

PROGRAMS RCN MOD36 / RCN2 (Mod 36)  
COMPUTATION OF ATOMIC RADIAL WAVEFUNCTIONS

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## I. SUMMARY OF PROGRAMS

### A. Introduction

This is a pair of FORTRAN 77 programs used on 64-bit-word CRAY or CDC CYBER 205 computers for the self-consistent-field calculation of atomic radial wavefunctions, and of various radial integrals involved in the calculation of atomic energy levels and spectra. RCN and RCN2 are easily adaptable to VAX, IBM RISC, SUN, Macintosh, and similar 32-bit-word computers because of the following coding features:

(1) IMPLICIT REAL\*8 (A-H,O-Z) statements have been included in all program units, so that floating-point variables will be double precision for 32-bit computers. (These statements can be commented out if necessary on 64-bit machines.)

(2) Generic names have been used for intrinsic functions, with arguments that are never numbers, but rather are variables defined by statements, such as HALF=0.5 or TWO=2.0, so that conversion to double precision will be automatically performed on 32-bit machines.

(3) Named common blocks of a given name have the same length in all subroutines. In all cases, there are an even number of integer storage spaces if followed by a floating-point variable.

RCN can be run singly, but RCN2 requires that RCN be run first to provide input wavefunctions, and the two are commonly run in succession to provide input for a third program RCG to compute atomic energy levels and spectra, giving the three possibilities:

RCN  
RCN/RCN2  
RCN/RCN2/RCG

The primary input information is always to RCN, and each program automatically provides input information to the succeeding program of the chain. Details of the programs will be described later (RCG in a separate writeup); here we outline only the basic purpose of each of the first two programs.

NOTE: The program RCN Mod36 still contains the possibility of feeding information into a modified version, HF8, of Charlotte Froese-Fischer's well-known Hartree-Fock program [Can. J. Phys. 41, 1895 (1963); Report ANL-7404 (1968); Comp. Phys. Commun. 1, 151 (1969)]. However, unlike in pre-1981 versions, RCN can itself calculate Hartree-Fock wave-functions. Therefore the program HF8 is no longer used, and is not supplied; the pertinent option in RCN has been retained for use by anyone desiring wavefunctions on the logarithmic radial mesh used by HF.

### B. Program RCN Mod36

Program RCN calculates single-configuration radial wavefunctions  $P_{nl}(r)$  for a spherically symmetrized atom via any one of the four following homogeneous-differential-equation approximations to the Hartree-Fock method.

(1) Hartree (H);

(2) Hartree-Fock-Slater, with any desired value of the coefficient for Slater's approximate exchange term, and either without (HFS) or with (HFSL) Latter's tail cutoff in the central-field potential-energy function;

(3) Hartree-plus-statistical-exchange (HX);

(4) Hartree-Slater (HS).

(5) RCN can also be used for true Hartree-Fock (HF) calculations, either for the spherically symmetrized atom (center-of-gravity energy of the configuration), or for the energy of a specific LS term of the configuration (LSD-HF) provided there exists only one LS term having that value of LS.

Normally, the center-of-gravity HF method is the only one used.

In addition to the radial wavefunctions, also calculated for each configuration are various radial integrals ( $r^m$ ,  $F^k$ ,  $G^k$ , ), and the total (spherically averaged) energy of the atom ( $E_{av}$ ) including approximate relativistic and correlation energy corrections. Relativistic terms can be included in the potential function of the differential equation (HXR or HFR) to give approximate relativistic corrections to the radial wavefunctions, as well as improved relativistic energy corrections in heavy atoms (important for outer orbitals only if  $Z > 50$ , and for inner orbitals if  $Z > 20$ ). Similarly, a correlation term can be included in order to make the potential function more negative, and thereby help to bind negative ions. Options are available to provide radial wavefunctions as input to either program RCN2 or program HF8.

### C. Program RCN2

Program RCN2 accepts radial wavefunctions (for one or more different configurations of one or more atoms or ions) from RCN, and for each atom calculates various two-configuration radial integrals: overlap integrals  $P_{n1}|P_{n'1'}$ , configuration-interaction Coulomb integrals  $R^k$  and spin-orbit integrals  $n|n'1'$ , and radial electric-dipole and electric-quadrupole integrals. In its most commonly used option, it automatically computes all quantities required for calculating energy levels and spectra of an atom, and writes a file containing this information in exactly the form required for input to program RCG, which performs these calculations. For plane-wave-Born calculations in RCG, calculation of radial multipole integrals in RCN2 is replaced by calculation of radial integrals of spherical Bessel functions.

For the theory behind all of the above programs, see Robert D. Cowan, The Theory of Atomic Structure and Spectra (University of California Press, Berkeley, 1981), Chap. 7, and Secs. 8-1, 16-1, and 18-13 -- hereafter referred to as TASS.

