PROGRAM RCG MOD11
CALCULATION OF ATOMIC ENERGY LEVELS AND SPECTRA

Robert D. Cowan
Los Alamos National Laboratory
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I.   Introduction

RCG is a FORTRAN77 program initially coded (1964-65) on the IBM 7030 ("Stretch"), and subsequently modified (with addition of many new features and options) to run on other IBM, CDC, and CRAY mainframes, various VAXs and MicroVAXs, SUN and IBM RISC workstations, and finally various Macintosh computers (using the Language Systems FORTRAN compiler) and PCs (using the free GNU g77 compiler). It has also been used by others on Apollo, Hewlett-Packard, and other computers. On 32-bit-word machines, it should be run in double-precision mode--preferably using, if available, a large-exponent-range option ($10^{\pm 350}$ rather than $10^{\pm 38}$) such as the VAX G_FLOATING compiler option. To make the program easily useable on both 64-bit and 32-bit machines, the following program modifications have been incorporated:

(1) PROGRAM cards have been included both with and without file-definition names included, and there have also been included file-name definitions via OPEN statements. On CRAY and CYBER machines, the simple PROGRAM card can be commented out and III in the main program set to 2, which causes the OPEN statements to be bypassed. On most other computers, the file-definition PROGRAM card is the one to be commented out, and III set to 1 to define all file names via OPEN statements. (On VAX machines, III may alternatively be set to zero, in which case some file names are set by typing them in interactively.)

(2) In all subroutines there are included IMPLICIT REAL*8(A-H,O-Z) statements, which may be commented out if necessary for 64-bit-word machines.

(3) Generic library subroutine names (e.g., MAX in place of AMAX1 or DMAX1) have been used so that the compiler will automatically use the single-precision or double-precision version, depending on the type of the argument variables. In all argument lists, constants have been replaced by variable names, the variable being given a value in a replacement statement such as TWO=2.0, so that in 32-bit-word machines it will automatically be converted to double precision.

(4) In subroutines PLEV and CALCFC, there were 25-fold-or-so nested DO loops, which exceeded the maximum size allowed in the VAX compiler (20-fold). This problem has been eliminated by moving the inner-most several DO loops to subroutines PLEVDOLP and CAFCDOLP, respectively.

(5) In subroutine SECONDS, there are included a single statement T=SECOND(T) appropriate to the CRAY, and also sets of timing-routine statements appropriate to VAXs or Macintoshes, PCs, SUNs, and IBM RISCs. Inappropriate sections of the routine are to be commented out (or a new one added as needed for the computer in question, or one can simply set T=0.0 if the computer has no internal timer clock).

(6) All ENCODE and DECODE statements used in older versions of the program have been removed. This has been facilitated by defining a number of variables as CHARACTER type.

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The basic purpose of RCG is to compute the angular factor
of various matrix elements in the theory of atomic structure and
spectra. The program employs Racah-algebra techniques, and input
decks containing coefficients of fractional parentage (cfp) for
each subshell l^w involved in each of the electron configurations

$$(n_1l_1)^{w_1} (n_2l_2)^{w_2} \quad (n_ql_q)^{w_q} \qquad (1)$$

present in the calculation. Any occupied subshell nl^w may be (and
in practice always is) deleted from the set (1) if it is filled
($w=4l+2$) in every configuration involved in a given calculation.
        A short description of the basic theory behind the program
(except for configuration-interaction effects) may be found in
R. D. Cowan, J. Opt. Soc. Am. <u>58</u>, 808 and 924 (1968). Full
details are given in R. D. Cowan, <u>The Theory of Atomic Structure
and Spectra</u> (University of California Press, Berkeley, 1981)--
especially Chapters 16 and 18--hereinafter referred to simply as
"TASS".
        The angular factors in question are:
        (a) the trivial (unit-matrix) coefficient of E_{av}, the
center-of-gravity energy of each configuration;
        (b) the coefficients f_k, g_k, and d of the single-
configuration direct and exchange Coulomb-interaction (F^k and G^k)
and spin-orbit-interaction ( ) radial integrals, and the
coefficients $r_d{}^k$ and $r_e{}^k$ of the direct and exchange configuration-
interaction Coulomb radial integrals R^k, which are involved in the
calculation of the Hamiltonian (energy-level) matrix elements;
        (c) the magnetic-dipole matrix elements, and the angular
coefficients of the electric-dipole ($t=1$) and electric-quadrupole
($t=2$) reduced radial matrix elements

$$\mathbf{P}_{ll'}{}^{(t)} = \langle l \| r^{(t)} C^{(t)} \| l' \rangle \qquad . \qquad (2)$$

Also possible are angular coefficients of certain effective-
Coulomb-interaction operators , , , T1, and T2, and "illegal-k"
operators F^k and G^k used in representing weak configuration-
interaction effects (TASS, Sec. 16-7), and also coefficients of
spherical-Bessel-function radial integrals

$$\langle l \| j_t(Kr) C^{(t)} \| l' \rangle \qquad , \qquad (3)$$

(TASS, Secs. 18-12 and 18-13).
     These angular coefficients may be used as input to programs
(such as RCE Mod 20) for least-squares fitting of experimental
energy levels.
        If numerical values of the radial integrals E_{av}, F^k, G^k, , R^k
are provided (either by considering them as adjustable parameters
determined by least-squares fitting of experimental levels, or
using ab initio theoretical values computed from atomic radial

wavefunctions), then energy levels and intermediate-coupling eigenvectors are computed. If numerical values of the electric-multipole integrals are supplied, then the energy levels and eigenvectors are used for computation of spectrum-line wavelengths and the associated oscillator strengths and radiative transition probabilities. In practice, values of these radial integrals (and indeed the entire RCG input file, ing11) are obtained via a calculation with the atomic-wavefunction programs RCN/RCN2.

   Options are available in RCG for the calculation of photoionization cross sections, autoionization transition probabilities, plane-wave-Born electron-impact collision strengths, and spherically averaged radial electron density distributions for each eigenvector-state (this last, provided single-configuration radial wavefunctions are available from an RCN calculation).

II.   Source Programs
   The following brief discussion of the function of each subroutine or function program provides a rough outline of the basic calculational procedure. For simplicity, the following discussion uses the default values of the various disk-file names, but these can be easily changed. In places, terminology will be used that dates from the time when computer input consisted of punched cards: The word "card" refers to a line (one record) of an input file or FORTRAN source file, and the word "deck" refers to an input file--set of cards--or portion thereof. Characters "punched" in specific columns of these cards are, of course, to be typed into the corresponding columns of the input line. Statements that various information is "printed" means that information is written to the output print file $IW=9$, but in many cases only if certain print options are in effect.

MAIN Reads various control cards from the input file, disk unit $IR=10$ (named ing11), and calls the various major subroutines according to the information thereon.

CUVFD (Calculate U,V,f,d) Defines three disk file numbers ID2, ID3,ID4 (normally 72,73,74). Reads coefficient-of-fractional-parentage (cfp) decks (including term quantum numbers $_iL_iS_i$ and parent quantum numbers $_i\bar{L}_i\bar{S}_i$) for each subshell $(l_i)^{w_i}$ that may be involved in any of the configurations (1) for which calculations are to be made later, computes coefficients of fractional grandparentage (cfgp) if pertinent, and writes all this on binary disk 72; calculates matrix elements of $U^{(r)}$ and $V^{(r1)}$ and writes them on disk 73; and calculates angular coefficients for $F^k(ii)$, for , , (also T,T1,T2 for d^w subshells) if so requested, and for $_i$, and writes them on disk 74.

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CIJKF   Calls S3J0SQ to calculate matrix elements

$$\langle l_i \| C^{(k)} \| l_j \rangle \quad . \tag{4}$$

LOCDSK   Locates the first record of information for l^w on disk 72, 73, or 74.

LNCUV (l^n,C,U,V)   Reads input cards specifying the subshells $l_i^{w_i}$ involved in each configuration, and calculates (via CIJKF) and prints a table of values of the matrix elements (4). This table is not used in further calculations, but is for information only.

PLEV (preliminary levels)   Using the $l_i^{w_i}$ values read by LNCUV, reads the terms of $l_i^{w_i}$ from disk 72, and vectorially adds quantum numbers $L_i S_i$ to set up tables of all possible quantum numbers $L_i S_i$ and J_i ($i \le q$).

PFGD   Sets up preliminary tables of the coefficients f_k, g_k, d, etc. of $F^k(ii)$, $\alpha, \beta, \gamma, T, T1, T2$, and ζ_i (obtained from disk 74) and of $F^k(ij)$ and $G^k(ij)$ (computed with the aid of subroutines CIJKF, RDIJ, and REIJ, using matrix elements of U and V obtained from disk 73), and writes these tables on disk 20.

PRK   Computes preliminary tables of coefficients r^k of the configuration-interaction parameters $R^k(ij,i'j')$ with the aid of cfp and cfgp from disk 72, U and V matrix elements from disk 73, and subroutines CLASS1 to CLAS11, RDIJ, and REIJ. Writes these tables on disk 20.

RDIJ   Used in computing coefficients f_k and $r_d^{\ k}$ of direct Coulomb-interaction parameters $F^k(ij)$ and $R^k(ij,i'j')$.

REIJ   Used in computing coefficients g_k and $r_e^{\ k}$ of exchange parameters $G^k(ij)$ and $R^k(ij,j'i')$.

CLASS1-CLAS11   Used in computing coefficients of R^k for the eleven possible classes of configuration interaction.

CALCFC (calculate final coefficients)   For each possible value of the total-angular-momentum quantum number J, selects those sets of quantum numbers $\alpha_i L_i S_i \mathcal{L}_i \mathcal{S}_i$ (1 $\le$ i $\le$ q) found by PLEV that can give this value of J, computes the LS-JJ transformation matrix, and writes all this on disk unit IL=31 (first parity) or IL=32 (second parity) and on IC=41 (both parities). Reads the preliminary tables of coefficients from disk 20, and sets up final coefficient matrices for all parameters (except E_{av}) and writes them on disk unit IC=41. Calls SPRIN to print matrices if desired, and also calls CPL37. If so requested, writes non-zero coefficient matrix elements on disk 19 for use by the Argonne National Laboratory least-squares level-fitting program.

CPL37 (coupling 3 to 7) If desired, calculates quantum numbers for, and transformation matrices to, coupling representations number 3 to 7 (**LS**=1, **JJ**=2--see JOSA article mentioned in Sec. I or page 15 below for definitions. Writes this information on disk IC=41.

SPRIN Multipurpose matrix-print routine, to print angular-coefficient matrices for F^k (KPAR=-1), G^k (0),   (+1), R^k (-2), for multipole transitions (+2), and for energy (+3) or eigenvector (+4) matrices, with more-or-less adequately labeled rows and columns. Also transforms energy-coefficient and mupole matrices when calculation in the JJ representation is desired, and computes and prints Landé g-values when called for **LS** eigenvectors. (Also, writes mupole matrices on disk IC=41.)

SPRN37 Called by SPRIN to read transformation matrices from disk IC=41, and transform and print eigenvectors in representations 3 to 7.

MUPOLE Reads quantum numbers from disks IL=31 and/or 32, cfp from disk 72, and $U^{(2)}$ from disk 73 (for electric quadrupole), and computes angular coefficients for line-strength calculations (or for plane-wave Born calculations). Calls SPRIN to print matrices and write on disk IC=41.

ENERGY Reads parameter values (E_{av}, and Coulomb and spin-orbit radial integrals) from data input cards on disk IR=10; for each **J**, reads quantum numbers and the **LS**-**JJ** transformation matrix from disk IC=41, reads coefficient matrices from IC and computes and diagonalizes the energy matrix, and writes eigenvalues (sorted in numerically increasing order) and eigenvectors on disk IE=31 (first parity) or 32 (second parity). Computes autoionization transition probabilities if appropriate, and writes them on disk IE. Calls SPRIN to print the energy and eigenvector matrices.

CALCV If so instructed, called by ENERGY (for each **J**) to calculate the diagonal elements of the coefficient matrices in the intermediate-coupling representation (the representation in which the energy matrix is diagonal). These elements represent the derivatives of the various eigenvalues with respect to the various parameters, providing information that can be used for a trial-and-error adjustment of the parameters to produce desired changes in the eigenvalues. (These are the elements that are calculated and used in least-squares programs such as RCE for the systematic iterative fitting of theoretical eigenvalues to experimental energy levels. In RCG, these elements are simply printed out for use in rough eye-ball parameter adjustments.)

LVDIST Called by ENERGY, if desired, to calculate the statistical distribution of energy-level statistical weight, and plot it on film via PLOJB (deleted in the present version of RCG). Also

calculates and plots that skewed-Gaussian curve that best fits the distribution (see TASS, Sec. 21-3 for definitions and examples).

SPECTR Called by ENERGY. Reads values of reduced mupole radial matrix integrals (2), calculated by RCN2, from the input file on disk 10. For each possible pair of values of (J,J'), reads the angular-coefficient mupole matrix from disk 41 and eigenvalues and vectors from disk IE=31 and/or 32, differences eigenvalues to compute wavelengths of spectrum lines, and multiplies the mupole matrix from either side by the appropriate eigenvector matrix (and multiplies the resulting matrix elements by the appropriate radial integral) to compute intermediate-coupling line strengths, oscillator strengths, and radiative transition probabilities. Spectrum-line information is printed after being sorted by (a) levels in the first set of configurations (first parity), (b) levels in the second set of configurations (second parity), and/or (c) wavelength. In the first two cases, a total transition probability and lifetime are computed for each level of the given set with resect to all possible transitions to lower-energy levels included in the opposite set.

WNDIST (wavenumber distribution) If desired, called from SPECTR to calculate [and plot] oscillator-strength distributions (see TASS, Sec. 21-4); writes this on disk unit 11 to provide input information for a separate program RADRATE.

BORN Can be called from ENERGY to calculate plane-wave-Born collision strengths (using interpolation routine AKNINT), and excitation rate coefficients (using routines RCOEFF, E1, and CSEVL).

UNCPLA and UNCPLB Compute the uncoupling coefficients U_a and U_b for reduced matrix elements, as defined in TASS, Eqs. (12.26) and (12.27).

RECPSH, RECPJP, RECPEX Compute the shift, jump, and exchange recoupling coefficients defined in TASS, Eqs. (13.64)-(13.66).

S3J0SQ, S9J, S6J, DELSQ, CALCFCT Compute the square of the 3-j symbol with magnetic quantum numbers all zero, the 9-j symbol, and the 6-j symbol, using a table of factorials computed by CALCFCT.

SORT, ORDER Sort an array of numbers into numerically increasing order, and correspondingly rearrange up to 12 additional arrays.

MLEW Dummy program (called by ENERGY) to call matrix-diagonalization routines TRED2 and TQL2.

RCEINP (RCE input) Called by ENERGY to write transformation and coefficient matrices on binary disk unit 2, and an input formatted file on disk 11, for the least-squares energy-level fitting program RCE.

ELECDEN Assumes the availability of the file tape2n computed by RCN, which contains one-electron radial wavefunctions for each orbital of each configuration in the present RCG calculation. Uses these wavefunctions to compute spherically averaged radial electron-density distributions for each configuration. Then uses each computed eigenvector to calculate a spherically averaged radial electron-density distribution for each configuration-interaction, intermediate-coupling eigenlevel.

