors in the coulomb basis
20 suppress the call to the bena package

****
*** INPUT DATA FOR BREIT ***
*** ENERGY ANALYSIS PACKAGE ***
****

FORMAT : 2 - 4 integers

(1) DS number of file containing MCBP coefficients - usually 11
(2) DS number of file containing wavefunctions - usually 9 or 10
(3) atomic weight - default infinity
(4) factor multiplying the velocity of light -
1.0E-03 will enable the long wavelength frequency limit to be obtained. Default : 1.0

==========

****
*** OSCL ***
****

FORMAT : Label "OSCL" , 0 - 20 integers

Options : -

1 print out the CSF matrix elements
2 print value of coulomb and gauge dependent integrals
3 print the integrand of the gauge dependent integrals
4 print the I and J integrals
5 print the integrands of the I and J integrals
6 print bessel functions
7 print 1-electron matrices
8 print MCT coefficients
9 use coulomb eigenvectors and eigenvalues (default)
10 use coulomb+breit eigenvectors and eigenvalues
11 use coulomb+breit+QED eigenvectors and eigenvalues
12 write out the hamiltonian eigenvectors and eigenvalues
20 suppress the call to the oscillator strengths routines

```
************************************
***     INPUT DATA FOR OSCL      ***
*** OSCILLATOR STRENGTHS PACKAGE ***
************************************
```

FORMAT : 2 - NCF+2 integers

(1) DS number of file containing MCT coefficients - usually 12
(2) DS number of file containing wave functions - usually 9 or 10
(3) List of levels between which matrix elements are to be calculated. The default is all levels.

```
================================================================================
========

***********
*** END ***
***********
```

End of input data. This card must be included !

VII) PREREQUISITES BEFORE RUNNING PROGRAM.

The following actions must be taken before attempting to run these programs.

1) A copy of all the JOB files mentioned above and listed below must be obtained through copying from one of the authors[#] CMS file space using the command: **RLINK CODE B RCODE** where code is supplied by the author. then copy the files with **COPY MCDF JOB B MCDF JOB A1** etc. copies of sample data files are also desireable and all the HFR package JOB and DATA files listed in section X of Report RL-83-030[8].

2) The JCL JOB files must be altered where they name OS. DATA-SETS. In those listed below all occurrences of **??** must be changed to the subproject name of the proposed user or the letters which appear before the first period in the user's OSDISK DATA-SET.

VIII) LISTINGS OF OUTPUT FROM MCDF HFR PROGRAMS AND SORTING AND COMPARISON PROGRAMS.

This section presents extracts from the output listings of the following programs and JOBS.

A) MCDF Selected pages of output from MCDF JOB A1. See Section II for more details.

The first page of output shows the beginning only of the complex relativistic form of input data (see Section VI for detail) prepared by the program, which is derived from the non-relativistic input (also re-printed). The next page is the start of the LS core and configuration definitions or 'designations', which were preceeded by JJ 'designations': which are not reproduced here. The term numbers associated with these 'designations' are used later later for indexing. No examples are given here of the next part of the output which includes dimensions, configuration mixing coefficients,eigenvalues and orbital properties. The MCDF output later prints a Summary of contributions to the energy levels both as computed and normalised to the lowest calculated level. They are repeated in AUs., Rydbergs, cm^{-1} and EV. Reproduced here is the start of the normalised energy level printout in cm^{-1} on which the Breit and QED components contributing to the energy levels are self evident. Both the energy levels without Breit and QED (in column headed "ZERO-ORDER" and with: (column "TOTAL") are used later and the LEVEL numbers are also cross references. Thus on the next MCDF sheet, which provides oscillator strengths, the level numbers correspond to the ZERO-ORDER levels in the table. In this table (only the start shown) spontanious transition probabilities and oscillator strengths (unweighted) are listed for all possible transitions both for COULOMB and BABUSKIN[13,14] gauge. The wavelength in Å and wavenumber in cm^{-1} (not AU) are given aswell as ‹//H//› the H matrix element which is analogous to the Racah dipole matrix elements applied in the HFR programs. The BABUSKIN gauge gives results similar to the HFR computations which apply the "length" type computations. The COULOMB

values have a similar mathematical basis to the "velocity" type computations. Both COULOMB and BABUSKIN are transmitted to the next section of the suite as added at RAL which converts them into weighted oscillator strengths gf in the form usually found in the literature. It should be noted that the eigenvector matrix and energy matrix output from the Oxford University version, which were not separated into individual matricies for each J value and parity, are not printed by the RAL version. The leading eigenvector components of levels can be conveniently be obtained from the sorting routine output by taking the square root of the level compositions.

B) HFR Output (Program Sections: RCN31, RCN2, and RCG) from MASTER JOB A1 or else SLPM JOB A1 and SPEC JOB A1 in series. Extracts from short "*DEFAULT OPTION*" print outs are shown. For further details of other "*OPTIONS*" see Report RL-83-030[8].

a) Output from first section RCN31 using "*DEFAULT OPTION*" input line residing in CMS file CANAD DATA A1:

200-5 2 10 1.0 5.E-08 1.E-11-2 130 1.0 0.65 0.0 0.50 0.0 0.70

The page (there will be one for each configuration) of output shows the expectation values $\langle r^{-3} \rangle$ $\langle r^{-2} \rangle$ to $\langle r^{6} \rangle$ (under (r-3) etc.) for each orbital and EE the corresponding eigenvalue in Rydbergs. The next lines below show sums and averages. Next follows "ZETA" spin-orbit information with the Blume-Watson component clearly labelled then ZETA(1/r(dv/dr)) under (R*VI) , then KE + e-n energy under I(RYD) then the mass-velocity, Darwin and total relativistic energy perturbations under EVEL, EDAR and EREL.

In the next few lines, which provide correlation correction data, EPS FGR is with relativistic corrections, N*R and N*RC are effective quantum numbers n* without and with correlation, ECT is total correlation energy for subshell, EC individual correlation energies and ETOTRL the total relativistic energy. After ETOT pairs of figs. correspond to no correlation energy,old correlation energy and new correlation energy.

Note that in a longer option print out would include wavefunctions, radial (PNL) ***and cancellation factor information under*** FRAC.

b) Output from the next section RCN2 on the next sheet using input "*DEFAULT OPTION*" line contained in CMS file LINEINP DATA A1:

G5INP23 0 0 00 0 000 1 9999999999 0000018 09

The page of output shows the direct configuration-interaction integral R^k_d under RDK and the exchange configuration-interaction integral R^k_e under REK. Next are printed values of the integral $\int rP_1P_2dr$ under R INTEGRAL and the Racah reduced radial dipole matrix elements under REDUCED MUPOLE ELEMENT.

The final combined output from RCN31 and RCN2 is arranged by binary program PPPBIN in the form required for input to RCG and printed as shown on the next sheet. The first line is the control line for RCG and lines giving occupation data for each configuration follow. Next are the values of

Slater Parameters with the last fig. indicating the type thus 0 is E_{av} , 1 or 3 are F^K , 2 for spin-orbit , 4 is G^K and 5 is R^K. These parameters will have been scaled according to the factors in the last columns (99 in this case represents no scaling). The Racah reduced radial dipole matrix elements mentioned above reappear on the next lines.

c) The output from RCG prints extensive information especially if certain "*OPTIONS*" are applied (see Report RL-83-030[8].) for more details. Here three pages are reproduced which contain perhaps the most used information.

The first page shows the Slater Parameters along with their scaling factors (no scaling in this case). The next page prints an eigenvector matrix: there is one for each J value of each parity. At the head of each column is a eigenvalue and the beginning of each row a basis-state label. At the base of each column appears the designation which has the largest eigenvector component for the eigenvalue heading the column. This may not be unique (see sorting routine in section F). These same designations are printed on the next sheet after the energy levels. Other columns give wavenumbers (in cm^{-1} , wavelengths in Å, weighted oscillator strengths "GF" and LOG GF, relative line strengths S/P**2 (where "S" is the Line strength and "P" is the Racah reduced radial dipole matrix element), then transition probabilities GA and cancellation factors. At the head of the page are printed the configuration labels used by this and following programs.

C) MC-Dirac-Fock output form DIRSORT JOB A1 (after previously running MCDF JOB A1) This output is first with Breit and QED then wthout. The four sheets shown are with Breit and QED.

a) The first sheet shows energy levels in cm^{-1} and their percentage composition for terms. Designations at this point are not necessarily unique and where duplication arises a warning is given. The term numbers 'TM NO' refer to the term order at the beginning of MCDF and the level numbers 'LVL NO' to the level orders in MCDF.

b) The next sheet shows the unique dominant terms chosen for designation. Term and level numbers are indexed.

c) The third output sheet gives ordered MCDF wavelengths (Å), wavenumbers in cm^{-1} gf's and terms. Term and level numbers are indexed.

a,b and c are repeated twice: firstly with Breit and QED included and with BABUSKIN gf values and then without Breit and QED and with COULOMB gf values.

d) The last DIRSORT output sheet arranges the output into multiplets and configurations printing wavelengths (Å), wavenumbers in cm^{-1} gf's and terms with Breit and QED included and with BABUSKIN gf values. The format is identical to the SLSORT HFR output and the BABUSKIN gfs are usually similar to the HFR '*length*' gfs.

D) Output of COMPAR JOB A1 in which MCDF (MCDF) and HFR ab initio calculations are compared . This output is first with Breit and QED then wthout. The two tables shown are with Breit and QED.

The example shows comparisons for the $3s3p^3$,$3s^23p3d$ and $3p^33d$

configurations in Si I in cm^{-1}. For the MCDF HFR comparisons interactions between the $3s3p^3$, $3s^23p3d$ and $3p^33d$ configurations were included. The first table combines all the configurations whereas the second compares each single $3p^33d$ configuration. Here is an explanation of the headings:

HF EN LEVEL HFR energy level. (1)
DF EN LEVEL MCDF energy level. (2)
DIFFERENCE (2)-(1)
AVERAGE Average of (2)-(1)
HF ENLV MOD (1)-AVERAGE. (3)
DIFF MOD (3)-(2)
STANDARD DEVIATION Applies to differences.

E) HFR output from SLSORT including that from SELECT which is the first part of SLSORT. (see Report RL-83-030[8] Section IX for further information)

The first sheet (there is one for each J value) shows precentage term composition of levels and dominant terms (J=2 shown here). Similar procedures are used in section C above. The last arranges the output into multiplets and configurations printing wavelengths (Å), wavenumbers in cm^{-1} gf's and terms. The format is identical to the DIRSORT MCDF output.

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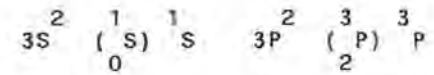
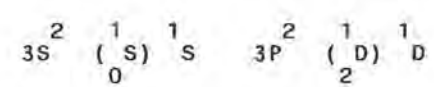
```
++++++++++ DATAIN ++++++++++

CARD INPUT

  1  =  FE XIII 3SN3PN3DN
  2  =  4 6 2

NON-RELATIVISTIC CONFIGURATIONS ARE DEFINED

  3  =    1S   2 2 2 2
  4  =    2S   2 2 2 2
  5  =    2P   6 6 6 6
  6  =    3S   2 1 2 0
  7  =    3P   2 3 1 3
  8  =    3D   0 0 1 1
  9  =   ANG
 10  =   -1

EQUIVALENT RELATIVISTIC INPUT DATA

 65    9
1S
2S
2P-
2P
3S     2  2  2  2  2  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2  2  2  C
       2  2  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  C
       0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
3P-    1  0  1  2  0  1  2  1  1  0  2  1  1  0  1  0  1  0  0  1  1  0  0  1  C
       0  0  0  1  2  1  1  1  0  2  2  1  1  1  1  1  0  0  2  2  1  1  1  1  C
       1  1  0  0  2  2  1  1  1  1  1  0  0  2  1  1  0
3P     1  2  1  0  2  2  1  2  2  3  1  2  2  3  2  1  0  1  1  0  0  1  1  0  C
       1  1  1  2  1  2  2  2  3  1  1  2  2  2  2  2  3  3  1  1  2  2  2  2  C
       2  2  3  3  1  1  2  2  2  2  2  3  3  1  2  2  3
3D-    0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  0  1  0  1  0  1  C
       1  0  1  0  0  1  0  0  0  1  0  1  0  1  0  0  1  0  1  0  1  0  1  0  C
       1  0  1  0  1  0  1  0  1  0  1  1  0  1  0  1  1
3D     0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1  1  0  1  0  1  0  1  0  C
       0  1  0  1  1  0  1  1  1  0  1  0  1  0  1  1  0  1  0  1  0  1  0  1  C
       0  1  0  1  0  1  0  1  0  1  0  0  1  0  1  0  0
ANG
  1     2
  2  2
  3     1
  5  0
  6  2        1   3
  7     2
  8  2        1   2
  9  2        0   2
 10     2
 11     1
 12  2        1   1
 13  0        1   1
 14     1
 15  0        0   0
 16     4
 17     3
 18     3
 19     3
 20     2
 21     2
 22     2
```

```
 23      2
 24      1
 25      1
 26      1
 27      0
 28 2         5/2 5
 29      4
 30 2         5/2 4
 31 2         5/2 4
 32 2         3/2 4
 33      4
 34      3
 35      3
 36 2         5/2 3
 37 2         5/2 3
 38 2         3/2 3
 39 2         3/2 3
 40 0         1/2 3
 41      3
 42      3
 43      2
 44      2
 45 2         5/2 2
 46 2         5/2 2
 47 2         3/2 2
 48 2         3/2 2
 49 0         1/2 2
 50 0         1/2 2
 51      2
 52      2
 53      1
 54      1
 55 2         5/2 1
 56 2         5/2 1
 57 2         3/2 1
 58 2         3/2 1
 59 0         1/2 1
 60      1
 61      1
 62      0
 63 2         5/2 0
 64 2         3/2 0
 65      0

 11  =  MCP 8
 12  =  MCDF
 13  =  8 0 10
 14  =  26.0
 15  =  55.85
 16  =  EAL
 17  =  MCT 12 1 -1
 18  =  MCBP 11
 19  =  BENA
 20  =  11 10 55.85 1.0
 21  =  OSCL
 22  =  12 10
 23  =  END


++++++++++ CFOUT ++++++++++
```