#### D. Computing Times

Approximate computing times for RCN on CRAY-1 computers are as listed below. Times on a CRAY-YMP would be two or three times shorter. Times on the CYBER 205 would be about the same as listed below; times on the CDC 7600 or IBM 360/95 or 370/195 would be about 3 times longer; times on modern (2005) PowerMacs and PCs are about 5 times shorter.

<u>Config.</u>	<u>Time (sec)</u>			
	<u>HX</u>	<u>HXR</u>	<u>HF</u>	<u>HFR</u>
Ar I 3p <sup>6</sup>	2	2	1	1
Kr I 4p <sup>6</sup>	3	3	3	3
Xe I 5p <sup>6</sup>	4	4		5
Dy I 4f <sup>10</sup> 6s <sup>2</sup>	6	7		10
Rn I 6p <sup>6</sup>	6	7		13
U I 5f <sup>3</sup> 6d7s <sup>2</sup>	7	9		17

Computing time for RCN2 is usually only a small fraction of that for RCN. However, if there are a large number of configurations on the TAPE2N input file to RCN2 (say, > 20) and the configurations in question are the ones with high serial number, read and rewind times can be uncomfortably long, especially if the file is on a tape rather than a disk unit.

## II. PROGRAM RCN36

### A. Program outline

This is a FORTRAN 77 program for the calculation of radial wavefunctions  $P_{n_l}(r)$  of a spherically symmetrized atom, corresponding to the center-of-gravity energy  $E_{av}$  of an electron configuration

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

Computed from these radial wavefunctions are the Coulomb integrals  $F^k$  and  $G^k$  and the spin-orbit integrals  $\zeta_{n_l}$ , along with radial integrals required to give kinetic and electron-nuclear energies, and rough relativistic and correlation corrections to both the one-electron binding energies and the total electronic binding energy  $E_{av}$ .

The program was originally (January 1964) based on the SHARE program 1417 (ML HFSS) described by Herman and Skillman, Atomic Structure Calculations (Prentice-Hall, 1963), and this reference may be used for a description of the radial integration mesh and basic numerical methods used in RCN. However, except for the subroutine CROSYM and part of SCHEQ, the original program has been changed beyond recognition [including notational changes from SNL(M,I) and SNLO(I) to PNL(I,M) and PNLO(I), and a redefinition of>NNLZ from  $100n+10l+const.$  to  $100n+1$ ]. Options are still available for making calculations via the Hartree-Fock-Slater approximation used by Herman and Skillman either with or without Latter's tail cutoff in the one-electron potential, using either Slater's original exchange coefficient  $3/2$  or Kohn and Sham's modified value of 1 (or any other value). However, these approximations are all considered to be unsatisfactory; a much better option utilizes the Hartree-plus-statistical-exchange (HX) approximation described in my book TASS, which should be consulted for theoretical discussions. Still further options are the HS approximation of Lindgren and Rosen [Int. J. Quant. Chem. S5, 411 (1971); Phys. Scripta 6, 109 (1972), or TASS], and full Hartree-Fock calculations. Hartree-Fock is the preferred option.

Normally, all radial functions are iterated to self-consistency. However, on configurations other than the first one, any desired number of inner orbitals can be held fixed (frozen-core approximation; see discussion below concerning the variable IBB1, and Secs. II-J and II-K).

The program is all in FORTRAN 77, and consists of a main program and thirty-odd subprograms.

RCN36 is the main program, and mostly just decides whether a normal calculation is to be performed, or one pertinent to dielectronic-recombination.

RCN is the main subroutine. It handles all input (for normal calculations) and some output, controls the self-consistent-field iteration, and does portions of the detailed calculation.

ANALYZ and SETCFG interpret the configuration-definition input and estimate initial values of the one-electron eigenvalues.

DIEL and ANALYZ1 are subroutines used to reduce handwork involved in setting up dielectronic-recombination runs; details are discussed in Sec. II-L.

SCHEQ integrates the one-electron radial wave equation, and controls the iteration on the one-electron eigenvalue  $E=EE(M)$  to give a radial wavefunction  $P_{n1}(r)$   $rR_{n1}(r)=PNLO(I)=PNL(I,M)$  that satisfies the boundary conditions at  $r=0$  and  $r=r_{max}$ . It also properly normalizes the function for either a bound electron ( $E < 0$ ) or a free electron ( $E > 0$ ); it will not handle the case  $E=0$ . The normalization for a free electron is likely to be inaccurate if  $E > 0.1$  rydberg (because of too coarse an integration mesh) unless  $EMX/10 \leq E \leq EMX$  and very large dimensions are used for  $PNL$ ,  $R$ , and other variables (see remarks below regarding continuum-wavefunction calculations--Sec. II-G). Appropriate small non-zero values of  $EMX$  also make possible calculation of  $P_{n1}$  for large  $n$  (about 15 to 40) by bringing into use the full 1801-point mesh instead of the 641-point mesh used when  $EMX=0$ ; too large a value of  $EMX$  (or too large  $n$ ) will result in convergence failure because even the 1801-point mesh will not extend to large enough radii.