III.   Input/Output Units
     Disk-storage unit numbers used, with external and internal names, are as follows:

Ext.	Int.	Default val.	Usage
ing11	ir	10	input
outg11	iw	9	printed output
tape2n		3	radial-wavefunction input (optional)
elecden		4	electron-density output
tape2e		2	coeffs. for use in least-squares prog. RCE
tapeci		8	Config.-interaction strengths from RCN2
outgine		11	formatted input for use in program RCE
tape72	id2	72	single-subshell quantum nos., cfp, and cfgp
tape73	id3	id2+1	$U(r)$, $V(r1)$
tape74	id4	id2+2	single-subshell Coulomb and spin-orbit coeffs.
		20	preliminary Coulomb and spin-orbit coefficients
	il	31,32	quantum nos., transformation matrices
	ic	41	quantum nos., transf. and final coef. matrices
	ie	31,32	energy levels, eigenvectors, autoionization transition probs.
		19	coeffs. for use in Argonne Natl Lab least-squares level-fitting program
		11	special-purpose level and osc.-strength output
		3,13	special-purpose dielectronic-recomb. output

     Normally, ID2-ID4 are small files; 20, IL, and IE are of intermediate length; IC is the largest. Actual sizes depend on the complexity of the set of configurations being run. Units 31 (ILA) and ID4 may share the same I/O buffer, as ILA is not used until ID4 is no longer needed. Default values may be readily changed by changing the six statements starting with statement 60 of the main program, by corresponding choice of the value of ID2T read from the input file at statement 85, and appropriate changes in the file numbers on the PROGRAM card or in OPEN statments.

<u>IV.   Input</u>
     We here discuss input-data setup for simple bound-state level and spectrum calculations. Modifications for special-purpose calculations involving continuum states will be discussed in Secs. XI to XIII. Sample input decks and output listings are provided in Sec. XV.
     Briefly, input data consist of the following:
          (1) Two types of optional control cards.
          (2) If requested by one of the above control cards, a set of cfp decks, followed by a card with a negative integer in columns 9-12 (signaling the end of the set of cfp decks).
          (3) An optional rescale card (see Sec. X).
          (4) One or more calculational decks (usually provided ready-to-run from output of an RCN/RCN2 calculation); each deck starts with a control card, and ends with a card containing "-99999999." in columns 21-30.
          (5) A card with a negative integer in columns 1-5, causing an exit from RCG. (This card is automatically provided by RCN2).
          (6) Any unused input data cards may be stored here if desired.

     NOTE: Before actual calculational runs can be made, a first RCG run must be made in which the input deck includes the cfp decks indicated in item (2) above; this results in the calculation of the files 72, 73, 74 discussed earlier, which are required in all subsequent calculations. An input file called ing11k is supplied that includes the cfp decks for this first calculation (with its name changed to ing11). This is discussed in greater detail in section (2) below, but it is suggested that on a first reading one skip the discussion of optional control cards, and at this point jump directly to the discussion of standard calculational decks in section (4) below.

     Details of the input are as follows.

     <u>(1a)</u> There may be one or two optional control cards of the following form:

cols.	variable	format
1-4	NCLSKP(K) 1	I4
5	K	I1
6-10	NOTKP(K)	I5
11-80	MULS1(I),LHS1(I)	14(I4,A1)

K must be 1 for configurations of the first parity, or 2 for configurations of the second parity. If NOTKP(K) is greater than zero then only those basis states (for configurations of parity K

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and serial number greater than or equal to NCLSKP(K) will be
retained that have one of the NOTKP(K) ("no. of LS terms to be
kept") values of multiplicity and total orbital angular momentum L
specified in columns 11 to 10+5*NOTKP; for example (using carats
to denote blank columns),

^^^12^^^^3^^^4s^^^2d^^^2s

means keep only ^{4}S, ^{2}D, and ^{2}S basis states for all configurations
of the second parity. These control cards need be included only
if LS-term truncation of this type is desired. [Notes: (a) If more
than one truncation control card with given K is included, only
the final one will be effective; (b) Truncation cards may appear
either before control card (1b), or following (1b) and the
associated cfp decks and end card (if any).]

   (1b)   There may be an optional control card of the form:

cols.	variable	format	comments
1-5	integer (=3)	I5	defines control card of type 1b
6-7	ILNCUV	I2	extra output print if > 0 (and ID2 > 0)
8-10	ID2	I3	file number (default=ID2DEF=72)
11-15	FLBDN	E5.1	default=0.001 Å
16-20	FLBDX	E5.1	default=500000 Å
21-30	DELEKEV	F10.5	default=0.0005 keV
31-40	EIONRY	F10.5	default=0.0 Ry
41-45	NPTKEV	I5	default=0
46-70	TKEV(I),I=2,6	5F5.3	default=0.0 keV [NTKEV (5) determined by the number of non-zero TKEV]
71-80	EMINA	F10.5	default=0.0 (same units as energy levels)

The variables FLBDN and FLBDX specify the minimum and maximum
wavelengths (lambda) of spectrum lines to be retained in
subroutine SPECTR; the variable DELEKEV is used in WNDIST in
defining the histogram bin-width for calculating the oscillator-
strength distribution; and the variables EIONRY, NPTKEV, TKEV, and
EMINA concern special-purpose dielectronic-recombination
calculations in SPECTR (see Sec. XII , pages 37 and 41). This
control card need be included only if cfp decks are included
and/or if non-default values of the other variables are desired;
there must be such a card (with ID2 non-zero) before a set of cfp
decks, and may be another (with ID2=0) following these decks.

   (2)   If ID2 is non-zero (normally=72), then this value will
determine values for the file numbers ID3(=ID2+1) and ID4(=ID2+2)
as well (see Sec. III). In addition, the control card (1b) must
then (and only then) be followed by a set of cfp decks, and by an
end card with negative integer in columns 9 to 12; the subroutine
CUVFD is called to process these cfp decks and write information
on disks ID2-ID4, and a non-zero ILNCUV produces printed output of

some of the computed information. Except as noted below, there
must be a cfp deck for each l^w involved in any configuration
specified in the calculational decks (4 below); if subshells l^w
and l^{w-2} will both be involved in a set of interacting
configurations, then a cfp deck for l^{w-1} must also be included (so
that cfgp for l^w can be computed). All decks of given l should be
grouped together, and must be arranged in order of increasing w.
Decks for l^0 and l^1 are needed only if cfgp for l^2 are required,
so that decks for g, h, i,   , electrons are normally never
needed. The input file ING11K provided with the program RCG
contains cfp decks for all s^w, p^w, d^w, f^0 to f^4 and f^{11} to f^{14},
and for g^0, g^1, g^2, h^0, h^1, and h^2. The file cfp contains also f^5
to f^{10} decks, but these require larger dimensions of several
variables than those used in the code provided (see the comment
cards near the beginning of the main program). Normally, all the
cfp decks included in ING11K can be used in calculation of disk
files ID2-ID4. (The presence of unneeded cfp decks causes no harm
except for extra computer time in CUVFD--see TASS, Tables 16-1 and
16-2--which needs to be executed only once, and a small amount of
extra disk search time in reading data from disks ID2-ID4 if
subshells of large l are needed in a given calculation.)
     The detailed format of each cfp deck need not be discussed
here. We need comment only on the form of the first card of each
deck, which contains:

        column 4:   the spectrosopic letter code for l
                     (s,p,d,f,g,h,i,k,   , according as the one-
                     electron angular momentum is
                      0,1,2,3,4,5,6,7,   , respectively.
     columns 5-8:   w   (format I4)
    columns 9-12:   number of LS terms of l^w (format I4)
   columns 13-16:   Number of parents (terms of l^{w-1})
                     (format (I4)

The size of a calculation (particularly for configurations
involving an f^w subshell) can be reduced by including only a
limited number of terms of the subshell l^w in setting up quantum
states of the complete configuration. To invoke such a
truncation, the number of terms of l^w to be included is placed in
columns 21-24, and the terms themselves are placed in columns 29-
32, 33-36,   73-76 (and if necessary in columns 1-4, 5-8,   of
succeeding cards). The first column for each term contains the
value of the multiplicity 2S+1, the second column contains the
letter symbol for L (S,P,D,F,G,H,I,K,   , except in lower case),
and the last two columns contain any necessary (left-adjusted)
serial number to distinguish different terms of the same LS; this
serial number must match that used in the body of the cfp deck,
which follows the convention used by C. W. Nielsen and G. F.
Koster, Spectroscopic Coefficients for the p^n, d^n, and f^n

Configurations (The M.I.T. Press, Cambridge, Mass., 1963). (Some examples are included in the cfp decks provided in ING11K for f^2, f^3, etc., though with the number of terms equal zero so that there is no truncation.)

The control card (1b) with ID2 > 0, together with cfp decks and end card, must be included on a first run of RCG--using, for example, ING11K for the input deck ING11--in order to produce the files ID2, ID3, and ID4 (normally TAPE72, TAPE73, and TAPE74). If these files, produced on such a run, are saved and made available to subsequent runs, then items (1b) and (2) may be deleted from all further runs [except, of course, that a (1b) card with ID2=0 must be included if non-default values are needed for variables other than ID2]. It will of course be necessary to recompute files ID2-ID4 if new subshells need to be added, or if truncation of LS terms is to be added or changed.

(3) For details of the optional rescaling card, see Sec. X).

(4) Calculational decks:
NOTE: In the most common usage of RCG, the calculational deck is automatically prepared by execution of programs RCN and RCN2, so that all the details below can be ignored except if one wishes to make changes for special purposes, or for some reason wishes to set up an input deck by hand. [The output deck from RCN2 is named "out2ing," and the name needs to be changed to "ing11" for use as the RCG input deck.]

Each calculational deck consists of the following:
(A) A control card, specifying among other things the number of configurations of each parity that are involved in the calculation.
(B) A set of configuration-definition cards, one for each configuration of the first parity.
(C) A set of configuration-definition cards, one for each configuration of the second parity. This will be an empty set if column 16 of the control card contains a zero.
(D) Zero, or one, or several, sets of parameter-value cards; a set may have any one of three forms:
(i) For a diagonalization, a set consists of:
(a) Parameter values for each configuration of the first parity.
(b) Configuration-interaction parameter values for each pair of interacting configurations of the first parity (if any).

(c) If IQUAD (col. 50 of the control card A) is 1 or >2, one or more sets of electric quadrupole reduced-matrix-element cards for

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configurations of the first parity.
- (d) Same as (a), for configs. of the second parity (if any).
- (e) Same as (b), for configs. of the second parity (if any).
- (f) If IQUAD 2, same as (c) except for the second parity.
- (g) If both parities are present, zero or more sets of electric-dipole reduced-matrix-element cards, for all pairs of configurations of opposite parity.

(ii) To write coefficient matrix elements for each parity on file 2, a single pseudo-parameter card containing "-55555555." in columns 21-30. If this option is used, then columns 9-10 of the control card (A) must contain a negative integer; the absolute value of this integer is the quantity NOCSET used in least-squares energy-level-fitting program RCE. This pseudo-parameter card may have one or more sets of genuine parameter cards (i) preceding it and/or following it.

(iii) A single pseudo-parameter card containing "-99999999." in columns 21-30 signals the end of the calculational deck (4). Any number of similar decks may follow.

A.   Calculational deck control card

The control card (A) is of the following form:

(i) If it contains a negative integer in columns 1-5, it is the data card (5) above, causing an exit from RCG. Any cards that follow are not read, but form part of the bone-pile (6).

(ii) If it contains a zero in columns 1-5, this is a rescaling card (see Sec. X below); it should be followed by a genuine card (iv) below.

(iii) If it contains a positive integer NOCSET in columns 8-10 and a 1 or 2 in column 5, this is a signal to search through the file on unit 2 until this CSET (set of coefficient matrices) is found. This pseudo control card is not followed by cards (B)-(D), but is immediately followed by a genuine control card (iv)-- normally containing a negative number in columns 9-10 to specify the serial number of a new CSET that is going to be added on to unit 2, to provide input for least-squares energy-level-fitting program RCE. [In practice, this option is never used, CSETs being computed as needed and written onto a new file on unit 2, rather than being added onto an old one.]

(iv) A genuine control card is of the following form:

cols.	format	variable name	normal value
1-5	I5	KCPL	1

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```
 6-7    I1,I2   NCK(K), K=1,2            blank
 9-10   I2      NOCET                   blank; see (iii) above
11-15   I1,2I2  NSCONF(I,1)