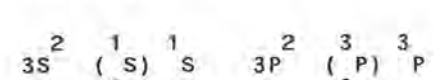
CONFIG. 1 EVEN PARITY J = 2



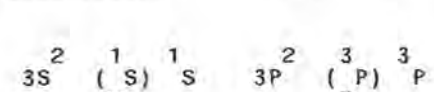
CONFIG. 2 EVEN PARITY J = 2



CONFIG. 3 EVEN PARITY J = 1

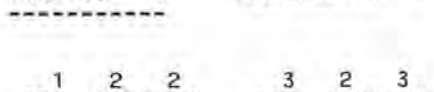


CONFIG. 4 EVEN PARITY J = 0



CONFIG. 5 EVEN PARITY J = 0

CONFIG. 6 ODD PARITY J = 3



CONFIG. 7 ODD PARITY J = 2

39	9.52888175D+00	-1.10817524D-02	9.51780000D+00	9.41590004D-04	-8.37292345D-03	-7.43133344D-03	9.5103686686301D+00
40	9.68020482D+00	-7.03048013D-03	9.67317434D+00	9.42577065D-04	-8.44672134D-03	-7.50414427D-03	9.6656701916088D+00
41	9.69797856D+00	-9.00928038D-03	9.68896928D+00	9.43018507D-04	-8.43323809D-03	-7.49021958D-03	9.6814790594828D+00
42	9.71980105D+00	-1.15626115D-02	9.70823844D+00	9.43514052D-04	-8.41301240D-03	-7.46949835D-03	9.7007689424860D+00
43	9.81048249D+00	-8.99089557D-03	9.80149160D+00	9.42446883D-04	-8.44205562D-03	-7.49960874D-03	9.7939919900688D+00
44	9.93780434D+00	-6.58197526D-03	9.93122236D+00	9.38663684D-04	-8.44841411D-03	-7.50975043D-03	9.9237126136131D+00
45	1.00095653D+01	-8.41291681D-03	1.00011524D+01	9.30141579D-04	-8.27562954D-03	-7.34548796D-03	9.9938068955301D+00
46	1.01342046D+01	-5.47759164D-03	1.01287270D+01	9.32412580D-04	-8.41977205D-03	-7.48735947D-03	1.0121239652591D+01
47	1.01609340D+01	-7.60221530D-03	1.01533318D+01	9.31876862D-04	-8.37714846D-03	-7.44527160D-03	1.0145886541817D+01
48	1.01619694D+01	-5.06135738D-03	1.01569081D+01	9.31160974D-04	-8.38949518D-03	-7.45833421D-03	1.0149449730702D+01
49	1.01712324D+01	-9.29177908D-03	1.01619406D+01	9.31176549D-04	-8.26123836D-03	-7.33006181D-03	1.0154610518292D+01
50	1.01828032D+01	-8.53886831D-03	1.01742643D+01	9.31720041D-04	-8.25589693D-03	-7.32417689D-03	1.0166940111547D+01
51	1.01852818D+01	-1.16105483D-02	1.01736713D+01	9.31611311D-04	-8.22388685D-03	-7.29227554D-03	1.0166378991202D+01
52	1.02115486D+01	-7.47978931D-03	1.02040688D+01	9.30765436D-04	-8.30339739D-03	-7.37263195D-03	1.0196696180430D+01
53	1.02190928D+01	-8.35828770D-03	1.02107345D+01	9.33045311D-04	-8.30562751D-03	-7.37258219D-03	1.0203361955006D+01
54	1.02854076D+01	-9.64212508D-03	1.02757655D+01	9.40597993D-04	-8.31565018D-03	-7.37505219D-03	1.0268390443077D+01
55	1.02859750D+01	-1.04353474D-02	1.02755396D+01	9.34254326D-04	-8.26514919D-03	-7.33089487D-03	1.0268208742021D+01
56	1.03228212D+01	-9.94249981D-03	1.03128787D+01	9.39457862D-04	-8.22791143D-03	-7.28845357D-03	1.0305590230013D+01
57	1.03301992D+01	-1.05364647D-02	1.03196627D+01	9.39043144D-04	-8.27469004D-03	-7.33564689D-03	1.0312327086932D+01
58	1.05898376D+01	-1.01606503D-02	1.05796770D+01	9.32079157D-04	-8.23462788D-03	-7.30254873D-03	1.0572374409514D+01
59	1.08331575D+01	-8.13780441D-03	1.08250197D+01	9.23215531D-04	-8.21214060D-03	-7.28892507D-03	1.0817730778735D+01
60	1.09461842D+01	-7.36102895D-03	1.09388232D+01	9.32717310D-04	-8.41084417D-03	-7.47812686D-03	1.0931345064474D+01
61	1.10279904D+01	-8.84313945D-03	1.10191473D+01	9.33833110D-04	-8.30247511D-03	-7.36864200D-03	1.1011778629118D+01
62	1.10763789D+01	-9.65387410D-03	1.10667251D+01	9.34730648D-04	-8.24468169D-03	-7.30995105D-03	1.1059415109294D+01
63	1.12834118D+01	-9.19362526D-03	1.12742182D+01	9.27928588D-04	-8.22755877D-03	-7.29963019D-03	1.1266918536950D+01
64	1.13379738D+01	-1.01486239D-02	1.13278252D+01	9.37979201D-04	-8.31650564D-03	-7.37852644D-03	1.1320446632275D+01
65	1.18027500D+01	-8.73331523D-03	1.17940167D+01	9.19404661D-04	-8.13874221D-03	-7.21933755D-03	1.1786797391659D+01

****

SUMMARY OF CONTRIBUTIONS TO ENERGY LEVELS. (UNITS = CM-1. 1 A.U. = 0.21947246D+06 CM-1)

LEVEL	ZERO-ORDER	BREIT	ZERO. + BREIT	VACUUM POLARIZ.	SELF ENERGY	Q.E.D.	TOTAL
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	9.36287245D+03	-3.12689700D+02	9.05018275D+03	2.21933673D-01	1.47578473D+01	1.49797810D+01	9.0651625308333D+03
3	1.93536569D+04	-5.87206435D+02	1.87664504D+04	3.57868694D-01	2.37970717D+01	2.41549404D+01	1.8790605367667D+04
4	5.24295766D+04	-6.65220545D+02	5.17643560D+04	4.36459387D-01	2.90230901D+01	2.94595495D+01	5.1793815565262D+04
5	1.04247867D+05	-5.66563691D+02	1.03681303D+05	4.43867345D-01	2.95156946D+01	2.99595619D+01	1.0371126284051D+05
6	1.90516454D+05	-3.02780983D+02	1.90213673D+05	5.17784946D+01	-4.50191496D+02	-3.98413002D+02	1.8981526038533D+05
7	2.66794057D+05	-2.99102041D+02	2.66494955D+05	4.63391802D+01	-4.03919233D+02	-3.57580053D+02	2.6613737535319D+05
8	2.67027384D+05	-3.33845669D+02	2.66693539D+05	4.64549221D+01	-4.04906829D+02	-3.58451907D+02	2.6633508688305D+05
9	2.69844239D+05	-5.80074954D+02	2.69264164D+05	4.66821370D+01	-4.00537405D+02	-3.53855268D+02	2.6891030920586D+05
10	3.14381437D+05	-3.61736641D+02	3.14019700D+05	4.61815712D+01	-3.95221011D+02	-3.49039440D+02	3.1367066093065D+05
11	3.14852036D+05	-5.14980006D+02	3.14337056D+05	4.49240875D+01	-3.82778816D+02	-3.37854728D+02	3.1399920148302D+05
12	3.14935098D+05	-4.64534118D+02	3.14470564D+05	4.61019837D+01	-3.93026220D+02	-3.46924236D+02	3.1412363989946D+05
13	3.43282217D+05	-8.76132555D+02	3.42406084D+05	3.34013453D+01	-2.75352911D+02	-2.41951565D+02	3.4216413250824D+05
14	4.02018475D+05	-2.42939890D+02	4.01775535D+05	5.33440632D+01	-4.68059976D+02	-4.14715913D+02	4.0136081909552D+05
15	4.15972974D+05	-9.71148688D+02	4.15001825D+05	2.45900049D+00	-1.32530035D+01	-1.07940030D+01	4.1499103082195D+05
16	4.23050668D+05	-1.28081011D+03	4.21769858D+05	2.25168848D+00	-3.78345999D+00	-1.53177151D+00	4.2176832625325D+05
17	4.33386651D+05	-1.67921111D+03	4.31707440D+05	2.42673551D+00	8.01132338D+00	1.04380589D+01	4.3171787812798D+05
18	4.33407153D+05	-5.81354062D+02	4.32825799D+05	4.71380856D+01	-3.95265749D+02	-3.48127664D+02	4.3247767110630D+05
19	4.86384858D+05	-8.53779244D+02	4.85531078D+05	1.40352208D+01	-1.20975801D+02	-1.06940580D+02	4.8542413778713D+05
20	4.94410464D+05	-9.23102414D+02	4.93487362D+05	8.08082213D+00	-6.16922123D+01	-5.36113902D+01	4.9343375014677D+05
21	4.99361478D+05	-1.14852876D+03	4.98212950D+05	1.65047331D+01	-1.24298728D+02	-1.07793995D+02	4.9810515556107D+05
22	5.01769985D+05	-1.13408198D+03	5.00635903D+05	8.25298512D+00	-4.57020066D+01	-3.74490215D+01	5.0059845358057D+05
23	5.06103977D+05	-1.19990851D+03	5.04904069D+05	8.58434298D+00	-4.91378058D+01	-4.05534628D+01	5.0486351508785D+05

TRANSITION	GAUGE	ENERGY A.U.	< // H // >	SPONT TRANS PROB. /SEC.	OSCILLATOR STRENGTH	
1 -> 7	COULOMB:	2.6679406D+05	3.00112D-03	7.33999D+08	4.63795D-02	374.821
	BABUSKIN:		3.94232D-03	1.26658D+09	8.00322D-02	
7 -> 1	COULOMB:	-2.6679406D+05	1.73270D-03	-2.20200D+09	-1.54598D-02	-374.821
	BABUSKIN:		2.27610D-03	-3.79975D+09	-2.66774D-02	
1 -> 12	COULOMB:	3.1493510D+05	2.61326D-03	6.56959D+08	2.97906D-02	317.526
	BABUSKIN:		3.45187D-03	1.14626D+09	5.19786D-02	
12 -> 1	COULOMB:	-3.1493510D+05	1.50876D-03	-1.97088D+09	-9.93019D-03	-317.526
	BABUSKIN:		1.99294D-03	-3.43879D+09	-1.73262D-02	
1 -> 14	COULOMB:	4.0201847D+05	-6.48036D-03	5.15701D+09	1.43512D-01	248.745
	BABUSKIN:		-8.43879D-03	8.74500D+09	2.43361D-01	
14 -> 1	COULOMB:	-4.0201847D+05	-3.74144D-03	-1.54710D+10	-4.78374D-02	-248.745
	BABUSKIN:		-4.87214D-03	-2.62350D+10	-8.11203D-02	
1 -> 18	COULOMB:	4.3340715D+05	1.36648D-03	2.47203D+08	5.91896D-03	230.730
	BABUSKIN:		1.68032D-03	3.73793D+08	8.94998D-03	
18 -> 1	COULOMB:	-4.3340715D+05	7.88936D-04	-7.41610D+08	-1.97299D-03	-230.730
	BABUSKIN:		9.70131D-04	-1.12138D+09	-2.98333D-03	
1 -> 20	COULOMB:	4.9441046D+05	-1.66426D-02	4.18297D+10	7.69648D-01	202.261
	BABUSKIN:		-2.04126D-02	6.29269D+10	1.15783D+00	
20 -> 1	COULOMB:	-4.9441046D+05	-9.60862D-03	-1.25489D+11	-2.56549D-01	-202.261
	BABUSKIN:		-1.17852D-02	-1.88781D+11	-3.85943D-01	
1 -> 23	COULOMB:	5.0610398D+05	5.31682D-03	4.37015D+09	7.67362D-02	197.588
	BABUSKIN:		6.44721D-03	6.42594D+09	1.12834D-01	
23 -> 1	COULOMB:	-5.0610398D+05	3.06967D-03	-1.31105D+10	-2.55787D-02	-197.588
	BABUSKIN:		3.72230D-03	-1.92778D+10	-3.76113D-02	
1 -> 27	COULOMB:	5.6592973D+05	-8.41336D-04	1.22364D+08	1.71835D-03	176.700
	BABUSKIN:		-8.22047D-04	1.16818D+08	1.64046D-03	
27 -> 1	COULOMB:	-5.6592973D+05	-4.85745D-04	-3.67093D+08	-5.72784D-04	-176.700
	BABUSKIN:		-4.74609D-04	-3.50453D+08	-5.46821D-04	
1 -> 29	COULOMB:	9.9202752D+05	-1.66646D-05	8.41525D+04	3.84594D-07	100.804
	BABUSKIN:		-5.60303D-05	9.51311D+05	4.34769D-06	
29 -> 1	COULOMB:	-9.9202752D+05	-9.62132D-06	-2.52458D+05	-1.28198D-07	-100.804
	BABUSKIN:		-3.23491D-05	-2.85393D+06	-1.44923D-06	
1 -> 35	COULOMB:	1.0307492D+06	-3.47731D-04	3.80709D+07	1.61165D-04	97.017
	BABUSKIN:		-7.12570D-04	1.59868D+08	6.76766D-04	
35 -> 1	COULOMB:	-1.0307492D+06	-2.00763D-04	-1.14213D+08	-5.37216D-05	-97.017
	BABUSKIN:		-4.11402D-04	-4.79604D+08	-2.25589D-04	
1 -> 44	COULOMB:	1.0905372D+06	-8.06206D-05	2.16514D+06	8.18820D-06	91.698
	BABUSKIN:		-2.53356D-04	2.13823D+07	8.08643D-05	
44 -> 1	COULOMB:	-1.0905372D+06	-4.65464D-05	-6.49543D+06	-2.72940D-06	-91.698
	BABUSKIN:		-1.46275D-04	-6.41469D+07	-2.69548D-05	
1 -> 46	COULOMB:	1.1120894D+06	9.93476D-04	3.35280D+08	1.21930D-03	89.921
	BABUSKIN:		2.10029D-03	1.49848D+09	5.44946D-03	
46 -> 1	COULOMB:	-1.1120894D+06	5.73584D-04	-1.00584D+09	-4.06434D-04	-89.921
	BABUSKIN:		1.21260D-03	-4.49543D+09	-1.81649D-03	
1 -> 52	COULOMB:	1.1205769D+06	3.46877D-04	4.11857D+07	1.47518D-04	89.240
	BABUSKIN:		6.07415D-04	1.26289D+08	4.52341D-04	
52 -> 1	COULOMB:	-1.1205769D+06	2.00270D-04	-1.23557D+08	-4.91728D-05	-89.240
	BABUSKIN:		3.50691D-04	-3.78868D+08	-1.50780D-04	
1 -> 54	COULOMB:	1.1286819D+06	-2.63769D-04	2.39869D+07	8.46863D-05	88.599
	BABUSKIN:		-3.49259D-04	4.20551D+07	1.48477D-04	
54 -> 1	COULOMB:	-1.1286819D+06	-1.52287D-04	-7.19606D+07	-2.82288D-05	-88.599
	BABUSKIN:		-2.01645D-04	-1.26165D+08	-4.94923D-05	
1 -> 59	COULOMB:	1.1887899D+06	1.48988D-03	8.06045D+08	2.56526D-03	84.119
	BABUSKIN:		5.65972D-03	1.16318D+10	3.70187D-02	
59 -> 1	COULOMB:	-1.1887899D+06	8.60181D-04	-2.41813D+09	-8.55088D-04	-84.119
	BABUSKIN:		3.26764D-03	-3.48955D+10	-1.23396D-02	

```
 FE    3P13D1            NCONF=  3    Z= 26    NCORES= 5    NVALES= 1    ION=12    R(I)/X(I)=0.29884981      CA1=0.700
TOLSTB=1.000   TOLK-2=1.00000   TOLEND= 0.5D-07   THRESH= 0.1D-10   KUT= 0    EXF=1.000   CORRF=0.0        CA0= 0.500

RCN MOD 31  IHF1= 2       MESH= 641   IDB= 641   RDB=1958.512   EMX=   0.00   R(MESH)=1958.512     IREL= 1     IB= 641
ENERGY = E(AV)

    T(RUN)=  2.33,     T(JOB)=   7.15 SECONDS
```