OUTPT handles most of the printed output (in part, via calls to POWER, ZETA1, and SLI1) and the wavefunction output to disk file 2 or (via a call to HFW RTP) to disk file 7, which provides input to program RCN2 or HF8, respectively.

SUBCOR calculates a modified free-electron correlation energy for a specified electron density.

CROSYM solves a system of linear equations to provide a value of

$$AZ = [ P_{n1}(r)/r^{l+1} ]_{r=0} . \quad (2)$$

POWER computes values of  $r^m$  for  $-3 \leq m \leq 6$  (except  $m=5$ ) for each orbital.

ZETA1 computes spin-orbit parameter values  $n1$  from the central-potential formula

$$n1 = \frac{1}{2} \int_0^{r_{max}} P_{n1}^2(r) \frac{1}{r} \frac{dV}{dr} dr , \quad (3)$$

and also via the Blume-Watson method [Proc. Roy. Soc. (London) A270, 127 (1962), A271, 565 (1963)]; the latter method gives much more accurate values and so provides the numbers used in practice. Also computed and printed are the one-electron kinetic-plus-

nuclear energy  $I_{n1}$ , and the relativistic mass-velocity and Darwin corrections. (Actually,  $I_{n1}$  is computed in RCN3S, and only printed in ZETA1.)

SLI1 computes and prints all Slater integrals  $F^k$  and  $G^k$  (in units of both rydbergs and  $\text{cm}^{-1}$ ); it also computes overlap integrals and calls RCN3S.

RCN3S prints the overlap integrals, and calculates (from the  $F^k$  and  $G^k$ , with the aid of subroutine S3J0SQ) and prints the Coulomb interaction energy between each pair of electrons. It then calculates correlation-energy corrections, and (using values of  $I_{n1}$  from ZETA1) calculates and prints one-electron binding energies and the total binding energy of the atom (see TASS for equations). It also prints those single-configuration parameter values  $E_{av}$ ,  $F^k(ii)$ ,  $F^k(ij)$ , and  $G^k(ij)$  required for the calculation of atomic energy levels; the total binding energy  $E_{av}$  is given in rydbergs, whereas all other parameter values are in kK (units of  $1000 \text{ cm}^{-1}$ ).

S3J0SQ calculates the square of the value of

$$\begin{array}{ccc} j1 & j2 & j3 \\ 0 & 0 & 0 \end{array} \quad \text{where} \quad \begin{array}{ccc} j1 & j2 & j3 \\ m1 & m2 & m3 \end{array}$$

is a 3-j symbol; though not used here, for other purposes there exists also a function routine S3J.

FCTRL calculates the factorial of an integer A, required by S3J0SQ and S3J.

HFWRTP interpolates values of each wavefunction from the (periodically doubled) linear mesh used by RCN to points on the logarithmic mesh used by HF8, and writes on tape 7 these wavefunctions and other input data for a Hartree-Fock calculation via program HF8.

HF POT calculates for a given orbital the Hartree-Fock potential (excluding the classical-potential terms, which are calculated in the main subroutine), written in the form of an effective homogeneous-equation local-potential function. (This is necessary because RCN is basically a homogeneous-equation program. The singularities that are present in the potential at zeroes of the orbital in question are smoothed out by means of a linear interpolation from the second mesh point below to the second mesh point above each zero.)

QUAD2 calculates the classical potential via a Simpson's-rule quadrature.

QUAD5 is a general-purpose five-interval quadrature routine.

QUADK is used by HF POT for the evaluation of Hartree's  $Y_k$  function.

ZETABW evaluates spin-orbit parameters via the Blume-Watson method, using function routines SM, SN, ZK, VK, and DYK patterned after those in HF8.

S6J evaluates the 6-j symbol

j1	j2	j3
l1	l2	l3

with the aid of a function routine DELSQ .

CLOCK is a subroutine used to call a CPU-time system-routine SECOND, which contains sections appropriate to a CRAY, VAX or Macintosh, PC, SUN, and IBM RISC; SECOND may be replaced by a dummy do-nothing routine if desired, as CLOCK output times are for information only.

PHSHIFT is a subroutine that for continuum orbitals computes and prints the phase shift of the (distorted-wave) continuum function relative to the phase of a pure (non-relativistic) Coulomb function. (This phase shift does not become quite constant at large  $r$ , indicating some inaccuracy in numerical integration of the differential equation. Because of this, and because of omission in each phase of a term consisting of the argument of a complex gamma function, only the phase shift is significant, not the distorted-wave and Coulomb phases individually.)