                        I=1,3    see below

16-20   I1,2I2  NSCONF(I,2)
21      I1      IABG                    blank
22      I1      IV                      blank
23-25   I3      NLSMAX                  blank
26-27   I2      NLT11                   blank
28-30   I3      NEVMAX                  blank
31-39   9I1     KCPLD(I), I=1,9         blank (except for Born calc.)
40      I1      IELPUN                  blank
41-44   2F2.1   SJNK(1), SJXK(1)        blank
45-48   2F2.1   SJNK(1), SJXK(2)        blank
49      I1      IMAG                    blank (for no M1 trans.)
50      I1      IQUAD                   blank (for no E2 trans.)
51-60   F10.5   UENRGY                  1000.0
61-65   F5.5    DMIN                    0.0
66      I1      ILNCUV                  blank
67      I1      IPLEV                   blank
68      I1      ICPC                    blank
69      I1      ICFC                    blank
70      I1      IDIP                    blank
71      I1      IENGYD                  0
72      I1      ISPECC                  7
73-74   I2      IW6                     -6   (blank for batch runs)
75-76   I2      IPCT                    blank
77-78   I2      ICTC                    blank
79-80   I2      ICTBCD                  blank
81-90   F10.5   CICRITERION             0.0 or blank
```

The significance of these quantities is as follows.

> KCPL: <0, an exit card, (i) above
>   =0, a rescaling card, (ii) above
>   =1, calculation to be done in **LS** (or **SL**) represent.
>   =2, calculation to be done in JJ representation

> NCK(K): If non-zero, then in all spectrum-line lists and
>   plane-wave-Born calculations, only those transitions
>   are included that involve levels belonging to the
>   first NCK(K) configurations. For parity-changing
>   (electric-dipole) transitions, K=1 and 2 represent
>   the first and second parities; for non-parity-
>   changing transitions, K=1 and 2 represent lower and
>   upper level, respectively. [Default is 50, except
>   NCK(1)=1 for plane-wave-Born calculations.]

> NOCSET: Must be blank or a negative integer; see under (iii)
>   above.

NSCONF(1,K): number of subshells for configurations of parity K

NSCONF(2,K):   number of configurations of parity K

NSCONF(3,K):   number of successive configurations for which
               interactions will be included [normally=NSCONF(2,K)].
               If NSCONF(3,K)=0, then following the configuration-
               definition cards there must be a card containing
               INTEST(I), I=1,80 (format 80I1); interaction will be
               included between configurations with serial numbers
               J1 and J2 if INTEST(I) > 0, where I is computed as
               follows:
                       J2X=NSCONF(2,K)
                       J1X=J2X-1
                       I=0
                       DO 799 J1=1,J1X
                       J2N=J1+1
                       DO 799 J2=J2N,J2X
                       I=I+1
                  799 CONTINUE
               If -7   NSCONF(3,K)   -1, interactions will be included
               if the first configuration has serial number

               J1   MAX(-NSCONF(3,K),IPCT).   If NSCONF(3,K)=-8, all
               interactions will be included. [Use this value with
               K=2 to calculate photoionization cross-sections.]
               If NSCONF(3,K)=-9, interactions will be included if
               the first configuration has serial number J1=1, or
               if the two configurations have successive serial
               numbers (J2=J1+1).
                   Note: A more satisfactory method of deleting
               weak configuration interactions is discussed under
               CICRITERION below.

        IABG: >0, include effective-operator parameters   (for p^w)
               or   , ,T,T1,T2 (for d^w), or   , , (for f^w); see
               TASS, Sec.16-7.
               =2 or 4, include illegal-k effective-operator
               parameters $F^k(ij)$ and $G^k(ij)$; TASS, Sec. 16-7.
                3, use **SL** instead of **LS** coupling (for straight **LS**
               coupling only; continue to use **LS** for compound
               couplings such as LSLK, LSJK, LSJLKS, etc.).

          IV: If non-zero, call CALCV to calculate and print V
               matrices (derivatives of eigenvalues with respect to
               parameter values).

      NLSMAX: Calculate eigenvectors in representations 3 to 7 if
               matrix size NLS is equal to or less than NLSMAX.

    The representations are [J. Opt. Sos. Am. 58, 808 (1968)]:

(1) LS: $\{[((\ _1L_1S_1)L_1S_1,\ \ _2L_2S_2)L_2S_2,\ \ \ \ \ \ _qL_qS_q]L_qS_q\}J_q$

(2) JJ: $\{[[(\ _1L_1S_1J_1)J_1,\ (\ _2L_2S_2J_2)]J_2,\ \ \ (\ _qL_qS_qJ_q)]\}J_q$

(3) JJJK: $\{[(\ \ \ \ \ J_{q-1})J_{q-1},\ L_q]K,S_q\}J_q$

(4) LSLK: $\{[((\ \ \ \ \ L_{q-1})L_{q-1},\ L_q)L_q,\ (\ \ \ \ \ S_{q-1})S_{q-1}]K,S_q\}J_q$

(5) LSJK: $\{[((\ \ \ \ \ L_{q-1})L_{q-1},\ (\ \ \ \ S_{q-1})S_{q-1})J_{q-1},L_q]K,\ S_q\}J_q$

(6) LSJLKJ: $\{[((\ \ \ \ L_{q-2})L_{q-2},\ (\ \ \ \ \ S_{q-2})S_{q-2})J_{q-2},$
$(L_{q-1}L_q)L]K,\ (S_{q-1}S_q)S\}J_q$

(7) LSJLSJ: $\{[(\ \ \ \ \ L_{q-2})L_{q-2},\ (\ \ \ \ S_{q-2})S_{q-2}]J_{q-2},$
$[(L_{q-1}L_q)L,\ (S_{q-1}S_q)S]J\ \}J_q$

NLT11: For all except the last configuration of each parity, include no more than the first NLT11 LS-terms of $l_1^{w_1}$ (default=119).

NEVMAX: For each J, print at most the eigenvectors having the NEVMAX smallest eigenvalues (default=500).

KCPLD(I): If > 0, do not print eigenvectors in the representation I (I=1 to 7) defined under NLSMAX. If KCPLD(3) 5, then a plane-wave-Born calculation is to be made, and KCPLD(3) to KCPLD(7) are interpreted differently; see Sec.XIII. If KCPLD(3) = 3 or 4, intermediate-coupling, CI radial electron-density distributions will be calculated provided tape2n from an RCN calculation is present; if = 3, cross-term contributions are not included.

KCPLD(9) IPRINT: If   7, delete energy-matrix print.
If   8, delete all eigenvector and purity prints.
If   9, delete eigenvalue and autoionization probability prints.

IELPUN: If = 1, write eigenvalues on unit 11 (special-purpose option).
If > 1, write multiplet level strengths on unit 19 (special-purpose option).

SJNK(K): For parity K, exclude matrices with J < SJNK(K) (default=0.0).

SJXK(K): For parity K, exclude matrices with J > SJXK(K) (default=99.0).
For example, to include only J=0 for first parity and J=1 for second parity, put .0.51.1. in columns 41-48.

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IMAG: If > 0, calculate magnetic-dipole transitions for
        the first, second, or both parities, according as
        IMAG=1, 2, or 3.

IQUAD: Similar to IMAG, except for electric quadrupole
        transitions (or parity-conserving plane-wave-Born
        excitations if KCPLD(3) 5). Note that the
        corresponding value of IQUAD must be used in column
        50 of the G5INP card in program RCN2 in order to
        calculate the required radial integrals.

UENRGY: Unit (in cm^{-1}) of all energy-parameter values on the
        parameter cards in this calculational deck
        (1000.0 if parameter values are in kilokaysers,
        8065.48 if in eV, 109737 if in Ry).

DMIN: Delete spectrum lines for which $S/X < DMIN$, where
        S is the line strength of the transition, and X is
        the largest $nl\,|\,r\,|\,n'l'^{\,2}$ for all of the transition
        arrays included in the calculation; S/X is the
        quantity printed in the spectrum line list in the
        column following the wavelength. Typical values of
        S/X for strong lines are 2 to 5; an appropriate
        value of DMIN to delete weak lines is 0.005 to 0.05.
        For modifications of these remarks in certain cases,
        see pages 25-26).

ILNCUV: If > 0, print $C^{(k)}$ matrix elements (4).

IPLEV: If > 0, print preliminary quantum numbers in
        subroutine PLEV.

ICPC: If > 0, print prelim. ang. coefs. in PFGD and PRK;
        if=1, print only parameter name and configuration(s),
        if=2, same as 1 plus single-configuration coeffs.,
        if=3, same as 1 plus config-interaction coeffs.,
        if=4, same as 1 plus all coeffs.

        If   5, write angular coefficients on unit 11 in a
        form suitable for input to program RCN, for making
        LS-term HF calculations.
        If = 9, skip matrix diagonalization part of program.
        (No parameter, multipole, nor "-99999999." cards are
        to be included in the input deck).

ICFC: If > 0, print coef. matrices in subroutine CALCFC;
        if=1, print only LS- and JJ-representation quantum
        numbers,
        if=2, print also the LS-JJ transformation matrix,
        if=3, same as 2 plus coef. matrices for single-conf.
        parameters,

if=4, same as 2 plus coef. matrices for CI params,
            if 5, same as 2 plus coef. matrices for all params.

    IDIP: If > 0, print J values of each multipole matrix;
            if > 1, print angular multipole matrix, and matrix
            of the squares of the elements.

  IENGYD: If = 0, print full energy matrix;
            if = 1, do not print matrix;
            if = 2, print only first NEVMAX rows and columns;
            if > 2, print first 11*IENGYD rows and columns.

  ISPECC: = 1, 3, 5, or 7, print spectrum lines sorted by
            levels of first parity
             = 2, 3, 6, or 7, print spectrum lines sorted by
            levels of second parity
            = 4 to 8, print spectrum lines sorted by wavelength
              8, call LVDIST and WNDIST;   sort printed only if 8.
            = 0, a variable IGDLEV is set to 7 (so that in the
            line list only lines involving the ground level are
            included), and then ISPECC is set to 8.
            Must be   6 to obtain values of BRNCH, etc.,
            see Sec. XII.

     IW6:   If < 0, information on the progress of the
            calculation is sent to unit 6 (the monitor screen).
            If > 0, normal output is sent to unit 6 instead of
            to unit 9; not a practical option because of the
            large volume of output.

    IPCT: Used only in connection with NSCONF(3,K), see above.

    ICTC: If not 0, use previously computed file on disk 41,
            skipping calls of PLEV, PFGD, PRK, CALCFC, and MUPOLE;
            TAPE72 is still required, but not TAPE73 nor TAPE74.

  ICTBCD: If > 0, write coefficient matrix elements on disk
            unit 19 for input to Argonne National Laboratory
            least-squares program.
            But if NOCSET not 0, set ICTBCD = 0 and write only
            disk 2, for input to least-squares program RCE.

CICRITERION: If greater than zero, configuration-interaction
            strengths for each pair of interacting configur-
            ations are read from tapeci (unit 4), written by
            program RCN2. Interactions for which the CI strength
            is less than CICRITERION will be omitted from all
            calculations in subroutines prk, calcfc, and energy.
            E.g., if CICRITERION=0.01, CI will be neglected for

configuration pairs in which the energy perturbation would have been less than about 1% of the energy spread within either configuration. Resulting time savings can be sizeable in cases involving many configurations. This is a more satisfactory method of deleting CI than the options described above involving NSCONF(3,K). [See the RCN2 writeup for definition of the cistrength.]

B-C.   Configuration Cards
     Each configuration is of the form

          $l_1{}^{w_1}\ l_2{}^{w_2}\qquad l_q{}^{w_q}$

and each of the NSCONF(2,1) + NSCONF(2,2) configuration cards is constructed accordingly in the form

          $l_1,\ w_1,\ l_2,\ w_2,\qquad l_q,\ w_q$

with format 8(A1,I2,2X), with l_j written as the appropriate letter symbol s,p,d,f,g,h,i,k,   , and w_i right-adjusted, even if less than 10. q must be   8, and w_j cannot be greater than 1 for j > 6. Any subshell that is filled in all configurations of this deck may be omitted.
     Certain restrictions must be observed in setting up the configurations. If only one parity is involved, then NSCONF(I,2)=0, all I; if both parities are present, then NSCONF(1,1)=NSCONF(1,2). For given i, l_i must be the same in all configurations, as must also be the principal quantum number, though it is not explicitly listed; there are three exceptions to this restriction, all pertaining to the case of a singly occupied subshell l_j [w_j=1] when all subsequent subshells in that configuration are empty:
     (1) For given parity, l_j may be the same in several configurations, with only the (unspecified) principal quantum number differing.

     (2) l_j may have different values for opposite parities. Thus, for example, the set of configurations $3s^2 3p^2$, $3s^2 3p4p$, $3s^2 3p5p$, $3s^2 3p4f$, $3s^2 3p5f$, $3s3p^3$, $3s^2 3p4s$, $3s^2 3p5s$, $3s^2 3p3d$, $3s^2 3p4d$, $3s23p5d$ in Si I could be set up in the form
s 2 p 2 p 0 f 0
s 2 p 1 p 1 f 0
s 2 p 1 p 1 f 0
s 2 p 1 p 0 f 1
s 2 p 1 p 0 f 1

```
s 1   p 3   s 0   d 0
s 2   p 1   s 1   d 0
s 2   p 1   s 1   d 0
s 2   p 1   s 0   d 1
s 2   p 1   s 0   d 1
s 2   p 1   s 0   d 1
```

and columns 11-20 of the control card would contain 4^5^54^6^6, where the carats represent blanks (or zeroes). [If one wished to include configuration interaction only between $3p^2$ and 3p4p, 3p4p and 3p5p, 3p5p and 3p4f, and 3p4f and 3p5f, the control numbers would be changed to 4^5^14^6^6, etc. For this and other options, see the discussion under NSCONF(3,K) and CICRITERION above.]

(3) If the final subshell j=q is never more than singly occupied, then l_j (as well, perhaps, as the principal quantum number) may be different in different configurations, even of the same parity. (To all intents and purposes, the dimensional limitation q 8 is then seldom any restriction whatever. In an RCN2 calculation, use of the minimum possible value of q may be forced by setting ICON = 2 on the G5INP control card.) In the example above, the outer p, f, s, and d electron may be placed in the third subshell in all configurations, with columns 11-20 of the control card then being 3^5^53^6^6 (or 3^5^13^6^6, etc.).

Dimensions of cfp, and of U and V matrix elements are such that any multiply occupied f^w subshell should be $l_1^{w_1}$ (even then, dimensions are too small for f^5 to f^{10}), and any multiply occupied d^w subshell should come next.

D.   Energy Parameter Cards

The first parameter card for each configuration contains any desired BCD identification (e.g., element and configuration) in columns 1-18. Columns 21-70 contain values of the first five parameters [format F10.5,4(F9.4,1X)], the value of E_{av} occupying columns 21-30; the total number of parameters may be placed in columns 19-20. Any additional parameter values are put on additional cards in columns 1-70 [format 7(F9.4,1X)]. Units for all parameters are defined by the number in columns 51-60 (in cm^{-1}) of the control card; for cards obtained from an RCN2 calculation, this number is 1000.0, and the energy unit for parameter values is kK (1000 cm^{-1}). Energy levels (eigenvalues) are printed in the same units as those used for the parameter values. The units need to be specified only for purposes of calculating wavelengths, oscillator strengths, and transition probabilities. [Note: The units used in calculating and printing can be changed from those on the parameter cards by means of the optional rescale control card; see Sec. X.]

Parameters for each configuration are arranged in the following order:

E_{av}

20

$F^k(l_1,l_1)$
$F^k(l_2,l_2)$

1
2

$F^k(l_1,l_2)$
$F^k(l_1,l_3)$

$F^k(l_2,l_3)$

$F^k(l_{q-1},l_q)$
$G^k(l_1,l_2)$
$G^k(l_1,l_3)$

$G^k(l_2,l_3)$

$G^k(l_{q-1},l_q)$

In this list, "F^k" represents F^2, F^4, F^m [m=min($2l_i,2l_j$)], and
"G^k" represents $G^{|l_i-l_j|}$, $G^{l_i+l_j}$, with index k incremented by 2.
There are no $F^k(l_i,l_i)$ unless 2 w_i $4l_i$; there are no $F^k(l_i,l_j)$
nor $G^k(l_i,l_j)$, i < j, unless 1 w 4l+1 for both w_i and w_j; and
there are no F^k of either type unless both l are greater than
zero. There is no $_i$ unless 1 w_i $4l_i$+1 and l_i > 0. If IABG > 0,
any parameters   TT1T2 for subshell i follow the corresponding

$F^k(l_i,l_i)$. If IABG = 2 or 4, then "F^k" represents F^1, F^2, F^3, F^m, and k likewise increases in unit steps for the G^k.

If desired, the first parameter card for each configuration may contain, in columns 71-72, BCD identification of the source of parameter values--for example, "LS" for least-squares, "HF" for Hartree-Fock, "HR" for HFR, "HX or XR" for Hartree-plus-statistical-exchange, etc. In columns 73-74, 75-76, 77-78, and 79-80 may be included two-digit scale factors for the $F^k(l_i,l_i)$, $_i$, $F^k(l_i,l_j)$, and $G^k(l_i,l_j)$, respectively; "50" means 0.50, "85" means 0.85, "99" means 1.00, and "01" means 0.001. These scale factors are factors that have already been applied to obtain the parameter values punched on the card, and are for identification only, except as discussed in Sec. X.

Configuration-interaction parameter cards are like single-configuration cards except that the parameter values are $R^k(ij,i'j')$ (all possible k) and $R^k(ij,j'i')$ (all possible k). If more than one set of values (ij,i'j') is possible, the order is an odometer order similar to that for the ij in $F^k(ij)$ and $G^k(ij)$. The only pertinent scale factor is that in columns 79-80.

For parameter-value cards output by RCN2, the tenth column of each parameter field (columns 30, 40,   70 on the first card;

columns 10, 20,   70 on continuation cards) contains a single-digit-integer code that provides correlation with the various scale factors in columns 73-80; see the discussion of parameter rescaling in Sec. X.

D. (cont)   Radial-Multipole-Integal Cards
These cards provide values of Racah's reduced matrix element

$$\mathbf{P} \quad l\|r^{(t)}\|l' \qquad\qquad \begin{matrix} l & t & l' \end{matrix}$$
$$= (-1)^l \left[(2l+1)(2l'+1)\right]^{1/2} \qquad \begin{matrix} & & & \int r^t P_l P_{l'} \, dr \quad (5) \\ 0 & 0 & 0 & \end{matrix}$$

(in units of $e^t a_0^t$); t = 1 or 2 for electric dipole or quadrupole radiation, respectively). No radial integral cards are needed for magnetic-dipole calculations.

Columns 1-18 and 21-38 contain BCD information (like that on the single-configuration parameter card) for the two configurations involved in the transition. In the case of quadrupole radiation, the two configurations may be the same or may be two different configurations of the same parity; if they are the same configuration, the code (incorrectly in some cases) uses a quadrupole integral only for electrons l_i in the last (greatest-i) non-s-electron, non-filled subshell. For electric radiation there is always one and only one card for each pair of configurations, even when the value of $\mathbf{P}$ is necessarily zero because of selection rules, as for example in the case of sp3 - s^2pp' or s^2ps - s^2pf. The value of $\mathbf{P}$ is punched in columns 41-50

(format F10.5); columns 51-64 contain "(nl//r^t//n'l')" where n and n' are two-digit integers and l and l' are BCD symbols (e.g., ^3p and ^3d, for identification only), and t is 1 or 2 as appropriate; the "(" and the value of t must be punched because the code uses these punches to distinguish between parameter and multipole cards.

Additional optional information is

$$\text{FRAC} \qquad \int r^t\, PP'\, dr \;\Big/\; \int \left| r^t\, PP' \right| dr \qquad (6)$$

in columns 65-70 (format (F6.4), and identification similar to that in columns 71-72 of the parameter cards.
    All of the above detail is automatically included on all input cards when the RCG input file is prepared by running RCN and RCN2.

D. (review): Detailed Arrangement of Parameter and Multipole Cards
    (1) Energy parameters for configurations of the first parity, one card (or set of cards if there are more than 5 parameters) for each configuration 1,2,3,4,   in succession.
    (2) Configuration-interaction parameter cards, one card (or set of cards) for each pair of configurations for which interactions are not identically zero (because of selection rules) and are not excluded through use of special values of NSCONF(3,K) (see A. above), in the order (1,2), (1,3), (1,4),   (2,3), (2,4), (3,4),   .
    (3) If IQUAD = 1 or 3, a set of quadrupole cards in the order (1,1), (1,2), (1,3), (1,4),   (2,1), (2,2), (2,3), (2,4), (3,1), (3,2),   .
    (3a) If desired, additional set(s) of quadrupole cards containing different values of P for the purpose of making parameter studies.
    (4) If configurations of both parities are included [NSCONF(2,2) > 0], then cards for the second parity analogous to (1), (2), and (if IQUAD > 1) (3); also,
    (5) A set of radial dipole-integral cards (optional), one card for each pair of configurations of opposite parity, arranged in the following order:

Serial number of configuration	
First parity	Second Parity
1	1
1	2
1	3
.	.
.	.