NL	WNL	EE	AZ	(R-3)	(R-2)	(R-1)	(R+1)	(R+2)	(R+3)	(R+4)	(R+6)
1S	2.	-553.80305	291.112	0.0	1.384D+03	2.599D+01	5.840D-02	4.586D-03	4.535D-04	5.418D-05	1.226D-06
2S	2.	-89.90988	90.071	0.0	1.344D+02	5.644D+00	2.628D-01	8.130D-02	2.863D-02	1.136D-02	2.472D-03
2P	6.	-80.10923	571.450	4.817D+02	4.130D+01	5.491D+00	2.328D-01	6.630D-02	2.239D-02	8.766D-03	1.959D-03
3S	2.	-28.56657	38.716	0.0	2.544D+01	2.011D+00	7.067D-01	5.664D-01	4.974D-01	4.743D-01	5.439D-01
3P	1.	-26.19515	257.703	8.675D+01	7.994D+00	1.936D+00	7.049D-01	5.705D-01	5.096D-01	4.974D-01	6.064D-01
3D	1.	-22.15051	275.891	1.177D+01	4.042D+00	1.808D+00	6.606D-01	5.076D-01	4.450D-01	4.383D-01	5.753D-01
	14.				3.348D+03	1.040D+02	4.818D+00	2.781D+00	2.142D+00	1.960D+00	2.286D+00
	1.				2.391D+02	7.427D+00	3.442D-01	1.986D-01	1.530D-01	1.400D-01	1.633D-01

NL	WNL	ZETA BLUME-WATSON (RYD)	ZETA BLUME-WATSON (CM-1)	ZETA (R*VI) (RYD)	ZETA (R*VI) (CM-1)	I (RYD)	EPS S	EVEL	EDAR	EVEL+EDAR	EREL
1S	2.	0.0	0.0	0.0	0.0	-681.79346	-549.09629	-31.16687	25.68812	-5.479	-554.57504
2S	2.	0.0	0.0	0.0	0.0	-167.57990	-88.41905	-3.72319	2.43682	-1.286	-89.70542
2P	6.	0.58878	64611.342	0.62184	68238.892	-165.13955	-80.01355	-0.50827	-0.01139	-0.508	-80.52182
3S	2.	0.0	0.0	0.0	0.0	-69.14668	-28.83534	-0.71971	0.44772	-0.272	-29.10734
3P	1.	0.10650	11687.118	0.11189	12278.049	-67.18535	-26.22671	-0.11862	-0.00213	-0.119	-26.34533
3D	1.	0.00996	1093.485	0.01184	1299.401	-64.48891	-22.31379	-0.02421	-0.00076	-0.024	-22.33800

NL	WNL	WITHOUT CORRELATION EPS FG	WITHOUT CORRELATION EPS FGR	CORR	WITH CORRELATION EPS FG	WITH CORRELATION EPS FGR	N*R	N*RC	ECT	EC
1S	2.	-553.80365	-553.80365-0.08250	-553.88615	-553.88615	0.5524	0.5524	-0.08210	0.0	-0.08210
2S	2.	-89.90987	-89.90987-0.08104	-89.99091	-89.99091	1.3710	1.3704	-0.22065	-0.05960	-0.07895
2P	6.	-80.10925	-80.10925-0.08129	-80.19054	-80.19054	1.4525	1.4517	-0.70482	-0.08013	-0.08046-0.08068-0.08085-0.08108
3S	2.	-28.56655	-28.56655-0.07618	-28.64273	-28.64273	2.4323	2.4290	-0.84027	-0.06141	-0.07403
3P	1.	-26.19514	-26.19514-0.07612	-26.27126	-26.27126	2.5400	2.5363	-0.91569	-0.07542	
3D	1.	-22.15050	-22.15050-0.07667	-22.22717	-22.22717	2.7622	2.7574	-0.99236	-0.07667	

```
                      ECORRT=  -1.11994 (OLD)                ECT=  -0.99236 (NEW)         ETOTRL=       0.0
```

ETOT=	-2416.55647	-2416.55647	-2417.67641	-2417.67641	-2417.54883	-2417.54883

```
FE    3P13D1          6  -2417.5488 0   11.6871 2    1.0935 2  142.2683 3  162.7660 4
  105.8349 4
```

```
RCN MOD 30

EE,EEE= -28.64273 -14.32137
EE,EEE= -25.91273 -27.27773

 SLATER INTEGRALS FOR FE    3P13D1          NCONF= 3          Z= 26   ION=12     EXF=0.650          IREL= 1
                      FE    3P33D1          NCONF= 4                  KUT=-1   CORRF=0.0          CLASS  0

        K          RDK( 3S, 3S, 3P, 3P)                    FRAC        K          REK( 3S, 3S, 3P, 3P)                    FRAC
        -     ---------------------------------------      -----        -     ---------------------------------------      -----

        1      1.69261145 RYD  =   185742.6269 CM-1   0.995          1      1.69261145 RYD  =   185742.6269 CM-1   0.995


 EIGENVALUE CONTRIBUTION OF   0.0    KK INCLUDED IN PARAMETER NUMBER  1


FE    3P13D1    -3P33D1          1   185.7426 5
SQRTDEL=    1.0000    1.0000        185.7426
```

Z	KUT	CA1	CA0	CONF1		CONF2	R INTEGRAL	REDUCED MUPOLE ELEMENT		FRAC	SIGMA SQ	OVER	FR1
26	-1	0.70	0.50	FE 3S23P2		FE 3S13P3	-0.702216	(3S//R1// 3P)=	0.70222 A0	-0.9993	0.164369	-0.981	-0.991
				SQRTDEL=	1.0000				0.70222				
26	-1	0.70	0.50	FE 3S23P2		FE 3P13D1	-0.652546	(3P//R1// 3D)=	0.92284 A0	-0.9790	0.028388	-0.873	-0.921
				SQRTDEL=	1.0000				0.92284				
26	-1	0.70	0.50	FE 3S23P2		FE 3P33D1	0.0	(//R1//)=	0.0 A0	0.0	0.0	0.0	0.0
				SQRTDEL=	1.0000				0.0				

```
                -99999999.0

FINISHED G5INP
   MAIN LINE68  -1
```

```
    123   3 1 13 3 300          1                  0 1000          0000018
S 2   P 2   S 0
S 1   P 3   D 0
S 2   P 1   D 1
S 0   P 3   D 1
FE     3S23P2         3    0.0    0 143.49071  11.70512   0.0    0   0.0    0HR99999999
FE     3S13P3         4 303.13070 143.22211  11.68882 186.31124   0.0    0HR99999999
FE     3P13D1         6 447.42500  11.68712   1.09352 142.26833 162.76604HR99999999
 105.83494
FE     3P33D1         71059.38520 142.73641  11.66052   1.08992 141.95083HR99999999
 162.49974 105.60414
3S13P3    -3P13D1     1 170.62035   0.0    5   0.0    5   0.0    5   0.0    5HR99999999
3S13P3    -3P33D1     2 170.65315 129.94355   0.0    5   0.0    5   0.0    5HR99999999
3P13D1    -3P33D1     1 185.74265   0.0    5   0.0    5   0.0    5   0.0    5HR99999999
FE     3S23P2          FE     3S13P3           0.70222( 3S//R1// 3P)-0.999HR -98 -99
FE     3S23P2          FE     3P13D1           0.92284( 3P//R1// 3D)-0.979HR -87 -92
FE     3S23P2          FE     3P33D1           0.0    (   //R1//   ) 0.0  HR   0   0
                       -99999999.0
```

```
FE    3S13P3          PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00 1.00 1.00 1.00)     1  S 1  P 3  D 0

                                EAV             F2(22)          ZETA 2          G1(12)

                              303.131           143.222          11.689          186.311

FE    3P13D1          PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00 1.00 1.00 1.00)     2  S 2  P 1  D 1

                                EAV             ZETA 2          ZETA 3          F2(23)          G1(23)
        G3(23)

                              447.425           11.687           1.093          142.268         162.766
        105.835

FE    3P33D1          PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00 1.00 1.00 1.00)     3  S 0  P 3  D 1

                                EAV             F2(22)          ZETA 2          ZETA 3          F2(23)
        G1(23)          G3(23)

                             1059.385           142.736          11.661           1.090         141.951
        162.500         105.604

3S13P3    -3P13D1       PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00)                     1  S 1  P 3  D 0  S 0  S 0  S 0  S 0  S 0
                                                                                             2  S 2  P 1  D 1  S 0  S 0  S 0  S 0  S 0

                                121D2213

                              170.620

3S13P3    -3P33D1       PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00)                     1  S 1  P 3  D 0  S 0  S 0  S 0  S 0  S 0
                                                                                             3  S 0  P 3  D 1  S 0  S 0  S 0  S 0  S 0

                                131D1223        132E1223

                              170.653           129.943

3P13D1    -3P33D1       PARAMETER VALUES IN  1000.0 CM-1 (HR TIMES 1.00)                     2  S 2  P 1  D 1  S 0  S 0  S 0  S 0  S 0
                                                                                             3  S 0  P 3  D 1  S 0  S 0  S 0  S 0  S 0

                                231D1122

                              185.743
```

ENERGY MATRIX (LS COUPLING) J= 1.0 FE 3S13P3 CONFIG 1 S 1 P 3 D 0 S 0 S 0 S 0 S 0 S 0

FE 3P33D1 3 S 0 P 3 D 1 S 0 S 0 S 0 S 0 S 0

TIME= 0.026 MIN

EIGENVALUES (J= 1.0)

	234.117	282.108	369.857	400.520	462.080	473.067	533.504	959.500	998.027	1058.419	1080.134
	1088.051	1095.880	1156.619	1182.979	1263.053						
CONFIG. NO.	1	1	1	1	2	2	2	3	3	3	3
	3	3	3	3	3						
G-VALUES	0.524	1.481	1.910	1.088	1.091	0.915	0.995	1.498	0.504	1.000	0.559
	1.460	1.485	1.995	0.507	0.995						

EIGENVECTORS (LS COUPLING)