```
.               .
2               1
2               2
2               3
.               .
.               .
.               .
```

(These cards are read in subroutine SPECTR, statements 104-110.
     (5a) Additional sets of dipole cards (5), if desired for
parameter studies.
     (6) Additional complete sets of cards (1)-(5) if desired
(for parameter studies, isoelectronic-sequence calculations,
etc.).
     (7) A card containing "-99999999." in columns 21-30. This
is a new first-configuration parameter card with a fictitious
value of the parameter E_{av}; it is a signal that there are no more
sets of input data (1)-(6), and that the program is to read a new
control card, etc. [cards (A)-(D), page 12].
     (8) A card containing a negative integer in columns 1-5.
This is a new control card (A) with "illegal" value of KCPL, and
is a signal for RCG to make a normal exit.

V.   Output
     The amount of output sent to the print file IW (internal disk
unit 9; external name OUTG11) is controlled by quantities punched
in columns 6-7 of the ID2 control card, and in columns 6-7, 21-50,
and 61-72 of the calculational-deck control card, as discussed in
the preceding section. In most cases, all these columns are left
blank, except that (a) for configurations in light elements where
LS coupling is a good approximation, column 32 may be non-zero to
delete printing of JJ-representation eigenvectors, and (b) if
columns 23-25 are non-zero to activate calculation of eigenvectors
in still other representations (numbers 3 to 7), then non-zero
punches can be used in columns 31 to 37 to delete printing of
eigenvectors in the corresponding undesired representations.
(Note: When using these options, any number in column 33 must be
less than 5 to avoid activating a plane-wave-Born calculation; see
Sec. XIII.)
     Information routinely printed in the normal case (columns 21-
50 and 61-71 blank or zero) consists of:
     (1) In CUVFD (if called as the result of inclusion of cfp
decks), a list of subshells for which cfp decks were included.
     (2) In PLEV, a list of dimensions actually used for certain
arrays. (If the array sizes specified in DIMENSION statements are
exceeded, a fatal-error STOP results.)
     (3) No output from PFGD and PRK unless ICPC > 0, in which case
a list of parameters for which coefficients have been computed is
printed, with array sizes and (for PRK) the configuration-
interaction class. In the parameter names "FK(i,j)" and
"GK(i,j)", the values of i and j refer to the serial numbers of
the subshells $l_i^{w_i}$ and $l_j^{w_j}$ involved; "ZETA(i)" is to be

interpreted similarly for i; and "mnkDiji'j'" and "mnkEiji'j'" refer to $R_d{}^k(ij,i'j')$ and $R_e{}^k(ij,i'j')$, where ij are subshell numbers for the configuration with serial number m, and i'j' are subshell numbers for configuration n.

(4) In CALCFC if ICFC > 0, for each J-matrix a list of quantum numbers for each row (or column) of the matrix in both the **LS** and **JJ** representations. In each case, symbols in parentheses refer to quantum numbers $l_i L_i S_i J_i$ for subshell $l_i{}^{w_i}$, and symbols not in parentheses refer to coupled quantum numbers $L_i S_i J_i$ as accumulated for coupling of successive subshells from left to right [TASS, Eqs. (12.1) and (12.2), or as listed under "NLSMAX" in Sec. IV above (page 15)].

(5) In ENERGY, a list of the parameter values read as input; for each J, the energy matrix, eigenvalues, Landé g-values, eigenvectors in both the **LS** and **JJ** representations (except as described in the first paragraph of this section, V, above), and eigenvector purities (square of largest eigenvector component) in each representation. Each eigenvector is tabulated vertically beneath its corresponding eigenvalue and g-value, in sets of eleven eigenvectors horizontally, with abbreviated basis-state labels at the left side of the page, and (immediately above each eigenvector) the configuration and basis-state label of the largest component; for complete basis-state definitions it may be necessary to consult the quantum-number listings in (4) above.

(6) In SPECTR, a list of the input radial multipole integrals, the number of spectrum lines for each J-J', and lists of the spectrum lines thenselves. For each spectrum line there is tabulated (after a serial number), the level value, the J value, the serial number of the dominant configuration, and the dominant eigenvector basis-state--first for the "first-parity" level, and then for the "second-parity" level (assuming dipole transitions between levels of opposite parity). Then comes the wavenumber in the same units as for the energy levels, the wavelength in Å, the line strength divided by the largest P^2 for any of the transition arrays present, the weighted oscillator strength gf and its common logarithm (for absorption oscillator strength f, g = statistical weight of the lower energy level, equal to 2J+1 or 2J'+1 as the case may be), the weighted Einstein transition probability gA in sec^{-1} (g = statistical weight of the higher energy level), and in the final column either an F-format number 1 [representing a cancellation factor in the calculation of line strength; TASS, Eq. (14.107)] or an E-format number usually of the order of 10^8 to 10^{14} [representing the quantity BRNCH involved in dielectronic-recombination problems--see Sec. XII(a)]. The line list is printed with lines sorted in the order of increasing energy of the "first-parity" energy levels, and/or in the order of increasing energy of the "second-parity" levels, and/or in the order of increasing wavenumber (decreasing wavelength), depending on the value of ISPECC (column 72 of the control card); in the first two cases, values are tabulated for the sum of oscillator strengths for all upward and for all downward transitions involving a given

level, as are the transition-probability sum for all downward
transitions and the radiative-decay lifetime corresponding to this
sum. [Note that these sums and lifetimes will not be correct if
the line-list storage dimension KLAM is not large enough to store
and process all lines in a single pass--see the following
section.]
        (7) In ELECDEN, values at intervals of 40 RCN radial mesh
points of the pure single-configuration electron density for each
configuration; then for each eigenstate (energy level), the
intermediate-coupling CI electron density for the diagonal terms
only and, if KCPLD(3) = 4, with cross-term contributions included.
        Sample output is included in Sec. XV at the end of this
document, and it is suggested that readers skip to that point.
The material in Secs. VI-XIV is highly specialized, and the reader
need refer to it only when and if he has need for information on
these special topics.

VI.   Array Dimensions
        It has already been mentioned that RCG allows up to 8
subshells. The limitation is only partly a matter of array
dimensions; a change would also involve some coding differences in
PLEV, and numerous do-loop-limit and format differences throughout
the program. [A 12-subshell version is available, but does not
contain the many upgrades made in the 8-subshell version since
1992.]
        Required dimensions for many array variables depend very
strongly on the complexity of the calculations that one wishes to
handle. Some dimensionally imposed limitations in MOD 11 as
currently provided are as follows:

Upper limit on:	Array variables	Dimensional parameter	Limit
Complexity of subshell 1	U1,V1,CFP1	KLSI	d^w or f^4
Complexity of subshell 2-3	U2,V2,CFP2	KLS2,3	d^w or f^3
Complexity of subshell 4-8	U3,U4,CFP2	KLS4-6	d^3 or g^2
No. of configs (first parity)	SOPI2,PMUP	KC	50
No. of configs (second parity)	NIJK,PMUP	KC	50
No. of parameters (each parity	PARNAM,VPAR	KPR	2100
Matrix size	C,CT4,TMX	KMX	300
No. of spectrum lines	T,TP,FLAM	KLAM	10000

        It should be noted that spectrum lines are processed in
batches, and that the dimension KLAM of T, TP, FLAM, etc. limits
only the maximum number of lines that can be processed in each
batch [ultimately, the number of lines arising from any one J-J'
matrix, excluding weak lines deleted by a non-zero value of DMIN
and short- and long-wavelength lines deleted by FLBDN and FLBDX
(page 10)]. However, if the total number of retained lines is so
great that processing is done in more than one batch, then one has
to manually combine multiple line lists to obtain (for example)
all lines involving a given upper level, and thereby obtain a
total downward transition probability and a correct radiative

lifetime. But note: If DMIN > 0, or NTKEV > 0, then DMIN is
automatically increased (in steps of 0.1 till DMIN=4.0, and then
by a factor of 2 at a time) until the number of spectrum lines is
small enough to be processed in one batch. For plane-wave-Born
calculations, DMIN must be zero, and is so set by the code
regardless of the value punched on the control card. Normally, a
non-zero value of DMIN deletes lines with S/X < DMIN, see page 15).
However, if a non-zero value of TEXCIT has been read in on a
rescale card (see page 30), then the cutoff is not on inherent
line strength, but rather on relative intensities in a light
source with effective excitation temperature TEXCIT (in the same
units as eigenvalues): If DMIN=0, DMIN is set initially to 10^4
and increased automatically by a factor 2 until the number of
retained lines is no more than KLAM; the cutoff is on

    gA*exp(-(max(EIG(L), EIGP(LP))-EMEAN)/TEXCIT)

less than DMIN, where EIG(L) and EIGP(LP) are the eigenvalues of
the levels involved in the transition, and EMEAN is the average of
the largest of all eigenvalues and the larger of the minimum
energies for the two parities.
      For most purposes, the dimensions can be considerably reduced
if storage is limited. If subshell 1 contains f electrons,
subshell 2 is not likely to be more complicated than d^2, and the
other subshells no more complex than p^w. Thus dimensions of U^2,
V^2, CFP2 can be reduced from 17 to 5 (there being only 5 LS-terms
in d^2), and those of U3,   V6 to 3. Except when computing
detailed Fano profiles in photoionization spectra, the number of
configurations usually need be at most 10 of each parity, the
number of parameters 100, matrix sizes about 75, and number of
spectrum lines 1000 or so. Other dimensions can also be decreased
greatly; e.g., those of ISER, PC, and PCI to 500, NOPCCC to 1200,
etc.
      Many required dimensions are very difficult to estimate, and
have to be ascertained more or less by trial and error (increasing
them whenever a run bombs because of exceeded dimensions).
      Nowadays, available fast memory on most computers is quite
large, and the dimensions in the current code are large enough to
handle most cases of interest, without any necessity for either
reducing them or having to increase them. However, if changes are
required, guides to estimating a few required values are as
follows:

      <u>Dimensions for f^5 to f^{10} subshells:</u> Dimension changes
required to be able to handle all f_i^w subshells (for i=1) are
given by comment cards near the beginning of the main program: one
needs to make the following changes in parameter statements
throughout the program:
                        KLSI=119
                        KJP=350
                        KMX=360   (or greater)
                        KTRN=3200   (or greater),

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the last two values being required to keep certain calculated
dimensions from being negative. Even with these changes, $f^w p$ or
$f^w d$ configurations may be so complex as to overflow many other
dimensions, and be completely impractical to compute unless the
number of terms kept for f^w is truncated (see page 11 above).

__Dimension of PCI:__ Given a set of terms $l_i^{w_i}$ $\nu L_i S_i$, the
required dimension is

$$(1/2) \text{ (no. of values of } \nu) \text{ (1+ no. of values of } \nu)$$
$$L_i S_i$$

A dimension of 21 will handle all d^w and f^3 and f^{11}. [PCI is also
used for spin-orbit parameters--see under PC.]

__Dimension of ISER:__ The dimension of ISER is computed
similarly to that for PCI, except that now we are considering a
sum over the different possible values of the total quantum
numbers __LS__, and in place of ν we have the total number of
different sets of quantum numbers $\nu L_i S_i L_i S_i$ having the given __LS__.
If the configuration involves only one open subshell, the result
is the same as for PCI; with more than one open subshell, the
result is greater--for example:

$$p^2 : \quad \text{terms } {}^1S \ {}^3P \ {}^1D \ ; \quad \text{PCI(3), ISER(3)}$$
$$d \ : \quad \text{terms } \quad {}^2D \quad ; \quad \text{PCI(1), ISER(1)}$$
$$p^2 d: \quad \text{terms } {}^4PDF, {}^2SPPDDDFFG,; \quad \text{PCI(3), ISER(17),}$$

where the 17 comes from

$$(1/2) \ (1 \cdot 2 + 1 \cdot 2 + 1 \cdot 2 + 1 \cdot 2 + 2 \cdot 3 + 3 \cdot 4 + 2 \cdot 3 + 1 \cdot 2)$$
.

__Dimension of PC:__ Must be at least as large as that of ISER.
However, PC is also used to store spin-orbit coefficients, and
this may require a larger dimension: for the most complex subshell
$l_i^{w_i}$, set up a table of all possible $\nu L_i S_i J_i$. Then the required
dimension is

$$(1/2) \text{ (no. of levels with } J_i = J) \text{ (1 + no. of levels with } J_i = J)$$
$$J$$

For example, $p^2 : \quad {}^1S_0 \ {}^3P_{012} \ {}^1D_2$,
$$\text{PC(7), where } \quad 7 = (1/2) \ (2 \cdot 3 + 1 \cdot 2 + 2 \cdot 3) \quad .$$

__Dimensions of CC(i,j):__ The dimension j must be as great as
the maximum number of different parameters R_d^k and R_e^k (for any
one pair of configurations, and any one set of four interacting
electrons). The dimension i must be inferred from the code of

PRK, statements 705-780; it is equal to the number of coefficients of R^k that are not inherently zero because of the **LS** selection rule, because of zero values of the cfp involved, because of incompatibility of intermediate quantum numbers, etc. The simplest and safest way to set the dimension i would be to consider only the **LS** rule; i.e., to find the maximum value, for all pairs of interacting configurations, of

$$\sum_{LS} \text{(no. of terms } LS \text{ in first conf.) (no. of terms } LS \text{ in second conf.)}$$

For example, $sp^4 - s^2p^2d$, terms of $sp^4 = {}^4P \ {}^2SPD$, terms of $s^2p^2d = {}^4PDF \ {}^2SPPDDDFFG$;

$$\text{dimension} = \underset{{}^4P}{1 \ 1} + \underset{{}^2S}{1 \ 1} + \underset{{}^2P}{1 \ 2} + \underset{{}^2D}{1 \ 3} = 7 \quad .$$

Of course, except for CC, the above sample dimensions become much greater when the presence of several configurations increases the number of terms of each **LS** or the number of levels of each **J**, dimensions going up roughly as the square of the number of configurations of given parity.

In modifying dimensions it is important to note that the labeled common block /C1/ is identical in all subroutines, but that blank common and several other labeled commons differ from one subroutine to another. This may lead to complications in the case of linker/loaders that require the first subroutine containing a given common to have the longest version of that common or that require all to be of the same length, though in RCG11 commons have been reorganized to minimize this problem.

VII.   Memory Requirements

Even with the code extensively overlayed and with small array dimensions, it was difficult to fit RCG into a 64K-word computer, such as the old CRAYS. On a Macintosh or PC, the executable file is about one Mbyte in size; with present array dimensions, execution requires about 25 Mbytes of RAM, which is no problem on modern-day desktop or laptop computers.

VIII.   Execution Times

Like required array dimensions, execution times vary tremendously, depending on the complexity of the problem--as measured especially by the number of parameters and the matrix sizes. Some examples are given in TASS, Tables 16-1 and 16-2. Generally speaking, CRAY Y-MP execution times are less than half a minute for problems involving no more than 40 parameters, matrices up to 50×50, and no more than a couple of thousand spectrum lines.

Modern `SUN`, `PowerMac`, and `PC times` **are several times smaller for state-of-the-art desktop computers.**

IX.   Modifications for Other Computers
     As noted in the Introduction, modifications for other
computers should be minor provided sufficient memory is available
or a virtual-memory system is in use, and this is generally true