1 (2D) 3D 1	-0.92233	-0.13974	-0.01672	-0.05254	-0.21231	-0.26460	0.04382	-0.00112	-0.01161	0.01177	0.04799
1 (2P) 3P 2	0.14224	-0.92030	0.05703	-0.00116	0.27114	-0.23260	-0.01365	-0.00358	0.00260	0.01014	-0.00388
1 (4S) 3S 3	-0.01084	0.06682	0.93048	-0.29061	0.02333	-0.01426	0.01841	0.00068	-0.00067	-0.00333	0.00242
1 (2P) 1P 4	-0.06031	-0.00495	0.28534	0.88887	-0.05108	0.00734	-0.31416	-0.00037	-0.00098	0.03458	-0.00172
2 (2P) 3D 5	0.33615	0.05592	0.01123	0.03059	-0.59158	-0.70931	0.11027	0.00772	0.02919	-0.02557	-0.09489
2 (2P) 3P 6	0.04873	-0.34380	0.04005	-0.03677	-0.70848	0.59447	0.05731	-0.01294	0.00961	0.03171	-0.01689
2 (2P) 1P 7	0.01943	-0.00494	-0.08169	-0.32735	-0.10904	-0.05982	-0.92352	-0.00040	-0.00161	0.03826	-0.00108
3 (4S) 5D 8	-0.00020	-0.00133	0.00009	-0.00012	-0.00078	0.00262	-0.00005	0.99552	-0.02709	0.03495	0.02675
3 (4S) 3D 9	-0.07655	-0.01192	-0.00131	-0.00423	-0.01610	-0.02139	0.00089	0.02669	0.64661	-0.09617	-0.34652
3 (2D) 3D 10	0.04830	0.00827	0.00073	0.00262	0.01419	0.01634	-0.00136	0.00791	0.73420	0.11403	0.51384
3 (2P) 3D 11	0.03436	0.00617	0.00137	0.00393	-0.08053	-0.09829	0.01704	-0.04487	-0.19200	0.18179	0.72180
3 (2D) 3P 12	-0.00083	0.00656	-0.00047	-0.00107	-0.00308	0.00215	0.00250	0.00059	-0.01361	0.04494	0.13500
3 (2P) 3P 13	0.01193	-0.08490	0.00638	-0.00407	-0.08368	0.07125	0.00772	0.07648	-0.06268	-0.22594	0.12809
3 (2D) 3S 14	0.00209	-0.01349	-0.19929	0.06417	-0.00639	0.00432	-0.00356	0.00247	-0.00262	-0.01186	0.01017
3 (2D) 1P 15	0.00003	0.00087	0.00058	0.00187	0.00146	-0.00099	0.01035	-0.00721	0.00259	0.91776	-0.21816
3 (2P) 1P 16	-0.00667	-0.00139	0.03313	0.09526	-0.02124	-0.00620	-0.17336	0.00182	0.00480	-0.20834	0.01516

1 (2D) 3D 1	-0.00772	-0.00632	0.00101	0.08302	0.01225
1 (2P) 3P 2	-0.03179	0.02408	0.00559	0.00100	0.00040
1 (4S) 3S 3	0.01746	-0.01357	0.20847	-0.00438	0.01008
1 (2P) 1P 4	0.01055	0.00163	0.00528	0.01887	-0.14759
2 (2P) 3D 5	0.01415	0.00682	0.00137	0.08175	0.00799
2 (2P) 3P 6	-0.11443	0.05547	0.01156	-0.00016	0.00080
2 (2P) 1P 7	0.01187	-0.00027	0.00653	0.01616	-0.12451
3 (4S) 5D 8	-0.07235	0.02872	0.00468	-0.01338	-0.00073
3 (4S) 3D 9	0.08740	0.03958	-0.00944	-0.65348	-0.09377
3 (2D) 3D 10	-0.02572	-0.06959	0.00143	0.41423	0.06224
3 (2P) 3D 11	-0.10435	-0.05844	-0.01133	-0.61012	-0.05213
3 (2D) 3P 12	0.43526	0.88762	0.01747	0.01419	0.04104
3 (2P) 3P 13	0.84612	-0.42181	-0.09671	-0.00457	-0.00055
3 (2D) 3S 14	0.07589	-0.05902	0.97159	-0.02005	0.04486
3 (2D) 1P 15	0.21337	-0.12707	-0.02139	-0.02712	0.21696
3 (2P) 1P 16	-0.06322	-0.00117	-0.04417	-0.11567	0.94670

1(2D)3D	1(2P)3P	1(4S)3S	1(2P)1P	2(2P)3P	2(2P)3D	2(2P)1P	3(4S)5D	3(2D)3D	3(2D)1P	3(2P)3D
3(2P)3P	3(2D)3P	3(2D)3S	3(4S)3D	3(2P)1P						

ELEC DIP SPECTRUM

1	FE	3S23P2	---	1	FE	3S13P3	
2			---	2	FE	3P13D1	
3			---	3	FE	3P33D1	

	LOW PAR LEVEL	JL	LPR TERM	UP PAR LEVEL	JU	UPR TERM	WAVENUMBER	WAVELENGTH	A	GF	LOG GF	S/P**2	GA(SEC-1)	CAN FAC
1	19442.429	2.0	1(1D)1D	157385.388	2.0	1(4S)5S	137942.96	724.937	0.0000	-4.5041	0.0001	3.976D+05	-0.0821	
2	71601.402	0.0	1(1S)1S	234117.499	1.0	1(2D)3D	162516.10	615.324	0.0001	-3.8877	0.0003	2.281D+06	-0.0073	
3	-13589.879	2.0	1(3P)3P	157385.388	2.0	1(4S)5S	170975.27	584.880	0.0014	-2.8572	0.0031	2.709D+07	-0.3455	
4	-23071.434	1.0	1(3P)3P	157385.388	2.0	1(4S)5S	180456.82	554.149	0.0008	-3.1236	0.0016	1.634D+07	-0.3934	
5	71601.402	0.0	1(1S)1S	282108.094	1.0	1(2P)3P	210506.69	475.044	0.0014	-2.8623	0.0025	4.059D+07	0.1706	
6	19442.429	2.0	1(1D)1D	234117.499	1.0	1(2D)3D	214675.07	465.820	0.0016	-2.8028	0.0028	4.841D+07	-0.1631	
7	19442.429	2.0	1(1D)1D	234294.123	2.0	1(2D)3D	214851.69	465.437	0.0018	-2.7394	0.0033	5.611D+07	-0.0481	
8	19442.429	2.0	1(1D)1D	236753.968	3.0	1(2D)3D	217311.54	460.169	0.0159	-1.7987	0.0283	5.007D+08	-0.1616	
9	-13589.879	2.0	1(3P)3P	234117.499	1.0	1(2D)3D	247707.38	403.702	0.0012	-2.9100	0.0019	5.034D+07	0.0242	
10	-13589.879	2.0	1(3P)3P	234294.123	2.0	1(2D)3D	247884.00	403.414	0.0110	-1.9586	0.0172	4.508D+08	-0.0241	
11	-13589.879	2.0	1(3P)3P	236753.968	3.0	1(2D)3D	250343.85	399.451	0.2213	-0.6551	0.3417	9.249D+09	-0.1477	
12	-23071.434	1.0	1(3P)3P	234117.499	1.0	1(2D)3D	257188.93	388.819	0.0268	-1.5716	0.0403	1.183D+09	-0.0737	
13	-23071.434	1.0	1(3P)3P	234294.123	2.0	1(2D)3D	257365.56	388.552	0.1611	-0.7928	0.2420	7.118D+09	0.1545	
14	19442.429	2.0	1(1D)1D	281847.358	2.0	1(2P)3P	262404.93	381.090	0.0071	-2.1468	0.0105	3.275D+08	-0.0191	
15	19442.429	2.0	1(1D)1D	282108.094	1.0	1(2P)3P	262665.66	380.712	0.0021	-2.6811	0.0031	9.590D+07	0.0849	
16	-31649.850	0.0	1(3P)3P	234117.499	1.0	1(2D)3D	265767.35	376.269	0.0772	-1.1123	0.1123	3.637D+09	0.1560	
17	19442.429	2.0	1(1D)1D	310028.917	2.0	1(2D)1D	290586.49	344.132	0.4997	-0.3013	0.6648	2.815D+10	0.2319	
18	-13589.879	2.0	1(3P)3P	281847.358	2.0	1(2P)3P	295437.24	338.481	0.2468	-0.6076	0.3230	1.437D+10	0.2149	
19	-13589.879	2.0	1(3P)3P	282108.094	1.0	1(2P)3P	295697.97	338.183	0.0375	-1.4260	0.0490	2.187D+09	0.1034	
20	71601.402	0.0	1(1S)1S	369857.025	1.0	1(4S)3S	298255.62	335.283	0.0088	-2.0576	0.0113	5.196D+08	-0.0711	
21	-23071.434	1.0	1(3P)3P	281715.746	0.0	1(2P)3P	304787.18	328.098	0.0573	-1.2417	0.0727	3.552D+09	0.2390	
22	-23071.434	1.0	1(3P)3P	281847.358	2.0	1(2P)3P	304918.79	327.956	0.0298	-1.5254	0.0378	1.849D+09	0.0567	
23	-23071.434	1.0	1(3P)3P	282108.094	1.0	1(2P)3P	305179.53	327.676	0.0817	-1.0878	0.1035	5.075D+09	-0.2580	
24	-31649.850	0.0	1(3P)3P	282108.094	1.0	1(2P)3P	313757.94	318.717	0.0521	-1.2832	0.0642	3.420D+09	-0.1350	
25	-13589.879	2.0	1(3P)3P	310028.917	2.0	1(2D)1D	323618.80	309.006	0.0041	-2.3898	0.0049	2.847D+08	-0.0094	
26	71601.402	0.0	1(1S)1S	400519.752	1.0	1(2P)1P	328918.35	304.027	0.2431	-0.6142	0.2857	1.754D+10	-0.2499	
27	-23071.434	1.0	1(3P)3P	310028.917	2.0	1(2D)1D	333100.35	300.210	0.0046	-2.3366	0.0053	3.409D+08	0.1371	
28	19442.429	2.0	1(1D)1D	369857.025	1.0	1(4S)3S	350414.60	285.376	0.0001	-4.1508	0.0001	5.788D+06	0.0002	
29	19442.429	2.0	1(1D)1D	383661.714	2.0	2(2P)3F	364219.28	274.560	0.0149	-1.8275	0.0158	1.316D+09	-0.7614	
30	19442.429	2.0	1(1D)1D	390280.517	3.0	2(2P)3F	370838.09	269.659	0.0015	-2.8229	0.0016	1.379D+08	0.1775	
31	19442.429	2.0	1(1D)1D	400519.752	1.0	1(2P)1P	381077.32	262.414	0.9522	-0.0213	0.9659	9.223D+10	0.9776	
32	-13589.879	2.0	1(3P)3P	369857.025	1.0	1(4S)3S	383446.90	260.792	1.2111	0.0832	1.2210	1.188D+11	-0.9323	
33	71601.402	0.0	1(1S)1S	462080.018	1.0	2(2P)3P	390478.62	256.096	0.0004	-3.4013	0.0004	4.036D+07	-0.0047	
34	-23071.434	1.0	1(3P)3P	369857.025	1.0	1(4S)3S	392928.46	254.499	0.6691	-0.1745	0.6583	6.890D+10	-0.8727	
35	-13589.879	2.0	1(3P)3P	383661.714	2.0	2(2P)3F	397251.59	251.730	0.0046	-2.3364	0.0045	4.852D+08	0.8346	
36	71601.402	0.0	1(1S)1S	473066.616	1.0	2(2P)3D	401465.21	249.088	0.0001	-4.0572	0.0001	9.423D+06	-0.0018	
37	-31649.850	0.0	1(3P)3P	369857.025	1.0	1(4S)3S	401506.87	249.062	0.2449	-0.6111	0.2357	2.633D+10	-0.7121	
38	-13589.879	2.0	1(3P)3P	390280.517	3.0	2(2P)3F	403870.40	247.604	0.0148	-1.8290	0.0142	1.613D+09	-1.0000	
39	-23071.434	1.0	1(3P)3P	383661.714	2.0	2(2P)3F	406733.15	245.861	0.0038	-2.4161	0.0036	4.233D+08	-0.9559	
40	-13589.879	2.0	1(3P)3P	400519.752	1.0	1(2P)1P	414109.63	241.482	0.0042	-2.3796	0.0039	4.772D+08	0.0113	
41	-23071.434	1.0	1(3P)3P	400519.752	1.0	1(2P)1P	423591.19	236.077	0.0745	-1.1276	0.0680	8.922D+09	0.6930	
42	-31649.850	0.0	1(3P)3P	400519.752	1.0	1(2P)1P	432169.60	231.391	0.0080	-2.0993	0.0071	9.910D+08	0.0488	
43	19442.429	2.0	1(1D)1D	454660.569	2.0	2(2P)3P	435218.14	229.770	0.8834	-0.0538	0.7847	1.116D+11	0.4963	
44	19442.429	2.0	1(1D)1D	462080.018	1.0	2(2P)3P	442637.59	225.918	0.0174	-1.7592	0.0152	2.275D+09	-0.3023	
45	19442.429	2.0	1(1D)1D	466596.548	2.0	2(2P)1D	447154.12	223.637	1.6578	0.2195	1.4332	2.211D+11	-0.7714	
46	19442.429	2.0	1(1D)1D	473066.616	1.0	2(2P)3D	453624.19	220.447	0.0299	-1.5247	0.0255	4.100D+09	1.0000	
47	19442.429	2.0	1(1D)1D	475447.257	3.0	2(2P)3D	456004.83	219.296	0.1094	-0.9611	0.0927	1.517D+10	0.2641	
48	19442.429	2.0	1(1D)1D	475851.263	2.0	2(2P)3D	456408.83	219.102	0.3353	-0.4746	0.2840	4.659D+10	1.0000	
49	71601.402	0.0	1(1S)1S	533504.495	1.0	2(2P)1P	461903.09	216.496	1.2909	0.1109	1.0803	1.837D+11	1.0000	
50	-13589.879	2.0	1(3P)3P	454660.569	2.0	2(2P)3P	468250.45	213.561	0.6766	-0.1697	0.5586	9.895D+10	-0.4010	

LEVELS THEIR PERCECTAGE COMPOSITION FOR TERMS

0.0	3P(1S)3P(	97.0%)	0.0	4	3P(1S)1S(	3.0%)	0.0	5	3P(1S)3P(	0.0%)	2.0	1	3P(1S)1D(	0.0%)	2.0	2
9065.2	3P(1S)3P(	100.0%)	1.0	3	3P(1S)3P(	0.0%)	2.0	1	3P(1S)1D(	0.0%)	2.0	2	3P(1S)3P(	0.0%)	0.0	4
18790.6	3P(1S)3P(	92.2%)	2.0	1	3P(1S)1D(	7.8%)	2.0	2	3P(1S)3P(	0.0%)	1.0	3	3P(1S)3P(	0.0%)	0.0	4
51793.8	3P(1S)1D(	92.2%)	2.0	2	3P(1S)3P(	7.8%)	2.0	1	3P(1S)3P(	0.0%)	1.0	3	3P(1S)3P(	0.0%)	0.0	4
103711.3	3P(1S)1S(	97.0%)	0.0	5	3P(1S)3P(	3.0%)	0.0	4	3P(1S)3P(	0.0%)	2.0	1	3P(1S)1D(	0.0%)	2.0	2
189815.3	3P(2S)5S(	99.0%)	-2.0	7	3P(2S)3P(	0.9%)	-2.0	10	3D(2P)3P(	0.0%)	-2.0	22	3P(2S)3D(	0.0%)	-2.0	8
266137.4	3P(2S)3D(	84.8%)	-1.0	12	3D(2P)3D(	11.2%)	-1.0	24	3P(2S)3P(	2.3%)	-1.0	13	3D(4S)3D(	0.6%)	-1.0	54
266335.1	3P(2S)3D(	83.7%)	-2.0	8	3D(2P)3D(	10.8%)	-2.0	21	3P(2S)3P(	3.9%)	-2.0	10	3D(4S)3D(	0.6%)	-2.0	44
268910.3	3P(2S)3D(	88.0%)	-3.0	6	3D(2P)3D(	11.0%)	-3.0	18	3D(4S)3D(	0.6%)	-3.0	35	3D(2D)3D(	0.2%)	-3.0	38
313670.7	3P(2S)3P(	87.5%)	-0.0	15	3D(2P)3P(	11.8%)	-0.0	27	3D(2P)3P(	0.7%)	-0.0	65	3D(2D)3P(	0.0%)	-0.0	63
313999.2	3P(2S)3P(	75.2%)	-2.0	10	3D(2P)3P(	11.3%)	-2.0	22	3P(2S)1D(	4.9%)	-2.0	9	3P(2S)3D(	3.8%)	-2.0	8
314123.6	3P(2S)3P(	84.4%)	-1.0	13	3D(2P)3P(	11.7%)	-1.0	25	3P(2S)3D(	2.2%)	-1.0	12	3D(2P)3P(	0.7%)	-1.0	60
342164.1	3P(2S)1D(	52.6%)	-2.0	9	3D(2P)1D(	37.2%)	-2.0	23	3P(2S)3P(	6.7%)	-2.0	10	3D(2D)1D(	1.6%)	-2.0	48
401360.8	3P(2S)3S(	85.4%)	-1.0	11	3P(2S)1P(	9.2%)	-1.0	14	3D(2D)3S(	3.9%)	-1.0	57	3D(2P)1P(	0.8%)	-1.0	26
414991.0	3D(2P)3F(	97.4%)	-2.0	20	3D(2P)3F(	1.6%)	-2.0	49	3P(2S)1D(	0.7%)	-2.0	9	3D(2P)3D(	0.2%)	-2.0	21
421768.3	3D(2P)3F(	97.7%)	-3.0	17	3D(2P)3F(	1.7%)	-3.0	40	3D(2P)3D(	0.3%)	-3.0	18	3D(2P)1F(	0.2%)	-3.0	19
431717.9	3D(2P)3F(	98.3%)	-4.0	16	3D(2P)3F(	1.7%)	-4.0	33	3D(2D)3F(	0.0%)	-4.0	31	3D(4S)5D(	0.0%)	-4.0	29
432477.7	3P(2S)1P(	78.0%)	-1.0	14	3D(2P)1P(	10.5%)	-1.0	26	3P(2S)3S(	9.5%)	-1.0	11	3D(2P)1P(	0.9%)	-1.0	61
485424.1	3D(2P)3P(	42.4%)	-2.0	22	3D(2P)1D(	23.5%)	-2.0	23	3P(2S)1D(	16.3%)	-2.0	9	3D(2P)3D(	9.1%)	-2.0	21
493433.7	3D(2P)3P(	48.2%)	-1.0	25	3D(2P)3D(	37.1%)	-1.0	24	3P(2S)3P(	7.0%)	-1.0	13	3P(2S)3D(	4.7%)	-1.0	12
498105.2	3D(2P)1D(	33.8%)	-2.0	23	3P(2S)1D(	21.4%)	-2.0	9	3D(2P)3P(	20.5%)	-2.0	22	3D(2P)3D(	16.2%)	-2.0	21
500598.4	3D(2P)3P(	86.4%)	-0.0	27	3P(2S)3P(	12.4%)	-0.0	15	3D(2P)3P(	1.2%)	-0.0	65	3D(2D)3P(	0.0%)	-0.0	63
504863.5	3D(2P)3D(	48.2%)	-1.0	24	3D(2P)3P(	37.5%)	-1.0	25	3P(2S)3D(	6.7%)	-1.0	12	3P(2S)3P(	5.7%)	-1.0	13
506601.9	3D(2P)3D(	86.1%)	-3.0	18	3P(2S)3D(	10.8%)	-3.0	6	3D(2P)3D(	1.7%)	-3.0	41	3D(2P)1F(	0.8%)	-3.0	19
507369.8	3D(2P)3D(	61.3%)	-2.0	21	3D(2P)3P(	22.8%)	-2.0	22	3P(2S)3D(	8.2%)	-2.0	8	3P(2S)3P(	3.8%)	-2.0	10
556640.4	3D(2P)1F(	97.0%)	-3.0	19	3D(2P)1F(	1.9%)	-3.0	42	3D(2P)3D(	0.8%)	-3.0	18	3D(2P)3F(	0.2%)	-3.0	17
564638.5	3D(2P)1P(	85.3%)	-1.0	26	3P(2S)1P(	9.8%)	-1.0	14	3D(2P)1P(	3.0%)	-1.0	61	3D(2P)3D(	1.3%)	-1.0	24
990236.0	3D(4S)5D(	99.0%)	-0.0	62	3D(2P)3P(	0.9%)	-0.0	65	3D(2P)3P(	0.0%)	-0.0	27	3D(2D)1S(	0.0%)	-0.0	64
990479.3	3D(4S)5D(	99.0%)	-1.0	53	3D(2P)3P(	0.7%)	-1.0	60	3D(2P)3D(	0.2%)	-1.0	59	3D(4S)3D(	0.1%)	-1.0	54
990874.3	3D(4S)5D(	98.5%)	-2.0	43	3D(2P)3D(	0.6%)	-2.0	50	3D(4S)3D(	0.3%)	-2.0	44	3D(2P)3P(	0.3%)	-2.0	51
991439.5	3D(4S)5D(	97.7%)	-3.0	34	3D(2P)3D(	0.7%)	-3.0	41	3D(2P)3F(	0.6%)	-3.0	40	3D(4S)3D(	0.5%)	-3.0	35
992512.3	3D(4S)5D(	98.3%)	-4.0	29	3D(2P)3F(	1.4%)	-4.0	33	3D(2D)3F(	0.2%)	-4.0	31	3D(2P)3F(	0.0%)	-4.0	16
1025221.1	3D(2D)3D(	42.9%)	-2.0	46	3D(4S)3D(	34.8%)	-2.0	44	3D(2D)3F(	10.6%)	-2.0	45	3D(2P)3D(	3.9%)	-2.0	50
1027353.5	3D(2D)3D(	49.7%)	-3.0	38	3D(4S)3D(	38.4%)	-3.0	35	3D(2P)3D(	4.4%)	-3.0	41	3D(2D)3F(	3.9%)	-3.0	37
1028993.7	3D(2D)3D(	53.8%)	-1.0	55	3D(4S)3D(	41.9%)	-1.0	54	3D(2P)3D(	3.7%)	-1.0	59	3D(2P)3P(	0.5%)	-1.0	60
1035690.3	3D(2D)3F(	70.6%)	-2.0	45	3D(2P)3F(	13.3%)	-2.0	49	3D(2D)3D(	9.8%)	-2.0	46	3D(4S)3D(	5.6%)	-2.0	44
1039032.1	3D(2D)3F(	78.0%)	-3.0	37	3D(2P)3F(	12.8%)	-3.0	40	3D(2D)3D(	4.3%)	-3.0	38	3D(4S)3D(	2.1%)	-3.0	35
1043261.5	3D(2D)1S(	98.5%)	-0.0	64	3D(2P)3P(	1.3%)	-0.0	65	3D(2D)3P(	0.1%)	-0.0	63	3D(4S)5D(	0.1%)	-0.0	62
1043632.0	3D(2D)3F(	83.7%)	-4.0	31	3D(2P)3F(	11.2%)	-4.0	33	3D(2D)3G(	3.8%)	-4.0	30	3D(4S)5D(	0.7%)	-4.0	29
1060674.2	3D(2D)3G(	94.5%)	-3.0	36	3D(2D)3F(	3.8%)	-3.0	37	3D(2P)1F(	0.8%)	-3.0	42	3D(2P)3F(	0.6%)	-3.0	40
1062409.0	3D(2D)3G(	93.2%)	-4.0	30	3D(2D)3F(	5.8%)	-4.0	31	3D(2P)3F(	0.9%)	-4.0	33	3D(2D)1G(	0.1%)	-4.0	32
1064525.8	3D(2D)3G(	100.0%)	-5.0	28	3P(1S)3P(	0.0%)	2.0	1	3P(1S)1D(	0.0%)	2.0	2	3P(1S)3P(	0.0%)	1.0	3
1074755.8	3D(2D)1G(	95.0%)	-4.0	32	3D(2P)3F(	3.1%)	-4.0	33	3D(2D)3F(	1.7%)	-4.0	31	3D(4S)5D(	0.1%)	-4.0	29
1088990.8	3D(2D)1P(	82.8%)	-1.0	58	3D(2P)3P(	5.4%)	-1.0	60	3D(2P)1P(	4.3%)	-1.0	61	3D(2P)3D(	3.9%)	-1.0	59
1096682.7	3D(2P)1D(	69.7%)	-2.0	52	3D(2D)1D(	18.1%)	-2.0	48	3D(2P)3F(	4.6%)	-2.0	49	3D(2D)3D(	2.6%)	-2.0	46
1110666.7	3D(2P)3D(	50.8%)	-1.0	59	3D(2D)3D(	26.2%)	-1.0	55	3D(4S)3D(	11.8%)	-1.0	54	3D(2D)1P(	5.5%)	-1.0	58
1113371.4	3D(2P)3P(	35.4%)	-2.0	51	3D(2D)3P(	29.3%)	-2.0	47	3D(2P)3D(	19.8%)	-2.0	50	3D(4S)3D(	5.3%)	-2.0	44
1113762.4	3D(2P)3P(	61.4%)	-0.0	65	3D(2D)3P(	35.4%)	-0.0	63	3D(2D)1S(	1.2%)	-0.0	64	3D(2P)3P(	1.2%)	-0.0	27
1114328.7	3D(2P)3F(	81.4%)	-3.0	40	3D(2D)3F(	12.7%)	-3.0	37	3D(2D)3G(	2.4%)	-3.0	36	3D(2P)3F(	1.3%)	-3.0	17
1115681.7	3D(2P)3F(	70.4%)	-2.0	49	3D(2D)3F(	15.6%)	-2.0	45	3D(2P)3P(	6.0%)	-2.0	51	3D(2P)3D(	2.6%)	-2.0	50
1115620.1	3D(2P)3F(	81.7%)	-4.0	33	3D(2D)3F(	8.6%)	-4.0	31	3D(2D)1G(	4.5%)	-4.0	32	3D(2D)3G(	2.9%)	-4.0	30
1118947.0	3D(2P)3P(	67.3%)	-1.0	60	3D(2D)3P(	22.0%)	-1.0	56	3D(2D)1P(	5.0%)	-1.0	58	3D(2P)3D(	1.5%)	-1.0	59
1119678.5	3D(2P)3D(	33.5%)	-2.0	50	3D(2P)3P(	21.7%)	-2.0	51	3D(2D)3D(	21.6%)	-2.0	46	3D(4S)3D(	7.6%)	-2.0	44
1126814.5	3D(2D)3P(	75.3%)	-1.0	56	3D(2P)3P(	20.8%)	-1.0	60	3D(2D)1P(	1.9%)	-1.0	58	3D(2D)3D(	0.5%)	-1.0	55
1126794.5	3D(2P)3D(	53.0%)	-3.0	41	3D(2D)3D(	27.6%)	-3.0	38	3D(4S)3D(	11.6%)	-3.0	35	3D(2P)1F(	3.1%)	-3.0	42
1130896.6	3D(2D)3P(	64.5%)	-0.0	63	3D(2P)3P(	34.3%)	-0.0	65	3D(2P)3P(	0.6%)	-0.0	27	3D(4S)5D(	0.3%)	-0.0	62
1131635.9	3D(2D)3P(	63.9%)	-2.0	47	3D(2P)3P(	31.5%)	-2.0	51	3D(2P)1D(	1.7%)	-2.0	52	3D(4S)3D(	1.0%)	-2.0	44
1160172.5	3D(2P)1F(	56.3%)	-3.0	42	3D(2D)1F(	35.0%)	-3.0	39	3D(2P)3D(	4.6%)	-3.0	41	3D(2P)1F(	1.2%)	-3.0	19