of even modest desktop computers these days. However, if memory
is a problem, the following modifications are possible.
     (1) Code storage space can be reduced by overlaying.
Suggested groupings of subroutines are indicated throughout the
RCG source program by commented OVERLAY and CALL OVERLAY cards.
If this feature is used, duplicate copies of the routines RDIJ and
REIJ in the PFDG overlay should be added to the PRK overlay.
     (2) Other possibilities in addition to reducing array
dimensions are:
          (a) If least-squares fitting of experimental energy
levels is of no interest, delete subroutine RCEINP and the call
thereof in ENERGY.
          (b) Delete CPL37, SPRN37, LVDIST, and WNDIST and calls
thereof.
          (c) If plane-wave-Born calculations are of no interest,
BORN, AKNINT, RCOEFF, E1, and CSEVL can be deleted, as can the
variable GOSS and several others.
          (d) The code could be broken into a chain of three
programs, containing essentially (i) CUVFD to prepare disks 72,
73, 74; (ii) LNCUV through MUPOLE to prepare disk 41; (iii) LNCUV
plus ENERGY and SPECTR to use disk 41 in the calculation of energy
levels and spectra.

X.   Rescaling of Input Data
     Most frequently, input data for an energy-level/spectrum
calculation will have been obtained via an RCN/RCN2 calculation.
The data will then be such that (1) the center-of-gravity energy
E_{av} of the first configuration will be zero, (2) all parameter
values (and hence all computed eigenvalues) will be in kilo-
kaysers (units of 1000 cm^{-1}), and (3) energy parameter values
other than E_{av} (and usually also spin-orbit parameters) will have
been scaled down by factors less than unity to allow for omitted
weak configuration-interaction effects (TASS, Sec. 16-2); these
scale factors appear in columns 73-80 of the parameter cards (see
Sec. IV-D above, pages 20-21), and the factor that has been used
for a given parameter is indicated by an integer JPAR in the tenth
column of the parameter-value field, as follows:

JPAR	kind of parameter	scale factor
0	E_{av}	–

1	$F^k(ii)$	columns 73-74
2		75-76
3	$F^k(ij)$	77-78
4	$G^k(ij)$	79-80
5	R^k	79-80

It is frequently desirable to shift all energy levels upward (by adding a constant to all E_{av}) to make the calculated ground level of the atom zero (as this is the convention used in tabulating experimental energy levels), to change the eigenvalue unit (to cm^{-1}, eV, or rydbergs, for example), or to modify the parameter scale factors to obtain better agreement with experiment. This can be done by using an editor to modify the data in the input file by hand, but it can be done much more easily with the aid of a rescaling card of the form:

cols.	format	variable	action
1-4	–	(blanks)	
5	I1	(zero)	defines a rescaling card
6	–	(blank)	
21-30	F10.5 (do not punch decimal point)	DELEAV	DELEAV (same units as on input para- meter cards) added to all E_{av}
31-40	5I2	IFACT0(5)	New scale factors, in percent (except 99 = 100 %, 01 = 0.1 %)
51-60	F10.5	UENRGY	New energy unit in cm^{-1} (8065.47 for eV, 109737.3 for Ry, etc.), applied <u>after</u> the addition of DELEAV
61-65	F5.2	TEXCIT	Effective light-source excitation temperature (in eigenvalue energy units) (see pages 25-26)

Default values are zero for DELEAV, no rescaling for any IFACT0(I) that is zero or blank, and the unit of energy specified on the normal control card <u>(A)</u> if UENRGY is zero or blank.
   Note that (1) the new scale factors represent exactly that, and <u>not</u> additional scaling over and above the scaling already present in the input parameter values; (2) old scale factors (columns 73-80 of the parameter cards) equal to zero are assumed to be unity; (3) non-zero values of IFACT0(I), I = 1 to 4, will not have the intended effect if the correct value of JPAR does not appear in the tenth column of each parameter field; (4) if scale factors are changed via IFACT0.ne.0, the value of DELEAV required to give zero energy for the ground level will in general be different from the value inferred from a previous run made with the old scale factors.
   A rescale card may be placed in front of any normal control card <u>(A)</u> of a calculational deck; it is read at statement 100 of the main program as a normal control card with KCPL=0, and reinterpreted as a rescale card. Non-default values read from a

rescale card remain in effect throughout the remainder of a
calculation until modified by another rescale card; a rescale card
containing default values (zeroes or blanks) for one or more
quantities returns program control to use of values of these
quantities specified in the individual calculational decks.

XI.   Photoionization Cross Sections Q
     A. Neglecting resonances, and for cases in which continuum-
continuum (intra-channel) configuration-interaction effects are
unimportant, photoionization-cross-section calculations are most
easily made with programs RCN/RCN2/RCG in the following way. (The
procedure will be illustrated using the special case of Ar XVII
$1s^2$ $-1s$ p, = kinetic energy of the free electron in rydbergs.)
     (1) Estimate the threshold value for photoionization, or
calculate it by making RCN runs for Ar XVII $1s^2$ and Ar XVIII 1s
and differencing values of E_{av}. In this case, a simple estimate
is: binding energy of a 1s electron = Z_c^2 = 17.5^2 = 306 Ry, and a
calculation gives $E_{av}(1s)$ - $E_{av}(1s^2)$ = -325.397 + 628.459 = 303
Ry.
     (2) Choose values of   at which the cross section is to be
computed. If one wishes a threshold value of Q, include a
continuum configuration with   = 1 to 5 % of the threshold energy.
In the argon case,   = 5 or 10 Ry is appropriate.
     (3) Make an RCN/RCN2 calculation. In order to be able to
interpolate across threshold, one can include bound configurations
1s np, say for n = 10 to 15. Larger n values get one closer to
threshold, but are more likely not to converge, so one might
choose n = 8 and 12. The input to RCN is then

cols. 4-5	9-10	11-23	27 (or greater) on	
18	17	Ar 17 1s2	1s2	
18	17	Ar 17 1s 8p	1s 8p	
18	17	Ar 17 1s 12p	1s 12p	
18	17	Ar 17 1s 5.p	1s 99p	5.0
18	17	Ar 17 1s 10.p	1s 99p	10.0
18	17	Ar 17 1s 25.p	1s 99p	25.0

etc.

On the RCN control card, EMX (columns 61-65) should be chosen such
that all values of   for which calculations are to be made lie in
the range from about EMX/10 to EMX. If the value of EMX is
inappropriate, or n for the bound states too large, the RCN runs
may fail to converge or bomb on an overflow. [If EMX is left zero
on the control card, RCN will set EMX equal to the largest value
of   on any input configuration card.]
     On the G5INP control card that is input to RCN2, columns 51-
60 [the empirical scale factors for $F^k(ii)$, $_i$, $F^k(ij)$, $G^k(ij)$, and

$R^k(ij,i'j')$] should have appropriate values, such as (for a highly ionized atom like Ar XVII) 9599959595. Column 72 of this card (and thereby column 72 of the RCG control card) should contain a one (for ease in using the RCG line-list output), and column 75 <u>must</u> be equal to 8.

     (4) Run RCG as usual, using as input the unmodified output file OUT2ING from RCN2 (with name changed to ING11).

     (5) Values of "f" in the RCG line-list output are oscillator strengths for bound-bound transitions ($1s^2$ - $1s\,8p$ and $1s^2$ - $1s\,12p$ in this example), and are values of df/d (in rydbergs) for bound-free transitions ($1s2$ - $1s\,5.0p$, etc.). For interpolation purposes, the bound-bound oscillator strengths can be converted to averaged (smeared-out-lines) values of $df/d = (df/dn) \div (d/dn)$ by taking

$$\frac{d}{dn}\quad \frac{d}{dn*} = \frac{d}{dn*}(-Z_C^2/n*^2) = 2Z_C^2/n*^3 \qquad\qquad (7)$$

with Z_C the spectrum number (1 for neutral) and $n*$ the effective quantum number (printed on the last page of the RCN listing for each configuration, under the heading "n*rc"), where it was calculated from

$$E = -\ Z_C^2/n*^2$$

with E = the binding energy ("eps fgr," with correlation) of the electron in Ry.

    Then

$$Q = 8.067\ 10^{-18}\ df/d \quad cm^2 \quad . \qquad\qquad (8)$$

Values of Q (correct only for the bound-free transitions) will be printed in the spectrum line list in place of gA, provided NSCONF(3,2) is negative, columns 51-64 are identical on the last two dipole-integral cards, and each of the dipole cards contains a number equal to 1.0 in columns 65-70.

    <u>(B) When resonances</u> (bound-free interactions) or free-free (intra-channel) configuration interactions are important, the set-up for RCG runs is much more complex, requiring introduction of many values of --in order to resolve the detailed shape of the resonance, for example. Calculations are then practical only for rather simple cases, such as those of Al I, Cl I, and Ba I in TASS, pages 539ff.

    One approach is the following (TASS, Sec. 18-8), though it involves a great deal of hand work.

    (1) Make an RCN/RCN2 run including all essential bound configurations, and continuum configurations in which the kinetic energy covers the range of interest or importance; if values of cover a range of more than 10:1, it may be necessary to make two or three runs, each of which includes the important bound

configurations but only one of several overlapping subsets of the continua, each covering a 10:1 energy range (with appropriate value of EMX in each case).

(2) Draw graphs like those in TASS, Fig.18-3, giving R^k and radial dipole integrals as functions of .

(3) Divide the energy range of the continuum into a number of segments, the ith segment having a width $_i$ rydbergs. [For an example in the case of neutral chlorine, see J. Opt. Soc. Am. <u>64</u>, 1474 (1974).]

(4) Read values of the radial integrals from the graphs at points $_i$ = center of each segment and multiply by $_i^{1/2}$, or by $_i^{1/2}$ $_j^{1/2}$ for free-free R^k. [Note that the values of   must be in rydbergs; values of R^k tabulated by RCN2 in "kK" have in all cases been converted from values in "Ry" by multiplying by 109.737, even though R^k has dimensions of $(energy)^{1/2}$ for bound-free interactions and has no energy dimension at all for free-free interactions (see TASS, Sec. 18-4)].

(5) Construct an appropriate RCG calculational deck, using the results (4), and using single-configuration parameter values for each "pseudo-discrete" configuration appropriate to the corresponding $_i$, and run in the usual way.

If NSCONF(3,2) is less than zero, the last two radial-dipole input cards contain the same information in columns 51 to 64, and each bound-free radial-dipole card contains the appropriate value of $_i^{1/2}$ in columns 65-70, RCG will calculate and print

photoionization cross sections SIGMA Q in place of weighted transition probabilities gA. These values will have been computed from Eq. (8) assuming d = $_i$ for all spectrum lines involving upper levels belonging to the configuration "i". This will be inappropriate if perturbations appreciably alter the mean energy spacing between adjacent configurations, and will be particlarly incorrect for bound-state autoionizing levels strongly mixed with continuum states.

An alternative method is available that involves no handwork in the preparation of the RCG input deck. This alternative requires that all desired bound and continuum configurations be included in a single RCN/RCN2 run, and that IDIP = 7 on the RCN2 control card; this may involve considerably more computer time than the hand method, and will not work if the desired values of principal quantum number n for bound functions and values of   for continuum functions cannot all be handled with a single value of EMX. (If this last is a problem, sometimes a compromise can be made, using a value of EMX smaller than the maximum , as the requirement EMX   largest   is somewhat conservative.)

The alternative method will be described by means of an example for neutral silicon, where the unperturbed position of $3s3p^3$ $^3P^o$ lies between $3s^23p$ nd $^3P^o$ for n = 4 and 5, but interactions of sp^3 are significant throughout the entire discrete

3p nd Rydberg series and well into the 3p εd continuum (which
thereby distorts the energy dependence of the photoionization
cross section). An appropriate set of input configurations might
be

Si I $3p^2$ – $3s3p^3$ + 3p3d + 3p4d + ··· + 3p9d + 3p10d + 3p12d
                   + 3p 0.036d + 3p 0.22d + 3p 0.58d   .

RCN2 recognizes the discontinuity between 10d and 12d as well as
the presence of continuum configurations, and sets up four pseudo-
discrete configurations with unmodified E_{av}, but with appropriate
values of $Γ_i$ to cover the energy range from just above 10d to well
beyond 0.58d. Values of R^k and radial dipole integrals are
automatically modified by appropriate "$Γ_i^{1/2}$" factors, which are
called "DEL" within RCN2, but printed out labeled "SQRTDEL".
      RCG can then be run using as input the unmodified output deck
from RCN2 provided IDIP on the RCN2 control card has the value 7.
The correct value of gf for 12d is obtained by dividing the listed
value of gf by $(SQRTDEL)^2$; i.e., "$Γ_i$" for bound configurations is
here not an energy width in rydbergs, but rather a weighting
factor related to the effective number of bound configurations
represented by the pseudo configuration. Photoionization cross
sections for the pseudo configurations derived from continuum
configurations will be printed explicitly, or may be obtained as
before from (8) by dividing the f obtained from the gf column by
$(SQRTDEL)^2$; i.e., "$Γ_i$" is here both a weighting factor and an
energy width in rydbergs.
      Note: The energies of the above set of three continuum
configurations were chosen because of primary interest in the low
bound configurations. For photoionization calculations, a larger
number of more closely spaced continua would be called for.

XII.   Autoionization Transition Probabilities
      RCG has the capability of computing autoionization transition
probabilities A^a (designated AA in the FORTARN program, or GAA for
the weighted transition probability gA^a). The basic theory is
discussed in TASS, Secs. 18-7 and 18-11, and in Appendix B of LA-
6220 by Merts, Cowan, and Magee, which also contains numerous
numerical examples.
      The calculation of values of A^a will be described by means of
an example in Fe XXI, which has the ground configuration $2s^22p^2$.
Suppose we wish to calculate A^a for the levels of Fe XXI $2s2p^215p$,
which all lie above the ionization limit Fe XXII $2s^22p$.
      (1) First, a preliminary RCN run is made for Fe XXI $2s2p^215p$
and Fe XXII $2s^22p$. From the computed total binding energies it
will be found that $E_{av}(2s2p^215p)$ lies 3.4 Ry above $E_{av}(2s^22p)$.
[See Table B-III of the above report LA-6220.]

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(2) The approximation is made that <u>all</u> levels of $2s2p^215p$ lie 3.4 Ry above the ionization limit, and a final RCN/RCN2 run is made for

> Fe XXI $2s2p^215p$
> Fe XXI $2s^22p\,3.4s$ (9)
> Fe XXI $2s^22p\,3.4d$,

parity and other selection rules permitting autoionization into only the s and d continua. [Preparation of the RCN input configuration cards involves punching "99s" or "99d" in the configuration-definition part of the card (<u>not</u> the configuration-label part), followed after at least one space by "3.4".] The G5INP control card in the RCN2 input deck should have an 8 or 9 in column 72 (ISPECC for the subsequent RCG run), and must have a 2 in column 73 and a 9 in column 75; these punches in columns 73 and 75 produce certain appropriate modifications in the RCN2 output for RCG input.
    (3) Output from the RCN/RCN2 run will include the usual punched-card RCG-input deck for the three interacting configurations (9). The three <u>printed</u> values of E_{av} will be equal (to within 0.05 Ry 5 kK). However, in the punched-card output (file out2ing) that is input for RCG, the values of E_{av} for the continuum configurations will have been changed to –9500 and –8500 (as a result of the 9 in column 75 of the G5INP control card).
    (4) Running RCG with these modified values of E_{av} will result in some eigenvalues being less than –4000 and hence a signal to the computer program (ENERGY, statement 362^+) that these belong to continuum states. After saving the bound-continuum CI matrix elements, the program zeroes these elements of the matrix so that diagonalization produces zero eigenvector mixing of discrete and continuum states. Values of A^a are computed in ENERGY, statements 360-380, using the perturbation theory expression