DOMINANT TERMS CHOSEN FOR DESIGNATION

TERMS	LEVELS	% COMP	J	TM NO	LVL NO
3D(2D)3G	1064525.8	100.0	-5.0	28	42
3D(2P)3F	431717.9	98.3	-4.0	16	17
3D(4S)5D	992512.3	98.3	-4.0	29	32
3D(2D)3F	1043632.0	83.7	-4.0	31	39
3D(2D)3G	1062409.0	93.2	-4.0	30	41
3D(2D)1G	1074755.8	95.0	-4.0	32	43
3D(2P)3F	1115620.1	81.7	-4.0	33	51
3P(2S)3D	268910.3	88.0	-3.0	6	9
3D(2P)3F	421768.3	97.7	-3.0	17	16
3D(2P)3D	506601.9	86.1	-3.0	18	24
3D(2P)1F	556640.4	97.0	-3.0	19	26
3D(4S)5D	991439.5	97.7	-3.0	34	31
3D(2D)3D	1027353.5	49.7	-3.0	38	34
3D(2D)3F	1039032.1	78.0	-3.0	37	37
3D(2D)3G	1060674.2	94.5	-3.0	36	40
3D(2P)3F	1114328.7	81.4	-3.0	40	49
3D(2P)3D	1126794.5	53.0	-3.0	41	55
3D(2P)1F	1160172.5	56.3	-3.0	42	58
3D(4S)3D	1199564.6	44.5	-3.0	35	60
3D(2D)1F	1242263.2	58.6	-3.0	39	64
3P(2S)5S	189815.3	99.0	-2.0	7	6
3P(2S)3D	266335.1	83.7	-2.0	8	8
3P(2S)3P	313999.2	75.2	-2.0	10	11
3P(2S)1D	342164.1	52.6	-2.0	9	13
3D(2P)3F	414991.0	97.4	-2.0	20	15
3D(2P)3P	485424.1	42.4	-2.0	22	19
3D(2P)1D	498105.2	33.8	-2.0	23	21
3D(2P)3D	507369.8	61.3	-2.0	21	25
3D(4S)5D	990874.3	98.5	-2.0	43	30
3D(2D)3D	1025221.1	42.9	-2.0	46	33
3D(2D)3F	1035690.3	70.6	-2.0	45	36
3D(2P)1D	1096682.7	69.7	-2.0	52	45
3D(2P)3P	1113371.4	35.4	-2.0	51	47
3D(2P)3F	1115681.7	70.4	-2.0	49	50
3D(2P)3D	1119678.5	33.5	-2.0	50	53
3D(2D)3P	1131635.9	63.9	-2.0	47	57
3D(4S)3D	1208391.1	42.6	-2.0	44	61
3D(2D)1D	1236389.2	73.7	-2.0	48	63
3P(2S)3D	266137.4	84.8	-1.0	12	7
3P(2S)3P	314123.6	84.4	-1.0	13	12
3P(2S)3S	401360.8	85.4	-1.0	11	14
3P(2S)1P	432477.7	78.0	-1.0	14	18
3D(2P)3P	493433.7	48.2	-1.0	25	20
3D(2P)3D	504863.5	48.2	-1.0	24	23
3D(2P)1P	564638.5	85.3	-1.0	26	27
3D(4S)5D	990479.3	99.0	-1.0	53	29
3D(2D)3D	1028993.7	53.8	-1.0	55	35
3D(2D)1P	1088990.8	82.8	-1.0	58	44
3D(2P)3D	1110666.7	50.8	-1.0	59	46
3D(2P)3P	1118947.0	67.3	-1.0	60	52
3D(2D)3P	1126814.5	75.3	-1.0	56	54
3D(2D)3S	1187097.0	94.2	-1.0	57	59
3D(4S)3D	1213618.5	42.4	-1.0	54	62
3D(2P)1P	1293438.7	89.5	-1.0	61	65
3P(2S)3P	313670.7	87.5	-0.0	15	10
3D(2P)3P	500598.4	86.4	-0.0	27	22
3D(4S)5D	990236.0	99.0	-0.0	62	28

WAVELENGTH A	WAVENUMBER	LOW LEVEL	LOW TERM	LOW J	LTN	UPP LEVEL	UPP TERM	UPP J	UTN	GF	LEVEL NOS		CONFIGURATIONS
615.665	162426.1	103711.3	3P(1S)1S	0.0	5	266137.4	3P(2S)3D	-1.0	12	0.000138	5	7	3S23P2--3S13P3
584.711	171024.6	18790.6	3P(1S)3P	2.0	1	189815.3	3P(2S)5S	-2.0	7	0.001480	3	6	3S23P2--3S13P3
553.250	180750.1	9065.2	3P(1S)3P	1.0	3	189815.3	3P(2S)5S	-2.0	7	0.000835	2	6	3S23P2--3S13P3
475.257	210412.4	103711.3	3P(1S)1S	0.0	5	314123.6	3P(2S)3P	-1.0	13	0.001500	5	12	3S23P2--3S13P3
466.541	214343.6	51793.8	3P(1S)1D	2.0	2	266137.4	3P(2S)3D	-1.0	12	0.001707	4	7	3S23P2--3S13P3
466.111	214541.3	51793.8	3P(1S)1D	2.0	2	266335.1	3P(2S)3D	-2.0	8	0.001945	4	8	3S23P2--3S13P3
460.582	217116.5	51793.8	3P(1S)1D	2.0	2	268910.3	3P(2S)3D	-3.0	6	0.018011	4	9	3S23P2--3S13P3
404.291	247346.8	18790.6	3P(1S)3P	2.0	1	266137.4	3P(2S)3D	-1.0	12	0.001278	3	7	3S23P2--3S13P3
403.968	247544.5	18790.6	3P(1S)3P	2.0	1	266335.1	3P(2S)3D	-2.0	8	0.009860	3	8	3S23P2--3S13P3
399.809	250119.7	18790.6	3P(1S)3P	2.0	1	268910.3	3P(2S)3D	-3.0	6	0.219390	3	9	3S23P2--3S13P3
388.996	257072.2	9065.2	3P(1S)3P	1.0	3	266137.4	3P(2S)3D	-1.0	12	0.026110	2	7	3S23P2--3S13P3
388.697	257269.9	9065.2	3P(1S)3P	1.0	3	266335.1	3P(2S)3D	-2.0	8	0.163938	2	8	3S23P2--3S13P3
381.380	262205.4	51793.8	3P(1S)1D	2.0	2	313999.2	3P(2S)3P	-2.0	10	0.007790	4	11	3S23P2--3S13P3
381.200	262329.8	51793.8	3P(1S)1D	2.0	2	314123.6	3P(2S)3P	-1.0	13	0.002196	4	12	3S23P2--3S13P3
375.746	266137.4	0.0	3P(1S)3P	0.0	4	266137.4	3P(2S)3D	-1.0	12	0.080034	1	7	3S23P2--3S13P3
344.388	290370.3	51793.8	3P(1S)1D	2.0	2	342164.1	3P(2S)1D	-2.0	9	0.498770	4	13	3S23P2--3S13P3
338.744	295208.6	18790.6	3P(1S)3P	2.0	1	313999.2	3P(2S)3P	-2.0	10	0.253100	3	11	3S23P2--3S13P3
338.601	295333.0	18790.6	3P(1S)3P	2.0	1	314123.6	3P(2S)3P	-1.0	13	0.036022	3	12	3S23P2--3S13P3
335.966	297649.6	103711.3	3P(1S)1S	0.0	5	401360.8	3P(2S)3S	-1.0	11	0.009930	5	14	3S23P2--3S13P3
328.293	304605.5	9065.2	3P(1S)3P	1.0	3	313670.7	3P(2S)3P	-0.0	15	0.058165	2	10	3S23P2--3S13P3
327.940	304934.0	9065.2	3P(1S)3P	1.0	3	313999.2	3P(2S)3P	-2.0	10	0.027191	2	11	3S23P2--3S13P3
327.806	305058.5	9065.2	3P(1S)3P	1.0	3	314123.6	3P(2S)3P	-1.0	13	0.086130	2	12	3S23P2--3S13P3
318.346	314123.6	0.0	3P(1S)3P	0.0	4	314123.6	3P(2S)3P	-1.0	13	0.051980	1	12	3S23P2--3S13P3
309.240	323373.5	18790.6	3P(1S)3P	2.0	1	342164.1	3P(2S)1D	-2.0	9	0.004900	3	13	3S23P2--3S13P3
304.167	328766.4	103711.3	3P(1S)1S	0.0	5	432477.7	3P(2S)1P	-1.0	14	0.243278	5	18	3S23P2--3S13P3
300.211	333099.0	9065.2	3P(1S)3P	1.0	3	342164.1	3P(2S)1D	-2.0	9	0.005190	2	13	3S23P2--3S13P3
275.333	363197.2	51793.8	3P(1S)1D	2.0	2	414991.0	3D(2P)3F	-2.0	20	0.017015	4	15	3S23P2--3P13D1
270.289	369974.5	51793.8	3P(1S)1D	2.0	2	421768.3	3D(2P)3F	-3.0	17	0.001687	4	16	3S23P2--3P13D1
262.685	380683.8	51793.8	3P(1S)1D	2.0	2	432477.7	3P(2S)1P	-1.0	14	0.956069	4	18	3S23P2--3S13P3
261.390	382570.2	18790.6	3P(1S)3P	2.0	1	401360.8	3P(2S)3S	-1.0	11	1.209163	3	14	3S23P2--3S13P3
256.593	389722.5	103711.3	3P(1S)1S	0.0	5	493433.7	3D(2P)3P	-1.0	25	0.000693	5	20	3S23P2--3P13D1
254.910	392295.7	9065.2	3P(1S)3P	1.0	3	401360.8	3P(2S)3S	-1.0	11	0.659176	2	14	3S23P2--3S13P3
252.398	396200.4	18790.6	3P(1S)3P	2.0	1	414991.0	3D(2P)3F	-2.0	20	0.005895	3	15	3S23P2--3P13D1
249.152	401360.8	0.0	3P(1S)3P	0.0	4	401360.8	3P(2S)3S	-1.0	11	0.243368	1	14	3S23P2--3S13P3
248.153	402977.7	18790.6	3P(1S)3P	2.0	1	421768.3	3D(2P)3F	-3.0	17	0.018571	3	16	3S23P2--3P13D1
246.350	405925.9	9065.2	3P(1S)3P	1.0	3	414991.0	3D(2P)3F	-2.0	20	0.004665	2	15	3S23P2--3P13D1
241.729	413687.1	18790.6	3P(1S)3P	2.0	1	432477.7	3P(2S)1P	-1.0	14	0.004602	3	18	3S23P2--3S13P3
236.176	423412.5	9065.2	3P(1S)3P	1.0	3	432477.7	3P(2S)1P	-1.0	14	0.083331	2	18	3S23P2--3S13P3
231.226	432477.7	0.0	3P(1S)3P	0.0	4	432477.7	3P(2S)1P	-1.0	14	0.008949	1	18	3S23P2--3S13P3
230.611	433630.3	51793.8	3P(1S)1D	2.0	2	485424.1	3D(2P)3P	-2.0	22	0.820846	4	19	3S23P2--3P13D1
226.429	441639.9	51793.8	3P(1S)1D	2.0	2	493433.7	3D(2P)3P	-1.0	25	0.018268	4	20	3S23P2--3P13D1
224.059	446311.3	51793.8	3P(1S)1D	2.0	2	498105.2	3D(2P)1D	-2.0	23	1.688819	4	21	3S23P2--3P13D1
220.717	453069.7	51793.8	3P(1S)1D	2.0	2	504863.5	3D(2P)3D	-1.0	24	0.035371	4	23	3S23P2--3P13D1
219.873	454808.1	51793.8	3P(1S)1D	2.0	2	506601.9	3D(2P)3D	-3.0	18	0.134178	4	24	3S23P2--3P13D1
219.502	455575.9	51793.8	3P(1S)1D	2.0	2	507369.8	3D(2P)3D	-2.0	21	0.352412	4	25	3S23P2--3P13D1
216.954	460927.2	103711.3	3P(1S)1S	0.0	5	564638.5	3D(2P)1P	-1.0	26	1.290610	5	27	3S23P2--3P13D1
214.301	466633.5	18790.6	3P(1S)3P	2.0	1	485424.1	3D(2P)3P	-2.0	22	0.681234	3	19	3S23P2--3P13D1
210.685	474643.1	18790.6	3P(1S)3P	2.0	1	493433.7	3D(2P)3P	-1.0	25	0.131290	3	20	3S23P2--3P13D1
209.926	476359.0	9065.2	3P(1S)3P	1.0	3	485424.1	3D(2P)3P	-2.0	22	0.840877	2	19	3S23P2--3P13D1
208.631	479314.5	18790.6	3P(1S)3P	2.0	1	498105.2	3D(2P)1D	-2.0	23	0.024190	3	21	3S23P2--3P13D1
206.454	484368.6	9065.2	3P(1S)3P	1.0	3	493433.7	3D(2P)3P	-1.0	25	0.030019	2	20	3S23P2--3P13D1
205.730	486072.9	18790.6	3P(1S)3P	2.0	1	504863.5	3D(2P)3D	-1.0	24	0.351993	3	23	3S23P2--3P13D1
204.997	487811.3	18790.6	3P(1S)3P	2.0	1	506601.9	3D(2P)3D	-3.0	18	3.662592	3	24	3S23P2--3P13D1
204.675	488579.2	18790.6	3P(1S)3P	2.0	1	507369.8	3D(2P)3D	-2.0	21	1.410388	3	25	3S23P2--3P13D1
204.482	489040.0	9065.2	3P(1S)3P	1.0	3	498105.2	3D(2P)1D	-2.0	23	0.908558	2	21	3S23P2--3P13D1
203.445	491533.3	9065.2	3P(1S)3P	1.0	3	500598.4	3D(2P)3P	-0.0	27	0.363066	2	22	3S23P2--3P13D1
202.661	493433.7	0.0	3P(1S)3P	0.0	4	493433.7	3D(2P)3P	-1.0	25	1.157868	1	20	3S23P2--3P13D1
201.695	495798.4	9065.2	3P(1S)3P	1.0	3	504863.5	3D(2P)3D	-1.0	24	0.921496	2	23	3S23P2--3P13D1
200.680	498304.6	9065.2	3P(1S)3P	1.0	3	507369.8	3D(2P)3D	-2.0	21	0.747540	2	25	3S23P2--3P13D1

TABLE XIII CALCULATED WL'S AND GF'S OF FE XIII EMISSION LINES

CONFIGURATIONS	TRANSITION	WAVENUMBER	WAVELENGTH	GF	LOW PAR LEVEL	HIGH PAR LEVEL
3S23P2--3S13P3	(1S)3P2--(2S)3D3	250119.700	399.809	0.219	18790.600	268910.300
3S23P2--3S13P3	(1S)3P1--(2S)3D2	257269.900	388.697	0.164	9065.200	266335.100
3S23P2--3S13P3	(1S)3P1--(2S)3D1	257072.200	388.996	0.026	9065.200	266137.400
3S23P2--3S13P3	(1S)3P0--(2S)3D1	266137.400	375.746	0.080	0.0	266137.400
3S23P2--3S13P3	(1S)3P2--(2S)3P2	295208.600	338.744	0.253	18790.600	313999.200
3S23P2--3S13P3	(1S)3P2--(2S)3P1	295333.000	338.601	0.036	18790.600	314123.600
3S23P2--3S13P3	(1S)3P1--(2S)3P2	304934.000	327.940	0.027	9065.200	313999.200
3S23P2--3S13P3	(1S)3P1--(2S)3P1	305058.400	327.806	0.086	9065.200	314123.600
3S23P2--3S13P3	(1S)3P1--(2S)3P0	304605.500	328.293	0.058	9065.200	313670.700
3S23P2--3S13P3	(1S)3P0--(2S)3P1	314123.600	318.346	0.052	0.0	314123.600
3S23P2--3S13P3	(1S)3P2--(2S)3S1	382570.200	261.390	1.209	18790.600	401360.800
3S23P2--3S13P3	(1S)3P1--(2S)3S1	392295.600	254.910	0.659	9065.200	401360.800
3S23P2--3S13P3	(1S)3P0--(2S)3S1	401360.800	249.152	0.243	0.0	401360.800
3S23P2--3S13P3	(1S)3P1--(2S)1P1	423412.500	236.176	0.083	9065.200	432477.700
3S23P2--3S13P3	(1S)1D2--(2S)3D3	217116.500	460.582	0.018	51793.800	268910.300
3S23P2--3S13P3	(1S)1D2--(2S)1D2	290370.300	344.388	0.499	51793.800	342164.100
3S23P2--3S13P3	(1S)1D2--(2S)1P1	380683.900	262.685	0.956	51793.800	432477.700
3S23P2--3S13P3	( )1S0--(2S)1P1	328766.400	304.167	0.243	103711.300	432477.700
3S23P2--3P13D1	(1S)3P2--(2P)3F3	402977.700	248.153	0.019	18790.600	421768.300
3S23P2--3P13D1	(1S)3P2--(2P)3D3	487811.300	204.997	3.663	18790.600	506601.900
3S23P2--3P13D1	(1S)3P2--(2P)3D2	488579.200	204.675	1.410	18790.600	507369.800
3S23P2--3P13D1	(1S)3P2--(2P)3D1	486072.900	205.730	0.352	18790.600	504863.500
3S23P2--3P13D1	(1S)3P1--(2P)3D2	498304.600	200.680	0.747	9065.200	507369.800
3S23P2--3P13D1	(1S)3P1--(2P)3D1	495798.300	201.695	0.921	9065.200	504863.500
3S23P2--3P13D1	(1S)3P0--(2P)3D1	504863.500	198.073	0.113	0.0	504863.500
3S23P2--3P13D1	(1S)3P2--(2P)3P2	466633.500	214.301	0.681	18790.600	485424.100
3S23P2--3P13D1	(1S)3P2--(2P)3P1	474643.100	210.685	0.131	18790.600	493433.700
3S23P2--3P13D1	(1S)3P1--(2P)3P2	476358.900	209.926	0.841	9065.200	485424.100
3S23P2--3P13D1	(1S)3P1--(2P)3P1	484368.500	206.454	0.030	9065.200	493433.700
3S23P2--3P13D1	(1S)3P1--(2P)3P0	491533.200	203.445	0.363	9065.200	500598.400
3S23P2--3P13D1	(1S)3P0--(2P)3P1	493433.700	202.661	1.158	0.0	493433.700
3S23P2--3P13D1	(1S)3P2--(2P)1F3	537849.800	185.926	0.131	18790.600	556640.400
3S23P2--3P13D1	(1S)3P2--(2P)1D2	479314.600	208.631	0.024	18790.600	498105.200
3S23P2--3P13D1	(1S)3P1--(2P)1D2	489040.000	204.482	0.909	9065.200	498105.200
3S23P2--3P13D1	(1S)1D2--(2P)3F2	363197.200	275.333	0.017	51793.800	414991.000
3S23P2--3P13D1	(1S)1D2--(2P)3D3	454808.100	219.873	0.134	51793.800	506601.900
3S23P2--3P13D1	(1S)1D2--(2P)3D2	455576.000	219.502	0.352	51793.800	507369.800
3S23P2--3P13D1	(1S)1D2--(2P)3D1	453069.700	220.717	0.035	51793.800	504863.500
3S23P2--3P13D1	(1S)1D2--(2P)3P2	433630.300	230.611	0.821	51793.800	485424.100
3S23P2--3P13D1	(1S)1D2--(2P)3P1	441639.900	226.429	0.018	51793.800	493433.700
3S23P2--3P13D1	(1S)1D2--(2P)1F3	504846.600	198.080	3.468	51793.800	556640.400
3S23P2--3P13D1	(1S)1D2--(2P)1D2	446311.400	224.059	1.689	51793.800	498105.200
3S23P2--3P13D1	(1S)1D2--(2P)1P1	512844.700	194.991	0.025	51793.800	564638.500
3S23P2--3P13D1	( )1S0--(2P)1P1	460927.200	216.954	1.291	103711.300	564638.500
3S23P2--3P33D1	(1S)3P2--(4S)3D3	1180774.000	84.690	0.124	18790.600	1199564.600
3S23P2--3P33D1	(1S)3P2--(4S)3D2	1189600.500	84.062	0.015	18790.600	1208391.100
3S23P2--3P33D1	(1S)3P1--(4S)3D2	1199325.900	83.380	0.075	9065.200	1208391.100
3S23P2--3P33D1	(1S)3P1--(4S)3D1	1204553.300	83.018	0.028	9065.200	1213618.500
3S23P2--3P33D1	(1S)3P0--(4S)3D1	1213618.500	82.398	0.035	0.0	1213618.500
3S23P2--3P33D1	(1S)1D2--(4S)3D3	1147770.800	87.125	0.017	51793.800	1199564.600
3S23P2--3P33D1	(1S)1D2--(4S)3D2	1156597.300	86.461	0.024	51793.800	1208391.100
3S23P2--3P33D1	(1S)3P2--(2D)3S1	1168306.400	85.594	0.153	18790.600	1187097.000
3S23P2--3P33D1	(1S)3P1--(2D)3S1	1178031.800	84.887	0.102	9065.200	1187097.000
3S23P2--3P33D1	(1S)3P0--(2D)3S1	1187097.000	84.239	0.037	0.0	1187097.000
3S23P2--3P33D1	(1S)3P2--(2D)1F3	1223472.600	81.735	0.017	18790.600	1242263.200
3S23P2--3P33D1	(1S)3P2--(2D)1D2	1217598.600	82.129	0.036	18790.600	1236389.200

HF COMPARED WITH MCDF PLUS BREIT AND QED FE XIII

TERM	J	HF EN LEVEL	DF EN LEVEL	DIFFERENCE	DFTERM
3(2D)3G	-5.0	1065444.011	1064525.800	-918.211	(2D)3G
2(2P)3F	-4.0	431518.820	431717.900	199.080	(2P)3F
3(4S)5D	-4.0	993357.561	992512.300	-845.261	(4S)5D
3(2D)3F	-4.0	1044416.051	1043632.000	-784.051	(2D)3F
3(2D)3G	-4.0	1063339.886	1062409.000	-930.886	(2D)3G
3(2D)1G	-4.0	1075786.132	1074755.800	-1030.332	(2D)1G
3(2P)3F	-4.0	1116212.287	1115620.100	-592.187	(2P)3F
1(2D)3D	-3.0	268403.818	268910.300	506.482	(2S)3D
2(2P)3F	-3.0	421930.367	421768.300	-162.067	(2P)3F
2(2P)3D	-3.0	507097.107	506601.900	-495.207	(2P)3D
2(2P)1F	-3.0	557242.329	556640.400	-601.929	(2P)1F
3(4S)5D	-3.0	992240.485	991439.500	-800.985	(4S)5D
3(2D)3D	-3.0	1028206.561	1027353.500	-853.061	(2D)3D
3(2D)3F	-3.0	1039873.669	1039032.100	-841.569	(2D)3F
3(2D)3G	-3.0	1061642.604	1060674.200	-968.404	(2D)3G
3(2P)3F	-3.0	1115111.530	1114328.700	-782.830	(2P)3F
3(2P)3D	-3.0	1127495.927	1126794.500	-701.427	(2P)3D
3(2P)1F	-3.0	1160887.394	1160172.500	-714.894	(2P)1F
3(4S)3D	-3.0	1201009.179	1199564.600	-1444.579	(4S)3D
3(2D)1F	-3.0	1243546.742	1242263.200	-1283.542	(2D)1F
1(4S)5S	-2.0	189035.238	189815.300	780.062	(2S)5S
1(2D)3D	-2.0	265943.973	266335.100	391.127	(2S)3D
1(2P)3P	-2.0	313497.208	313999.200	501.992	(2S)3P
1(2D)1D	-2.0	341678.767	342164.100	485.333	(2S)1D
2(2P)3F	-2.0	415311.564	414991.000	-320.564	(2P)3F
2(2P)3P	-2.0	486310.419	485424.100	-886.319	(2P)3P
2(2P)1D	-2.0	498246.398	498105.200	-141.198	(2P)1D
2(2P)3D	-2.0	507501.113	507369.800	-131.313	(2P)3D
3(4S)5D	-2.0	991598.026	990874.300	-723.726	(4S)5D
3(2D)3D	-2.0	1026202.704	1025221.100	-981.604	(2D)3D
3(2D)3F	-2.0	1036497.245	1035690.300	-806.945	(2D)3F
3(2P)1D	-2.0	1097514.450	1096682.700	-831.750	(2P)1D
3(2P)3P	-2.0	1114637.191	1113371.400	-1265.791	(2P)3P
3(2P)3F	-2.0	1116429.625	1115681.700	-747.925	(2P)3F
3(2P)3D	-2.0	1120472.263	1119678.500	-793.763	(2P)3D
3(2D)3P	-2.0	1132135.263	1131635.900	-499.363	(2D)3P
3(4S)3D	-2.0	1209629.888	1208391.100	-1238.788	(4S)3D
3(2D)1D	-2.0	1237565.076	1236389.200	-1175.876	(2D)1D
1(2D)3D	-1.0	265767.349	266137.400	370.051	(2S)3D
1(2P)3P	-1.0	313757.944	314123.600	365.656	(2S)3P
1(4S)3S	-1.0	401506.875	401360.800	-146.075	(2S)3S
1(2P)1P	-1.0	432169.602	432477.700	308.098	(2S)1P
2(2P)3P	-1.0	493729.868	493433.700	-296.168	(2P)3P
2(2P)3D	-1.0	504716.466	504863.500	147.034	(2P)3D
2(2P)1P	-1.0	565154.345	564638.500	-515.845	(2P)1P
3(4S)5D	-1.0	991149.480	990479.300	-670.180	(4S)5D
3(2D)3D	-1.0	1029676.654	1028993.700	-682.954	(2D)3D
3(2D)1P	-1.0	1090069.035	1088990.800	-1078.235	(2D)1P
3(2P)3D	-1.0	1111783.384	1110666.700	-1116.684	(2P)3D
3(2P)3P	-1.0	1119701.121	1118947.000	-754.121	(2P)3P
3(2D)3P	-1.0	1127530.253	1126814.500	-715.753	(2D)3P
3(2D)3S	-1.0	1188269.310	1187097.000	-1172.310	(2D)3S
3(4S)3D	-1.0	1214629.256	1213618.500	-1010.756	(4S)3D
3(2P)1P	-1.0	1294702.864	1293438.700	-1264.164	(2P)1P
1(2P)3P	-0.0	313365.596	313670.700	305.104	(2S)3P
2(2P)3P	-0.0	500204.800	500598.400	393.600	(2P)3P
3(4S)5D	-0.0	990881.092	990236.000	-645.092	(4S)5D

3(2D)1S	-0.0	1044031.724	1043261.500	-770.224	(2D)1S
3(2P)3P	-0.0	1114669.328	1113762.400	-906.928	(2P)3P
3(2D)3P	-0.0	1131222.225	1130896.600	-325.625	(2D)3P
1(3P)3P	0.0	0.0	0.0	0.0	(1S)3P
1(1S)1S	0.0	103251.252	103711.300	460.048	(1S)1S
1(3P)3P	1.0	8578.416	9065.200	486.784	(1S)3P
1(3P)3P	2.0	18059.971	18790.600	730.629	(1S)3P
1(1D)1D	2.0	51092.279	51793.800	701.521	(1S)1D