$$A_{ji}{}^a = (4\,{}^2/h) \mid j|H|i \mid^2$$

$$= (4\,{}^2/h) \mid \sum_{bb'} j|b\ b|H|b'\ b'|i \mid^2 \quad . \quad (10)$$

The intermediate-coupling eigenvector components $j|b$ for the pure-discrete (but potentially autoionizing) state j and the components $b'|i$ for the pure continuum state i are obtained from the energy-matrix diagonalization; the basis-state configuration-interaction matrix elements $b|H|b'$ prior to diagonalization have been saved in the block CI at statement 255. [Note: At statement 363^+, A^a is calculated in units of 10^{13} sec^{-1} by using h/2 $(10^{-13}/2066)$ Ry-sec, and using the factor 1/109.735 to convert

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$\langle b|H|b'\rangle$ from the incorrect units put out by RCN2 (see pages 32-33 above) to units of $Ry^{1/2}$.]

It is essential in the RCG input deck (and hence in the RCN input deck also) that all discrete configurations come first, and all continuum configurations come last. For any given value of the total-angular-momentum quantum number J, let the matrix size be NLS, and let LX ($<$ NLS) be the number of discrete levels and JX-1 $\equiv$ NLS-LX be the number of continuum levels. Then the minimum permissable block size for the variable CI is LX by JX-1, for the variable CII is NLS by NLS, and for AA is NLS by JX+1. After completion of the matrix diagonalization (which leaves the eigenvalues in the order of increasing value), the continuum eigenvalues will be numbers 1 through JX-1 and the discrete eigenvalues will be numbers JX through NLS. The value of $A_{ji}{}^a$ is stored in AA(j,i) [JX $\leq$ j $\leq$ NLS, 1 $\leq$ i $\leq$ JX-1]. The value of $\sum_i AA(j,i)$ is in AA(j,JX) for all $E_i < -8000$ and in AA(j,JX+1) for all $E_i < -4000$; the distinction between these two sums, $A_j{}^{a1}$ and $A_j{}^{a2}$, respectively, is for special purposes having to do with dielectronic recombination. All results are written on disk unit IE (= 31 or 32, depending on parity) for use in SPECTR.

(a) Branching ratios and dielectronic recombination

If configurations of both parity are included, for example

$$
\begin{array}{l}
\text{Fe XXI } 2s^2 2p\, 15p \\
\text{Fe XXI } 2s 2p^2\, 15p \\
\text{Fe XXI } 2s^2 2p\, 3.4s \\
\text{Fe XXI } 2s^2 2p\, 3.4d \quad ,
\end{array}
\tag{11}
$$

then spectral transitions are computed as usual, but only between levels with E $\geq$ -4000 kK. Provided ISPECC (column 72 of the RCG control card) is 6,7,8, or 9, then for each spectrum line L = j $\to$ k, a quantity

$$
B_{jk}{}^r \equiv \text{BRNCH(L)} = \frac{g_j A_j{}^{a1} A_{jk}{}^r}{A_j{}^{a2} + \sum_{k'} A_{jk'}{}^r}
\tag{12}
$$

is computed in SPECTR, and printed in the final column of the line list (in place of the cancellation factor normally printed there). The factor $g_j A_j{}^{a1}$ is proportional to the total rate of dielectronic capture of free electrons by ions initially in states having E_{av} less than -8000 (in practice, ions in the ground configuration), and the remaining factor in (12) is the branching ratio for radiative decay to stable (non-autoionizing) levels, including the effect in $A_j{}^{a2}$ of possible autoionization to excited ion states defined by $-8000 < E_{av} < -4000$. The quantity $B_{jk}{}^r$ is

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equal to g_j times the final fraction in TASS, Eq. (18.120) [or equal to $G_m F^{jk}$ in Eq. (B.21) of LA-6200, where G_m g_m is the total statistical weight of the ground configuration of the recombining ion], and the contribution of the levels j and k to the dielectronic-recombination rate coefficient is given by (18.120).

Also computed in SPECTR (called BRNCHR in the code, and printed as "GM*FRBAR) is the quantity

$$B^r \qquad _{jk} B_{jk}{}^r \quad , \tag{13}$$

which provides the <u>total</u> contribution of all levels j and k to the dielectronic-recombination rate coefficient via TASS, Eq. (18.116).

In equation (18.120) mentioned above, there has been assumed a mean kinetic energy E_s (i.e., a mean energy of autoionizing levels above the ionization limit). When the energy spread of autoionizing levels j is not small compared with the plasma electron temperature of interest, this is a poor approximation. The appropriate correction factor is computed for each of NTKEV (5) temperatures TKEV (in units of keV) read in on the type-b optional control card (page 10). If NPTKEV (read in on this card) is 1 or greater than 2, then there will be written on unit 13 the value of B^r/G_m together with the temperature correction factors, and also the values of $_j B_{jk}{}^r/G_m$ for each lower level k with the corresponding correction factor. If NPTKEV is greater than 1, then there will be written on the normal print file IW the value of B^r and of B^r times each correction factor. EIONRY is the ionization energy (in rydbergs) from the ground level of the recombining ion; this is used to compute (and write on 13) the center-of-gravity energy of the autoionizing levels (with G_m and B^r/G_m), and the energies of the individual levels k (with J_k and $_j B_{jk}{}^r/G_m$), all relative to the ground level of the recombined ion. In order for this to work correctly, it is essential that the (final) continuum input parameter card contain the kinetic energy in rydbergs in columns 7-12 (format F6.2), and that therefore the corresponding RCN input configuration card contain this information in columns 17-22.

Note that the DIEL feature in RCN (Sec. II.L of the RCN writeup) makes it possible to set up input for dielectronic-recombination calculations such as that in (11) without having to explicitly make a preliminary calculation to obtain the free-electron kinetic energy nor figure out by hand the possible values of the free-electron angular momentum. At the same time, RCN automatically puts the kinetic energy in columns 17-22 of the continuum-configuration cards to satisfy the above requirement.

A non-zero value of EMINA is intended for handling problems in which some levels of a configuration have too low an energy to

lie above the bottom of a continuum to which they might otherwise
autoionize. Consider, for example levels of 2s2p(^{1}P)nl that lie
above 2s2p(^{3}P), and therefore can autoionize to 2s2p(^{3}P) l' but not
to 2s2p(^{1}P) l'.   If EMIN 0, RCG allows autoionization only if the
bound level has energy greater than EMINA, and the continuum level
either has energy less than -8000 or has an energy less than or
equal to the center-of-gravity energy of the configuration to
which it belongs. In the above example, EMINA should be the
energy of 2s2p(^{3}P) [determined by means of a preliminary
calculation], E_{av} should be greater than -8000 for each 2s2p l'
configuration , and E_{av} should be less than -8000 for $2s^2$ l".
(Obviously the code is not general; one would run into difficulty
if the spin-orbit splitting of the ^{3}P were large, or in more
complex cases such as $2s2p^2$ l'.

    If ISPECC (column 72 of the control card) is 8 or 9, SPECTR
calls WNDIST: the latter calculates and punches (on disk unit 11),
in the form of a histogram, the normalized [(12) divided by (13)]
energy distribution of radiation resulting from excited levels j
produced by dielectronic recombination in low-density plasmas.
The quantity DELEKEV (read in the main program from columns 21-30
of the type-b optional control card, page 10) specifies the width
of the histogram bins. (If no A^a calculations are being
performed, the histogram gives the normalized distribution of gf
rather than of B_{jk}^r, representing approximately the energy
distribution of radiation resulting from collisional excitations
in low-density plasmas, assuming the optical approximation
(excitation rates proportional to oscillator strengths). Both
types of punched deck constitute input for a computer program
RADRATE; for sample output of this program, see TASS, Figs. 19-12
and 19-13.

    It should be noted that calculation of B_{jk}^r and related
quantities will be incorrect if there are too many spectrum lines
for SPECTR to store and process them all in one pass (i.e., if
statement 560 is reached from the IF statement following statement
511 or 550 rather than from the IF that follows 200), because the
summation over k' in (12) cannot be correctly evaluated. [This is
not a program bug, but just an inherent storage limitation.] If
DMIN > 0 or if NTKEV > 0, DMIN is automatically increased until
enough weak lines have been deleted so that this storage
limitation is not encountered (see pages 25-26).

(b) Autoionization contributions to collisional ionization
    Electron-impact ionization may take place either by direct
ejection of an electron from an atom (or ion), or by collisional
excitation of an inner-subshell electron to a level j lying above
the ionization limit, followed by autoionization. For this second
(indirect) process, one needs to know excitation-rate coefficients
to all possible levles j, together with the branching ratios

$$\sum_m A_{jm}^a$$

$$B_j{}^a = \frac{}{\sum_m A_{jm}{}^a + \sum_{k'} A_{jk'}{}^r}$$

$$= \frac{g_j A_j{}^{a2}}{g_j A_j{}^{a2} + g_j \sum_{k'} A_{jk'}{}^r} \tag{14}$$

for autoionization to all possible states of the ion; see, for example, R. D. Cowan and J. B. Mann, Astrophys. J. 232, 940 (1979).

If an RCG run is made as described in the preceding subsection, values of $g_j \sum A_{jk'}{}^r$ are printed as "SUMGA" in the spectrum line list sorted by second-parity levels, and $g_j A_j{}^{a2}$ and $B_j{}^a$ are printed as "GAATOT" and "BRION" in the following line. [Note that these prints will be obtained only if ISPECC = 2,3,6,7,8, or 9, and that if equal to 9 then the lines themselves are not printed.]

(c) Autoionization contributions to collisional excitation

Similarly to collisional ionization, excitation (or de-excitation) can take place either directly, or indirectly via dielectronic capture of the impacting electron into a highly excited state, followed by autoionization into a state of the target atom different from the original one. Computation of the indirect process involves much the same quantity as that (12) for dielectronic recombination, except that the required branching ratio is for autoionization instead of radiative decay:

$$B_{mji}{}^a = \frac{(g_j A_{jm}{}^a)(g_j A_{ji}{}^a)}{g_j A_j{}^{a2} + g_j \sum_{k'} A_{jk'}{}^r} \quad ; \tag{15}$$

unlike (12), we have not summed over states m involving the ground configuration of the target atom to give $A_j{}^{a1}$, and the quantities $A_{jm}{}^a$ and $A_{ji}{}^a$ in the numerator of (15) are the values printed by subroutine ENERGY as "AA" in all but the last two lines (which are $A_j{}^{a1}$ and $A_j{}^{a2}$).

States m and i of the (N+1)-electron system --target atom plus free electron--will be basically JJ coupled, and we denote them by

$$m = [(J_t)_m, (J_l)_m]J$$
and $\tag{16}$
$$i = [(J_t)_i, (J_l)_i]J \quad ,$$

where J_t defines the target-atom state with total angular momentum J_t, the free electron l has orbital angular momentum l and total

angular momentum (l+s) of J_l, and the total (N+1)-electron angular momentum (J_m or J_i) is necessarily equal to the value J J_j of the resonance-capture state j. If we sum (15) over the two possible values $J_l = l \pm 1/2$, and redefine m and i to represent the sum of the two states:

$$m = [(J_t)_m, l_m]J$$
and   (17)
$$i = [(J_t)_i, l_i]J   ,$$

then values of the quantities in parentheses in the numerator of (15) are printed by ENERGY as an array of numbers "GAAXC" ("gA^a excitation"), labeled on the left by the serial number of the free-electron configuration target+ l and the energy "EXC" of the target level J_t (relative to E_{av}).

In SPECTR, the above values are combined with the denominator of (15) and summed over all levels j [including thereby a summation over the quantum number J in (17)] to obtain values

$$"BRNCHX(m,i)" = \sum_{j\ (J_l)_m\ (J_l)_i} B_{mji}^a \qquad (18)$$

printed in a square array, labeled similarly to the GAAXC array (as to both row and column), except with rows and columns sorted in order of increasing configuration serial number and increasing value of EXC.

This array (which of course forms a symmetric matrix) gives maximum physically significant detail for the collisional excitation/de-excitation problem, as it provides the total contribution for all levels j and for all possible couplings of the free electron (with given l) to the target state. (Diagonal elements pertain to resonant-state contributions to elastic scattering.)

Actually, the l of the free electron is really only of mathematical (not physical) interest, so in a second array, columns are combined to give the summation of (18) over the possible values of l_i. [This array is printed only if it is actually narrower than the first one.] It is left to the user to perform the corresponding sum over rows (l_m) to give total values from one target level to another; the result is the quantity

$$g_m F_{mi} \qquad (19)$$

involved in Eqs. (2) and (3) of R. D. Cowan, J. Phys. B. <u>13</u>, 1471 (1980). [There, m and i have been further redefined to refer only to the levels J_t of the N-electron target.]

Still a third array is printed (if narrower than the second) in which a summation has been carried out over levels i of each target <u>configuration</u>. The user may manually sum rows over l_m to obtain the total excitation rate from a given target level to all

levels of the excited configuration. Or he may also sum over the
levels of the initial configuration to obtain the quantity

$$\sum_m \sum_i g_m F_{mi} \equiv \overline{G_m F^a} \quad . \tag{20}$$

If this is divided by the total statistical weight $G_m \equiv \sum_m g_m$ of
all levels of the ground configuration of the target, one has a
quantity proportional to the mean total excitation rate, summed
over all levels i and averaged over all levels m; this is
appropriate for application to moderate-density plasmas, where the
(metastable) levels of the ground configuration may be more or
less statistically populated. The quantity (20) is printed as

$$\text{"GM*FABAR"} \equiv \sum_j \frac{g_j A_j^{a1}(A_j^{a2} - A_j^{a1})}{A_j^{a2} + \sum_{k'} A_{jk'}^r} \quad . \tag{21}$$

In some cases (as for example the O IV case discussed in the
above JPB paper), not all levels j of the excited configuration
will lie above the ionization limit, and the summations over j in
(18) and (21) must correspondingly be limited appropriately. (RCG
does not inherently have enough information to set A_{jm}^a to zero
for levels lying below the limit.) The necessary modifications
may be accomplished (as described earlier) by introducing the
quantity EMINA (format F10.5) read from columns 71-80 of the
type-b optional control card (pages 10 and 37). If EMINA $\neq$ 0 and
the continuum level has energy greater than -8000, then A^a will be
set to zero if the level j has energy less than EMINA, or if the
continuum level has energy greater than E_{av} for the continuum
configuration in question. The second of these two restrictions
was introduced in order to compute excitations from $2s^2$ l to
$2s2p(^3P)$ 'l' via autoionizing levels $2s2p(^1P)n"l"$ [i.e., in order
to exclude continuum levels $2s2p(^1P)$ 'l'], and may not always be an
appropriate restriction--in which case the code will have to be
changed accordingly.

XIII.   Plane-Wave-Born Collision Strengths
     If KCPLD(3) (column 33 of the calculational-deck control
card) is greater than 4, then columns 33 to 37 are interpreted not
as KCPLD(3) to KCPLD(7), but rather as

column	format	variable
33	I1	IGEN
34	I1	IRNQ ($\geq$ 0)
35	I1	IRXQ ($\geq$ IRNQ)
36	I1	IRND ($\geq$ 1)
37	I1	IRXD ($\geq$ IRND)

and plane-wave-Born collision strengths will be computed [from levels of only the first configuration of the first parity unless NCK(1)--column 6 of the control card--is greater than one], via calls near the end of ENERGY to subroutine BORN.

The amount of printed output is smaller the larger the value of IGEN from 5 to 9 (9 is recommended). If collision strengths for optically forbidden excitations are desired for the first, second, or both parities, then IQUAD must be 1, 2, or 3, respectively, and IRNQ and IRXQ (even integers) must specify the minimum and maximum values of t for the Bessel-function matrix elements

$$l_i \| j_t(Kr) \, C^{(t)} \| l_k \qquad\qquad (22)$$

that will be involved for the jumping electron in any of the excitations specified by NCK(1) and NCK(2). Similarly, if optically allowed (electric-dipole allowed) excitations are to be calculated, then IRND and IRXD (odd integers) must be specified appropriately. [See TASS, Secs. 18-12 and 18-13 for details.] This same set of five integers (and IQUAD) must be punched on the G5INP control card for RCN2 in order that the latter compute the matrix elements (22) in place of the normal electric multipole matrix elements

$$l_i \| r^t \, C^{(t)} \| l_k \qquad , \qquad (t = 2 \text{ or } 1) \qquad , \qquad (23)$$

and also to set up a card containing various other required quantities (SPECTR, format 8).

The basic printed output consists of:

(i) a table of values of the momentum transfer K;

(ii) for each spectrum line (or rather, each J–J' excitation), a table of values of the weighted generalized oscillator strength $gf_{JJ'}(K)$, and a table containing X kinetic energy of the impacting electron ( ) in units of the excitation energy (E), the kinetic energy in rydbergs, the unmodified collision strength , and two modifications of that should be physically more accurate at small X--specifically,

$$M1(X) = \begin{cases} W(3)\,F(X) & , \quad X < 3 \\[2mm] W(X)\,F(X) & , \quad X \; 3 \end{cases}$$

$$\text{where} \quad F(X) = 1 - 0.2\,\exp[0.07702(1 - X)] \quad ,$$

and

$$M2(X) = W(X + 3/(1+X)) \quad ,$$

with M_2 generally being more accurate than M_1. Also printed is
a table of excitation-rate coefficients computed from M_2 by
integration over a Maxwellian distribution, at electron
temperatures ranging from T=1 to 2000 eV for low excitation
energies (low ionization stages) or from T=5 to 10000 eV for high
excitation energies (highly ionized atoms). (The quantity labeled
"CORR" is the percentage of the printed rate coefficient
contributed by extrapolating $M_2(X)$ from the largest tabulated
value of X to infinity.)

  (iii) for each transition array, the array-average optical
oscillator strength f_a [TASS, Eq. (14.97), evaluated by numerical
summation of the individual weighted oscillator strengths] if
IGEN = 5, three alternative values for the array-average excitation
energy (the first being E_{av}, the second being E_{av} for the higher
configuration minus the lowest energy of the lower configuration,
and the third being an average of the individual excitation
energies weighted with the unmodified collision strength at the
largest X value being calculated), and a table of values of X and
the unmodified and modified values of collision strength (summed
over all levels of both the lower and the upper configuration).
Rate coefficients are tabulated as in (ii).

XIV. List of Principal Variables
   Sections of code: A = all
            C = cfp-deck calculations (CUVFD)
            P = preliminary calcs. (LNCUV,PLEV,PFGD,PRK)
            F = final J matrices (CALCFC,CPL37)
            M = line-strength matrix elements (MUPOLE)
            E = energy diag.(ENERGY,CALCV,LVDIST)
            S = spectrum calculation (SPECTR,WNDIST)
            B = plane-wave-Born (BORN)

Variable	Sections	Significance
AA(L,J)	E	autoionization transition probability from bound state L to continuum level J
AA(L,JX)	E	total A^a from L to all continuum levels with E < -8000 (= A^{a1})
AA(L,JX+1)	E	total A^a from L to all continuum levels with E < -4000 (= A^{a2})
AA(L)	S	A^{a1} for level L of first parity
AAP(LP)	S	A^{a1} for level LP of second parity
AAT(L)	S	A^{a2} for level L of first parity
AAPT(LP)	S	A^{a2} for level LP of second parity
ALF	CP	in $_iL_iS_i$ (BCD serial number for terms of l^w with given $\overline{LS}$)
ALFBR	C	in $\overline{LS}$ (BCD serial number for terms $\overline{}$

			of l^{w-1} with given LS)
ALF3	E		skewness parameter α_3 in skewed Gaussian
AVCG(K)	E		$(2J+1)$-weighted average of Eav for all levels of parity K
AVEIG(K)	E		$(2J+1)$-weighted average of all eigenvalues of parity K [should equal AVCG(K)]
AVP(M,K)	E		average purity of all eigenvectors of parity K for coupling M
BIGKS	SB		$\ln K$, where K = momentum transfer
BRION	S		branching ratio (14) for autoionization
BRNCH(L)	S		quantity (12) for contribution of line L to dielectronic recombination
BRNCHA	S		quantity (21) for total contribution to collisional excitation
BRNCHR	S		quantity (13) for total contribution to dielectronic recombination
BRNCHX	S		collisional-excitation quantity (18), and partial sums thereof
C	FMES		coefficient (f_k, etc.), multipole, energy, or eigenvector matrix
CAVE	P		correction to diagonal coeff. matrix elements to give zero contribution to E_{av}
CC,CCC	P		temporary storage for config.-interaction matrix elements
CFGP,CFGPT	C		coefficient of fractional grandparentage
CFGP1	PM		coef. of frac. grantparentage (subshell 1)
CFGP2	PM		coef. of frac. grantparentage (subshells 2-6)
CFP	CPM		coef. of fractional parentage (l^w)
CFPM1	C		coef. of fractional parentage (l^{w-1})
CFP1	CPM		coef. of fractional parentage (subshell 1)
CFP2	CPM		coef. of fractional parentage (subshells 2-6)
CIJK	P		$l_i\|\mathcal{C}(k)\|l_j$
COUPL	A		BCD label for coupling type (LS,JJ,etc.)
CPURTY(L,J)	E		purity of configuration J in level L
CS(I,J)	B		collision strength at X_i for transition array J
CSM	B		collision strength (modification one)
CSM2	B		collision strength (modification two)
CTA	B		temporary storage for matrix products, etc.
CT4	all		temporary storage for matrix products, etc.
C1(I)	B		collision strength at Xi for specific transition
C2(I)	B		collision strength at Xi (modification one)
D	S	l	ine strength (dipole, etc.) matrix, D = S**1/2
EIG	ES		eigenvalue
EIGP	S		eigenvalue, second parity ("eigenvalue prime")
ELEM	ES		BCD name of element and configuration (from parameter-value card)
FJ(L,I)	F		J_i for Lth row of coefficient matrix
FJS1	F		J_i for Lth row of coefficient matrix (maybe not

		literally the first subshell, but rather the first occupied subshell with $2 \le w \le 2l$)
EXC	ES	excitation energy of target (relative to Eav)
FJT(I),FJTP(I)	S	$J_q, J_{q'}$ for Ith spectrum line
FK	F	quantum number K for LK coupling
FKJ	F	quantum number K for JK coupling
FK6	F	quantum number K for coupling number 6 (LSJLKS)
FL	CPF	L_i (preliminary set of LS quantum numbers)
FLBR	C	L_i bar (in parent term $alpha_{bar}$, L_{bar}, S_{bar})
FLAM	S	wavelength of spectrum line (floating-point lambda)
FLL(I)	CP	l_i (floating-point little el) for the subshell I and the parity under consideration
FLLIK(I,K)	P	l_i for subshell I and parity K
FLLIJK(I,J,K)	P	l_i for subshell I and configuration J of parity K
FNU(I)	S	wavenumber nu (= sigma) of Ith spectrum line
GA	S	weighted radiative transition probability gA^r
GAA(I)	S	weighted autoionization transition probability gA^{a1} for level of first parity in spectrum line I
GAAP(I)	S	gA^{a1} for level of second parity in line I
GAAT(I)	S	gA^{a2} for level of first parity in line I
GAAPT(I)	S	gA^{a2} for level of second parity in line I
GAAXC(J,I)	ES	gjA_{ji}^a for bound level J to continuum level I (summed over J_l of continuum electron)
GF	SB	weighted oscillator strength gf
GOSS(I,IT)	B	weighted generalized oscillator strength for transition I and momentum transfer IT
IBK	SB	number of values of momentum transfer K
ICS	B	number of transition arrays
IC	A	disk unit number (=41) for coefficient matrices and transf. mxs. for cpls. 3-7 and mupole mxs.)
IE	ES	disk unit number (=30+K) for eigenvalues and vectors, parity K)
IL	F	disk unit number (=30+K) for quantum numbers and LS-JJ transformation matrix, parity K
ISER(M)	P	serial number of the term of subshell i for the Mth preliminary basis function
ISER(I)	S	serial number of level of second parity for spectrum line I

IPNT(J)	C	serial number I of parent for cfp of Jth term; $(alpha_i L_i S_i\ bar|\}alpha_j L_j S_j)$
ITRM(M)	C	serial number of Ith input term of lw for Mth truncated term
JEXC(I)	E	serial number of configuration for target level with energy EXC(I)
K or KK	A	K=1 for first parity, K=2 for second parity
KCPL	A	kind of coupling (1=LS, 2=JJ, etc.)
KCPLD(J)	A	If KCPLD(J) > 0, transformations to this kind of coupling are to be deleted
KPAR	A	kind of parameter (or matrix--see comment cards in subroutine SPRIN)
LBCD(M,I)	P	BCD symbol for Li for Mth set of preliminary quantum numbers [SPDFG, etc.]
LBRBCD	C	BCD symbol for Lbar [SPDFG, etc.]
LBCDI(M)	P	L (BCD) for Mth term of lw
LCDLT(L)	ES	serial no. of dominant configuration for level L
LCDLTP(LP)	S	serial no. of dominant configuration for level LP
LHS1	FE	script L1 (Hollarith=BCD, used for matrix and eigenvector labeling, subshell 1--maybe not literally the first subshell, but rather the first occupied subshell with 2.le.w.le.2l)
LHS4	FE	script L (Hollarith=BCD, used for matrix and eigenvector labeling, for the final subshell)
LHS1J	FE	script L_i (same as LHS1, except for labeling in JJ representation)
LHS4J	FE	not used
LHQQ	FE	script L (BCD label used in coupling number 6)
LL	A	BCD symbol (spdfg, etc.) analogous to FLL
LLIK	A	BCD symbol (spdfg, etc.) analogous to FLLIK
LLIJK	A	BCD symbol (spdfg, etc.) analogous to FLLIJK
MULSI(M)	P	multiplicity of Mth term of l^w
MULS1	FE	multiplicity 2(script S1) + 1 for subshell 1 (cf. LHS1)
MULS4	FE	multiplicity 2(script S) + 1 for final subshell (cf. LHS4)
MULS1J	FE	multiplicity 2(script S1) + 1 for subshell 1 (cf. LHS1J)
MULT(M,I)	PF	multiplicity $2S_i + 1$ for Mth set of preliminary quantum numbers
MULTBR	C	multiplicity $2\,S_{bar} + 1$ for parent term

		alpha$_{bar}$, L$_{bar}$, S$_{bar}$
MULTQQ	F	multiplicity used in label for cplg. #6 (cf. LHQQ)
NALS(L,I)	F	serial number of term $a_i L_i S_i$ for Lth matrix row (LS coupling)
NALSJI(M)	CP	serial number of term aiLiSi for Mth term $a_i L_i S_i J_i$ of $l_i{}^{w}i$ (JJ coupling)
NALSJ(L,I)	F	serial number of term $a_i L_i$Si for Lth matrix row (JJ coupling)
NALSJP(M,I)	PF	serial number of term $a_i L_i S_i$ for Mth set of preliminary quantum numbers (JJ coupling)
NALSP(M,I)	PF	serial number of term $a_i L_i S_i$ for Mth set of preliminary quantum numbers (LS coupling)
NBIGKS	SB	number of values of momentum transfer BIGKS
NCFG(L)	F	configuration serial number for matrix row L
NCFGJP(M)	PF	configuration serial number for Mth set of preliminary quantum numbers (JJ)
NCFGP(M)	PF	configuration serial number for Mth set of preliminary quantum numbers (LS)
NCSER(I)	S	serial number of dominent configuration, level of first parity for spectrum line I
NCSERP(I)	S	same, second parity
NDIFFJ(I)	P	number of different values of J_i for subshell i (considering diff. configs. to imply diff. J_i)
NDIFFT	CP	number of different LS terms (i.e., number of different possible values of script $L_q S_q$, (considering diff. configs. to imply diff. $L_q S_q$)
NDIFSJ	F	total number of sets of values of $\{J_i\}$ (all i) for given script J_q
NENRGS	SB	number of energies at which to calc. coll. strength
NI(I)	CP	occupation number w_i of subshell i ($l_i{}^{w}i$)
NIJK(I,J,K)	A	occupation number w_i of subshell i for configuration J of parity K
NIJKP(I,J)	P	similar to NIJK, for subshell I of configuration J (used in PRK)
NJJ	F	number of basis states for given script J_q (JJ representation)
NJK(K,I)	P	number of basis states for Kth value of J_i (see NDIFFJ)
NLASTT(I)	P	serial number of last term of $l_i{}^{w}i$ retained in setting up basis states
NLS	F	number of basis states for given script J_q (LS

		representation)--hence matrix size for that J_q
NOPC	CP	number of coefficients (f_k, g_k, etc.) in preliminary tables
NOPCCC	P	serial number of r_k coefficient (PRK 755)
NOSUBC	A	no. of subshells ("subconfigurations")=NSCONF(1,K)
NOTOTJ(I)	P	total number of basis functions for subshell I (all configurations)
NTOTJJ(I,J)	P	total number of basis functions for subshell I, summed through configuration J-1
NOTOTT	P	total number of basis functions (all q subshells and all configurations)
NTOTTJ(J)	P	total number of basis functions, all subshells, summed through configuration J-1
NOTSJ1(I,J)	P	number of LS terms for subshell I, summed through configuration J-1
NOTSJP	M	number of LS terms for subshell I, summed through configuration J-1 (second parity)
NPAR	PFE	total number of energy parameters (including Eav's) for current parity
NPARJ(I,J)	PE	number of single-configuration parameters for configuration I (=J), or number of configuration-interaction parameters for interaction I-J
NPARK(K)	E	value of NPAR for parity K
NPAV(J)	E	serial number of parameter Eav for Jth config.
NSCONF	A	see writeup Section IV. A
NSCRJ8	F-S	number of different values of script J_q for current parity
NTI	P	same as NTRMK
NTRMK(L)	CPF	number of LS terms with given value of script $L_q S_q$ (serial number L) for any given config.
PC(M)	C	cfp
PC(M)	PF	preliminary coefficient (f_k, g_k, etc.)--M=serial number--including off-diagonal coefficients (also used for assorted tempoary storage)
PCI	P	similar to PC
PJ, PJI	P	similar to PC, except for zeta coeffs. in JJ repr.
PMUP(I,J)		electric dipole or quadrupole reduced matrix element, $\langle l_i \| r^t C(t) \| l_j \rangle$
PSCRL(L,I)	P	script L_i for Lth LS term
PSCRS(L,I)	P	script S_i for Lth LS term
S(L,I)	CPF	S_i for Lth LS term of ith subshell, $l_i{}^{w_i}$ (cf. FL)

SBR	C	S_i bar for Lth LS term (cf. FLBR)
S2(I)	S	line strength (except for factor P**2) for Ith line
SCRJ(L,I)	F	script J_i for Lth row of matrix (JJ representation)
SCRJ8	F	script J_q (total J value for given matrix)
SCRJ8P	MS	script J_q (total J value for given matrix), 2nd parity
SCRL(L,I)	F	script L_i for Lth row of matrix (LS representation)
SCRS(L,I)	F	script S_i for Lth row of matrix (LS representation)
SCRL6	F	script L for coupling representation number 6
SCRS6	F	script S for coupling representation number 6
SOABSS(I)	S	cancellation factor (S/|S|) with sign of S**1/2 for spectrum line I
SOPI2(I,J)	MS	sum of line strengths (divided by P**2) for array I-J
SUMGA	S	sum of radiative gA^r for given energy level
SUMGAA	E	sum of $gA^{a}1$ for all levels up to current J value
SUMGAAT	E	same, for $gA^{a}2$
SUMGAR	S	sum of gA^r for all levels
T(I)	S	term (energy level, first parity) for Ith line
TP(I)	S	term (energy level, second parity) for Ith line
TMX	F	transformation matrix (LS to JJ, or LS to ...)
TMXP	M	transformation matrix, second parity
U1,U2,...U6	P	matrix elements of $U^{(k)}$ for 1st,2nd,...subshells
V1,V2,...V6	P	matrix elements of $V^{(k1)}$ for 1st,2nd,...subshells
V	S	eigenvector matrix
V	E	V matrix (derivatives of eigenvalues with respect to parameter values
VECT	E	energy matrix; eigenvector matrix
VPAR(I,K)	E	energy parameter values (E_{av},F^k,etc.) for Kth parity
X	S	temporary storage

XV. Program Usage and Example

   The primary storage location for the various programs is an anonymous
FTP directory on the Los Alamos t4 network. To obtain the files using a
Web browser such as Netscape or Internet Explorer, go to
      http://www.t4.lanl.gov
and follow links to my programs, or go directly to
       ftp://aphysics.lanl.gov/pub/cowan
The FORTRAN files are named rcn.f, rcn2.f, rcg.f, and rce.f . Various
sample input files have fairly obvious names starting with "in". The
files rcng.UNIX and rcng.VMS are procedure files for running rcn, rcn2,
and rcg in succession for a sample test run in five-fold-ionized potassium,

and also contain sample input; output from such a run is given in file OutputK+5. The files diel.UNIX and diel.VMS are similar procedure files for making an autoionization/dielectronic-recombination run for Se+24, and output is contained in file OutputSe+24. Of course, the three programs can also be run one at a time with appropriate input files, instead of using these procedure files. The file "readme" contains further information regarding compilation, file sizes, and execution times.

   The file rcg.f uses dimensions adequate for all s, p, and d subshells, and for all f subshells except f5 to f10, and the file ing11k contains cfp decks for all such subshells; when renamed ing11, it can be used for a first RCG run to calculate the binary files tape72, tape73, and tape74. The file rcglg.f is a source file for RCG with dimensions large enough to make runs with all f subshells, and cfp decks for calculation of tapes 72-74 for all subshells are contained in the file "cfp". [However, rcglg.f is based on an older version of rcg.f, so it might best be used only as a guide to making appropriate dimension changes in the current rcg.f. Likewise, included 12-subshell versions of rcg and rcn2 are not up to date.]

XVI. Sample Input and Output
<u>RCN input file in36</u> for a K VI $3s^2 3p^2 + 3p^4 - 3s^2 3p 3d$ run