STANDARD DEVIATION	AVERAGE	STDEVN N-1
600.9	-465.2	605.6

CONFIGURATION 3P33D1 FE XIII

TERM	J	HF EN LEVEL	DF EN LEVEL	DIFFERENCE	DFTERM	HF ENLV MOD	DIFF MOD
3(2D)3G-5.0		1065444.011	1064525.800	-918.211	(2D)3G	1064557.938	-32.138
3(4S)5D-4.0		993357.561	992512.300	-845.261	(4S)5D	992471.488	40.812
3(2D)3F-4.0		1044416.051	1043632.000	-784.051	(2D)3F	1043529.978	102.022
3(2D)3G-4.0		1063339.886	1062409.000	-930.886	(2D)3G	1062453.813	-44.813
3(2D)1G-4.0		1075786.132	1074755.800	-1030.332	(2D)1G	1074900.059	-144.259
3(2P)3F-4.0		1116212.287	1115620.100	-592.187	(2P)3F	1115326.214	293.886
3(4S)5D-3.0		992240.485	991439.500	-800.985	(4S)5D	991354.412	85.088
3(2D)3D-3.0		1028206.561	1027353.500	-853.061	(2D)3D	1027320.488	33.012
3(2D)3F-3.0		1039873.669	1039032.100	-841.569	(2D)3F	1038987.596	44.504
3(2D)3G-3.0		1061642.604	1060674.200	-968.404	(2D)3G	1060756.531	-82.331
3(2P)3F-3.0		1115111.530	1114328.700	-782.830	(2P)3F	1114225.457	103.243
3(2P)3D-3.0		1127495.927	1126794.500	-701.427	(2P)3D	1126609.854	184.646
3(2P)1F-3.0		1160887.394	1160172.500	-714.894	(2P)1F	1160001.321	171.179
3(4S)3D-3.0		1201009.179	1199564.600	-1444.579	(4S)3D	1200123.106	-558.506
3(2D)1F-3.0		1243546.742	1242263.200	-1283.542	(2D)1F	1242660.669	-397.469
3(4S)5D-2.0		991598.026	990874.300	-723.726	(4S)5D	990711.953	162.347
3(2D)3D-2.0		1026202.704	1025221.100	-981.604	(2D)3D	1025316.631	-95.531
3(2D)3F-2.0		1036497.245	1035690.300	-806.945	(2D)3F	1035611.172	79.128
3(2P)1D-2.0		1097514.450	1096682.700	-831.750	(2P)1D	1096628.377	54.323
3(2P)3P-2.0		1114637.191	1113371.400	-1265.791	(2P)3P	1113751.118	-379.718
3(2P)3F-2.0		1116429.625	1115681.700	-747.925	(2P)3F	1115543.552	138.148
3(2P)3D-2.0		1120472.263	1119678.500	-793.763	(2P)3D	1119586.190	92.310
3(2D)3P-2.0		1132135.263	1131635.900	-499.363	(2D)3P	1131249.190	386.710
3(4S)3D-2.0		1209629.888	1208391.100	-1238.788	(4S)3D	1208743.815	-352.715
3(2D)1D-2.0		1237565.076	1236389.200	-1175.876	(2D)1D	1236679.003	-289.803
3(4S)5D-1.0		991149.480	990479.300	-670.180	(4S)5D	990263.407	215.893
3(2D)3D-1.0		1029676.654	1028993.700	-682.954	(2D)3D	1028790.581	203.119
3(2D)1P-1.0		1090069.035	1088990.800	-1078.235	(2D)1P	1089182.962	-192.162
3(2P)3D-1.0		1111783.384	1110666.700	-1116.684	(2P)3D	1110897.311	-230.611
3(2P)3P-1.0		1119701.121	1118947.000	-754.121	(2P)3P	1118815.048	131.952
3(2D)3P-1.0		1127530.253	1126814.500	-715.753	(2D)3P	1126644.180	170.320
3(2D)3S-1.0		1188269.310	1187097.000	-1172.310	(2D)3S	1187383.237	-286.237
3(4S)3D-1.0		1214629.256	1213618.500	-1010.756	(4S)3D	1213743.183	-124.683
3(2P)1P-1.0		1294702.864	1293438.700	-1264.164	(2P)1P	1293816.791	-378.091
3(4S)5D-0.0		990881.092	990236.000	-645.092	(4S)5D	989995.019	240.981
3(2D)1S-0.0		1044031.724	1043261.500	-770.224	(2D)1S	1043145.651	115.849
3(2P)3P-0.0		1114669.328	1113762.400	-906.928	(2P)3P	1113783.255	-20.855
3(2D)3P-0.0		1131222.225	1130896.600	-325.625	(2D)3P	1130336.152	560.448

STANDARD DEVIATION	AVERAGE	STDEVN N-1
235.6	-886.1	238.7

LEVELS THEIR PERCECTAGE COMPOSITION FOR TERMS OF J= 3.0

236.754	1(2D)3D(88.0%)	2(2P)3D(11.1%)	3(4S)3D(0.6%)	3(2D)3D(0.2%)	3(2P)3D(0.1%)	
390.281	2(2P)3F(97.8%)	3(2P)3F(1.7%)	2(2P)3D(0.2%)	2(2P)1F(0.2%)	1(2D)3D(0.1%)	
475.447	2(2P)3D(86.1%)	1(2D)3D(10.9%)	3(2P)3D(1.7%)	2(2P)1F(0.8%)	2(2P)3F(0.4%)	
525.592	2(2P)1F(97.1%)	3(2P)1F(2.0%)	2(2P)3D(0.8%)	2(2P)3F(0.1%)	1(2D)3D(0.1%)	
960.591	3(4S)5D(98.0%)	3(2P)3D(0.6%)	3(2P)3F(0.5%)	3(4S)3D(0.4%)	3(2D)3D(0.2%)	
996.557	3(2D)3D(50.2%)	3(4S)3D(38.7%)	3(2P)3D(4.4%)	3(2D)3F(3.5%)	3(2P)3F(1.6%)	
1008.224	3(2D)3F(78.8%)	3(2P)3F(13.0%)	3(2D)3D(3.9%)	3(2D)3G(1.9%)	3(4S)3D(1.9%)	
1029.993	3(2D)3G(95.2%)	3(2D)3F(3.4%)	3(2P)1F(0.7%)	3(2P)3F(0.5%)	3(2D)1F(0.1%)	
1083.462	3(2P)3F(81.7%)	3(2D)3F(12.9%)	3(2D)3G(2.1%)	2(2P)3F(1.3%)	3(2P)3D(1.1%)	
1095.846	3(2P)3D(53.7%)	3(2D)3D(27.6%)	3(4S)3D(11.7%)	3(2P)1F(2.7%)	3(2D)1F(1.9%)	
1129.238	3(2P)1F(56.8%)	3(2D)1F(35.4%)	3(2P)3D(3.9%)	2(2P)1F(1.2%)	3(2P)3F(0.7%)	
1169.359	3(4S)3D(44.6%)	3(2P)3D(33.3%)	3(2D)3D(16.9%)	3(2D)1F(3.2%)	1(2D)3D(0.7%)	
1211.897	3(2D)1F(58.9%)	3(2P)1F(37.0%)	3(4S)3D(1.6%)	3(2P)3D(1.2%)	2(2P)1F(0.6%)	

DOMINANT TERMS CHOSEN FOR DESIGNATION J= 3.0 PARITY=1

TERMS	LEVELS	% COMP
1(2D)3D	236.753968	88.0
2(2P)3F	390.280517	97.8
2(2P)3D	475.447257	86.1
2(2P)1F	525.592479	97.1
3(4S)5D	960.590635	98.0
3(2D)3D	996.556711	50.2
3(2D)3F	1008.223819	78.8
3(2D)3G	1029.992754	95.2
3(2P)3F	1083.461680	81.7
3(2P)3D	1095.846077	53.7
3(2P)1F	1129.237544	56.8
3(4S)3D	1169.359329	44.6
3(2D)1F	1211.896892	58.9

TABLE I CALCULATED WL'S AND GF'S OF EMISSION LINES

CONFIGURATIONS	TRANSITION	WAVENUMBER	WAVELENGTH	GF	LEVELS CM-1 LOW PAR LEVEL	HIGH PAR LEVEL
3S23P2--3S13P3 (	)3P2--(4S)5S2	170975.267	584.880	0.001	-13589.879	157385.388
3S23P2--3S13P3 (	)3P1--(4S)5S2	180456.822	554.149	0.001	-23071.434	157385.388
3S23P2--3S13P3 (	)3P2--(4S)3S1	383446.904	260.792	1.211	-13589.879	369857.025
3S23P2--3S13P3 (	)3P1--(4S)3S1	392928.459	254.499	0.669	-23071.434	369857.025
3S23P2--3S13P3 (	)3P0--(4S)3S1	401506.875	249.062	0.245	-31649.850	369857.025
3S23P2--3S13P3 (	)1S0--(4S)3S1	298255.623	335.283	0.009	71601.402	369857.025
3S23P2--3S13P3 (	)3P2--(2D)3D3	250343.847	399.451	0.221	-13589.879	236753.968
3S23P2--3S13P3 (	)3P2--(2D)3D2	247884.002	403.414	0.011	-13589.879	234294.123
3S23P2--3S13P3 (	)3P2--(2D)3D1	247707.378	403.702	0.001	-13589.879	234117.499
3S23P2--3S13P3 (	)3P1--(2D)3D2	257365.557	388.552	0.161	-23071.434	234294.123
3S23P2--3S13P3 (	)3P1--(2D)3D1	257188.933	388.819	0.027	-23071.434	234117.499
3S23P2--3S13P3 (	)3P0--(2D)3D1	265767.349	376.269	0.077	-31649.850	234117.499
3S23P2--3S13P3 (	)3P2--(2D)1D2	323618.796	309.006	0.004	-13589.879	310028.917
3S23P2--3S13P3 (	)3P1--(2D)1D2	333100.351	300.210	0.005	-23071.434	310028.917
3S23P2--3S13P3 (	)3P2--(2P)3P2	295437.237	338.481	0.247	-13589.879	281847.358
3S23P2--3S13P3 (	)3P2--(2P)3P1	295697.973	338.183	0.038	-13589.879	282108.094
3S23P2--3S13P3 (	)3P1--(2P)3P2	304918.792	327.956	0.030	-23071.434	281847.358
3S23P2--3S13P3 (	)3P1--(2P)3P1	305179.528	327.676	0.082	-23071.434	282108.094
3S23P2--3S13P3 (	)3P1--(2P)3P0	304787.180	328.098	0.057	-23071.434	281715.746
3S23P2--3S13P3 (	)3P0--(2P)3P1	313757.944	318.717	0.052	-31649.850	282108.094
3S23P2--3S13P3 (	)3P2--(2P)1P1	414109.631	241.482	0.004	-13589.879	400519.752
3S23P2--3S13P3 (	)3P1--(2P)1P1	423591.186	236.077	0.074	-23071.434	400519.752
3S23P2--3S13P3 (	)3P0--(2P)1P1	432169.602	231.391	0.008	-31649.850	400519.752
3S23P2--3S13P3 (	)1D2--(2D)3D3	217311.539	460.169	0.016	19442.429	236753.968
3S23P2--3S13P3 (	)1D2--(2D)3D2	214851.694	465.437	0.002	19442.429	234294.123
3S23P2--3S13P3 (	)1D2--(2D)3D1	214675.070	465.820	0.002	19442.429	234117.499
3S23P2--3S13P3 (	)1D2--(2D)1D2	290586.488	344.132	0.500	19442.429	310028.917
3S23P2--3S13P3 (	)1D2--(2P)3P2	262404.929	381.090	0.007	19442.429	281847.358
3S23P2--3S13P3 (	)1D2--(2P)3P1	262665.665	380.712	0.002	19442.429	282108.094
3S23P2--3S13P3 (	)1D2--(2P)1P1	381077.323	262.414	0.952	19442.429	400519.752
3S23P2--3S13P3 (	)1S0--(2P)3P1	210506.692	475.044	0.001	71601.402	282108.094
3S23P2--3S13P3 (	)1S0--(2P)1P1	328918.350	304.027	0.243	71601.402	400519.752
3S23P2--3P13D1 (	)3P2--(2P)3F3	403870.396	247.604	0.015	-13589.879	390280.517
3S23P2--3P13D1 (	)3P2--(2P)3F2	397251.593	251.730	0.005	-13589.879	383661.714
3S23P2--3P13D1 (	)3P1--(2P)3F2	406733.148	245.861	0.004	-23071.434	383661.714
3S23P2--3P13D1 (	)3P2--(2P)3D3	489037.136	204.483	3.691	-13589.879	475447.257
3S23P2--3P13D1 (	)3P2--(2P)3D2	489441.142	204.315	1.417	-13589.879	475851.263
3S23P2--3P13D1 (	)3P2--(2P)3D1	486656.495	205.484	0.346	-13589.879	473066.616
3S23P2--3P13D1 (	)3P1--(2P)3D2	498922.697	200.432	0.766	-23071.434	475851.263
3S23P2--3P13D1 (	)3P1--(2P)3D1	496138.050	201.557	0.928	-23071.434	473066.616
3S23P2--3P13D1 (	)3P0--(2P)3D1	504716.466	198.131	0.131	-31649.850	473066.616
3S23P2--3P13D1 (	)3P2--(2P)3P2	468250.448	213.561	0.677	-13589.879	454660.569
3S23P2--3P13D1 (	)3P2--(2P)3P1	475669.897	210.230	0.144	-13589.879	462080.018
3S23P2--3P13D1 (	)3P1--(2P)3P2	477732.003	209.322	0.794	-23071.434	454660.569
3S23P2--3P13D1 (	)3P1--(2P)3P1	485151.452	206.121	0.022	-23071.434	462080.018
3S23P2--3P13D1 (	)3P1--(2P)3P0	491626.384	203.406	0.363	-23071.434	468554.950
3S23P2--3P13D1 (	)3P0--(2P)3P1	493729.868	202.540	1.139	-31649.850	462080.018
3S23P2--3P13D1 (	)3P2--(2P)1F3	539182.358	185.466	0.107	-13589.879	525592.479
3S23P2--3P13D1 (	)3P2--(2P)1D2	480186.427	208.252	0.013	-13589.879	466596.548
3S23P2--3P13D1 (	)3P1--(2P)1D2	489667.982	204.220	0.938	-23071.434	466596.548
3S23P2--3P13D1 (	)3P2--(2P)1P1	547094.374	182.784	0.001	-13589.879	533504.495
3S23P2--3P13D1 (	)3P1--(2P)1P1	556575.929	179.670	0.003	-23071.434	533504.495
3S23P2--3P13D1 (	)3P0--(2P)1P1	565154.345	176.943	0.001	-31649.850	533504.495
3S23P2--3P13D1 (	)1D2--(2P)3F3	370838.088	269.659	0.001	19442.429	390280.517
3S23P2--3P13D1 (	)1D2--(2P)3F2	364219.285	274.560	0.015	19442.429	383661.714
3S23P2--3P13D1 (	)1D2--(2P)3D3	456004.828	219.296	0.109	19442.429	475447.257
3S23P2--3P13D1 (	)1D2--(2P)3D2	456408.834	219.102	0.335	19442.429	475851.263