```
2   5    2   10  1.0    5.e-08    1.e-11-2   090   1.0  0.65  0.0 0.00   -6
    19    6K VI  3s2 3p2       3s2 3p2
    19    6K VI  3p4           3p4
    19    6K VI  3p 3d          3s2 3p 3d
    -1
```

<u>RCN2 input file in2</u>

```
g5inp  0 0000  0.000  000     1100000   00000000 9099909090.0000     07229
       -1
```

<u>RCG monitor output</u>
   Times are for a 1.25 MHz PowerMac G4; times would be similar for PCs.

```
rcg mod 11    LS coupling    nsconf= 3 2 2   3 1 1   iabg=0  iv=0   119
000000000 99.0 99.0  print=00000 500 2 0 0 0    0.00000
```

```
Finished lncuv at   0.001 min
Finished plev at    0.001 min
Finished pfgd at    0.001 min
Finished prk at     0.001 min
Finished calcfc at  0.002 min
```

Finished plev at   0.002 min
Finished pfgd at   0.002 min
Finished prk at   0.002 min
Finished calcfc at   0.003 min
Finished mupole matr for J=0.0 and Jp=1.0 at time=0.004 min, Matr size= 4 by 3
Finished mupole matr for J=1.0 and Jp=0.0 at time=0.004 min, Matr size= 2 by 1
Finished mupole matr for J=1.0 and Jp=1.0 at time=0.004 min, Matr size= 2 by 3
Finished mupole matr for J=1.0 and Jp=2.0 at time=0.004 min, Matr size= 2 by 4
Finished mupole matr for J=2.0 and Jp=1.0 at time=0.004 min, Matr size= 4 by 3
Finished mupole matr for J=2.0 and Jp=2.0 at time=0.004 min, Matr size= 4 by 4
Finished mupole matr for J=2.0 and Jp=3.0 at time=0.004 min, Matr size= 4 by 3
Finished energy for J= 0.0 at time= 0.004 min, Matrix size=   4
Finished energy for J= 1.0 at time= 0.004 min, Matrix size=   2
Finished energy for J= 2.0 at time= 0.004 min, Matrix size=   4
Finished energy for J= 0.0 at time= 0.005 min, Matrix size=   1
Finished energy for J= 1.0 at time= 0.005 min, Matrix size=   3
Finished energy for J= 2.0 at time= 0.005 min, Matrix size=   4
Finished energy for J= 3.0 at time= 0.005 min, Matrix size=   3
Finished energy for J= 4.0 at time= 0.005 min, Matrix size=   1
Finished first-parity sort at time=   0.006 min
Finished second-parity sort at time= 0.006 min
Finished wavelength sort at time=   0.006 min

time= 0.006 min   for Pmax= 1.70752,   10.0000   10.00000
                                 sums2,sumgf=   10.0000   10.00000   22.3585
                                        sumf=   7.3938
sumgAr= 9.6958E+11
                                      s2min=   0.00000

              0 lines omitted, with max s2=   0.00000

              0 lines omitted, with lambda.gt. 500000.0000
              0 lines omitted, with lambda.lt.   0.0010
              0 lines omitted, insuff storage
              0 lines omitted, conf serial nos .gt. 50, 50

STOP (normal exit)

Appendix--Notes on basis-state and level designations

 Some details regarding basis-state labeling and level designations
will be given, using an example from singly ionized argon, containing
two configurations of odd parity and five configurations of even parity.
 At the beginning of the output from subroutine spectr, there is
a list of radial dipole integrals (nl//r1// n'l'), together with
the names of the corresponding configurations and the serial numbers
of the configurations:

serial no.	conf.	serial no.	conf.	dipole integral
1	Ar II 3p5	1	Ar II 3p4 4s	(3p//r1// 4s)=
1	Ar II 3p5	2	Ar II 3p4 5s	(3p//r1// 5s)=
1	Ar II 3p5	3	Ar II 3p4 3d	(3p//r1// 3d)=
1	Ar II 3p5	4	Ar II 3p4 4d	(3p//r1// 4d)=
1	Ar II 3p5	5	Ar II 3p4 5d	(3p//r1// 5d)=
2	Ar II 3p4 4p	1	Ar II 3p4 4s	(4p//r1// 4s)=
2	Ar II 3p4 4p	2	Ar II 3p4 5s	(4p//r1// 5s)=
2	Ar II 3p4 4p	3	Ar II 3p4 3d	(4p//r1// 3d)=
2	Ar II 3p4 4p	4	Ar II 3p4 4d	(4p//r1// 4d)=
2	Ar II 3p4 4p	5	Ar II 3p4 5d	(4p//r1// 5d)=

 Then a bit later, the list of (the first five) configurations is

repeated, together with configuration serial number:

serial no.	conf.		conf.
1	Ar II 3p5	---	Ar II 3p4 4s
2	Ar II 3p4 4p	---	Ar II 3p4 5s
3		---	Ar II 3p4 3d
4		---	Ar II 3p4 4d
5		---	Ar II 3p4 5d

There follows the line list itself, of which I give a few of the lines below:

O	E	J	Conf		Ep	Jp	Confp		delta e
1	153.4484	2.5	2 (3P)	4P	131.5956	3.5	3 (3P)	4D	21.8528
2	155.2788	3.5	2 (3P)	4D	131.5956	3.5	3 (3P)	4D	23.6832
3	55.7404	2.5	2 (3P)	4D	131.5956	3.5	3 (3P)	4D	24.1448
8	-0.4039	1.5	1 (2P)	2P	131.7381	2.5	3 (3P)	4D	132.1420
9	153.4484	2.5	2 (3P)	4P	131.7381	2.5	3 (3P)	4D	21.7103
61	-0.4039	1.5	1 (2P)	2P	132.7190	2.5	1 (3P)	4P	133.1228
62	153.4484	2.5	2 (3P)	4P	132.7190	2.5	1 (3P)	4P	20.7295
74	172.7695	1.5	2 (1D)	2P	141.4790	2.5	3 (3P)	4F	31.2905
75	192.6821	1.5	2 (1S)	2P	141.4790	2.5	3 (3P)	4F	51.2031

For each line, the first column is a line serial number, which has no
physical significance--it is given only so that one can see how many lines
there are. The next two columns give the energy and total J value for the
level of first parity (odd parity, in this example), and the next column
is the configuration serial number--1 means $3p^5$ and 2 means $3p^4$ 4p.
Now comes the complicated part. As an example, in (3P) 4P, the 3 and 4
should be read as superscripts; the part in () being the term of $3p^4$, and
the final part, 4P, being the overall LS term--that is, the total multiplicity
2S+1 (=4) and the total L (P=one unit of angular momentum).
   The part (3P) is in the present example always the multiplicity and
angular momentum of the first subshell of the configuration; for $3p^4$, the
only possible values are ^{3}P, ^{1}D, and ^{1}S, as in lines 62, 174, and 175.

   For configuration 1 ($3p^5$), there is only one subshell, and so the
quantity in () is always the same as the total LS.
   For cases in which there are more than two subshells, the quantity in

() is the LS for the outermost (last) subshell that contains at least two electrons and at least two holes; if there is no such subshell, then the LS in () is the total LS (vectorially) for the next-to-last subshell. [The computer code involved is that in subroutine calcfc, statements 350 to 420 (or to 460 for jj coupling).]

The above information for the first-parity level is followed by the corresponding information for the second-parity level of the spectrum line, and thus includes the serial number of the second-parity configuration.

Clearly, the amount of information given in the line list, limited by space considerations to only one intermediate LS (for a single subshell, or for the vector sum of all but the final subshell), is not generally sufficient to specify the level designation completely. In such cases, the only way of obtaining complete information is the following:

(1) On the g5inp control card for RCN2 or on the RCG control card, a value of ICFC=1 in column 69 will result in all details of the basis-state quantum numbers for each state being written to the file outg11.

(2) For the eigenvalue and J value of interest, one goes to the output of eigenvalues and eigenvectors for this J value. The desired eigenvector lies below the desired eigenvalue, in the same column; the configuration serial number and (abbreviated) level designation lie in this same column in between the eigenvalue and eigenvector.

(3) In the eigenvector, find the eigenvector component that corresponds to the term label in the line list--this is usually (but not always) the component with the largest magnitude, but in any case, the configuration serial number and name and the basis-state label are given in the left-hand portion of the eigenvector-component row. Note the row number of this eigenvector component.

(4) Going back in the file outg11 to the place where basis-state quantum numbers are listed for the J value in question, the desired full set of quantum numbers is that for the row number just mentioned. [Note, however, that for a given energy level, the correct row number will in general not be the same for the jj-representation eigenvector as it will be for the LS-representation eigenvector, because the dominant eigenvector component will in general lie in a different row.]

Two levels may sometimes appear to have the same level designation; this is not supposed to happen, but the computer code may not be infallible. However, such apparent duplication may be because the levels actually belong to two different configurations, or may result because of

the missing parts of the level designations in the case of more than two subshells.