VINTI computes values of the Vinti integrals and associated weighting factors and sum (see Sec. II-H).

EBREIT, BRTINT , and S3J are used for evaluation of approximate Breit magnetic and retardation energies, if  $IREL=2$ . The approximation is poor and inclusion of this option seems to provide no improvement between theory and experiment; if one wishes to save storage space, he can change the dimensions of the approximate small-component relativistic wavefunction QNL(KMSHQ,KOQ) from (1801,20) to (1,1), in which case the Breit energies will not be computed even with  $IREL=2$ .

## B. Input

For simplicity in the following, terminology will be used in places that dates from the time when computer input consisted of punched cards: The word "card" may be used to refer to a line of an input file or FORTRAN source file, and the word "deck" to refer 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 9, but in many cases only if certain print options are in effect.

Normal input, read in subroutine RCN, consists of a control "card," and one configuration "card" for each configuration to be computed (not necessarily all of the same element nor ion stage)--additional cards are required if an LS-term HF calculation is to be done; see Sec. II-F. Normally, the control card is nearly universal and is seldom changed from one run to the next, except to switch from non-relativistic (HF) to relativistic (HFR)

calculations, or to include or delete correlation corrections in the effective central-field potential function.

(1) Control card: this is read at statement 200 of the main subroutine, and contains the following quantities.

cols	format	variable	normal value			
			RCN36		RCN36 + HF8	
			HX	HF	HX+HF	HF only
1	I1	ITPOW	2	2	2	0
2	I1	IPTVU	0	0	0	0
3	I1	IPTEB	0	0	0	0
4-5	I2	NORBPT	-9	-9	-9	-9
6	I1	IZHXBW	0	0	0	0
7-8	I2	IPHFWF	0	0	0	0
9-10	I2	IHF	0	2	1	1
11-13	I3	IBB	0	0	0	0
14-15	F2.1	TOLSTB	1.0	1.0	1.0	1.0
16-20	E5.1	TOLKM2	<b>2.0</b>	<b>2.0</b>	<b>2.0</b>	<b>2.0</b>
21-30	E10.1	TOLEND	5.E-08	5.E-08	5.E-08	5.E-02 <sup>a</sup>
31-40	E10.1	THRESH	1.E-11	1.E-11	1.E-11	1.E-05 <sup>a</sup>
41-42	I2	KUTD	-2	-2	-2	-2
43-44	I2	KUT1	0	0	0	0
45	I1	IVINTI	0	0	0	0
46	I1	IREL <sup>b</sup>	0	0	0	0
47-48	I2	MAXIT	90	90	90	90
49-50	I2	NPR	0	0	0	0
51-55	F5.5	EXF10	1.0	1.0	1.0	1.0
56-60	F5.5	EXFM1	0.65	0.65	0.65	0.65
61-65	F5.5	EMX <sup>c</sup>	0.0	0.0	0.0	0.0
66-70	F5.5	CORRF <sup>d</sup>	1.0	1.0	1.0	1.0
71-75	I5	IW6 <sup>e</sup>	0	0	0	0

<sup>a</sup>Use 5.E-08 and 1.E-11 if IREL=0, and HX relativistic energy corrections to  $E_{av}$  are desired.

<sup>b</sup>Use IREL=1 for HXR or HFR; use IREL=2 to include Breit energies.

<sup>c</sup>See notes regarding continuum-wavefunction calculations, p. 6 and Sec. II-G.

<sup>d</sup>See Sec. II-I below.

<sup>e</sup>Use IW6=-6 if output to the monitor screen is desired on the progress of the calculation. The value used here for IW6 is automatically carried through to subsequent programs RCN2, RCG, and RCE.

The first seven quantities and NPR control the amount of printed output, as follows:

ITPOW:       =1 or 3, print SCF iteration information (NITER, DELT, ALFM); this information is sent to the monitor screen if IW6 < 0.  
               2, call POWER to print  $r^m$

ITPVU:      1, print  $F^k$  and  $G^k$   
              2, print Coulomb interaction energies  
              3, print wavefunction overlap integrals  
              4, print HFS potentials (RU, RUEE, etc)  
              5, print HX or HF potentials ( $v^{nl}$ )  
              6, in SCHEQ, print relativistic contribution to  
    potential

IPTEB:      1, print EE, JJJ, R(JJJ), AZ  
              2, print  $E_{kin}$  , etc

NORBPT:    <0, do not print wavefunctions  
              >0, print first two and last NORBPT wavefunctions at  
    every fifth mesh point  
              6, print continuum wavefunctions at every mesh point  
    (for configurations 1, 5, 10, 15,            only,  
    if  $0 < \text{NORBPT} < 6$ )  
              any, write on tape 2 or 7 the last  $|\text{NORBPT}|$   
    wavefunctions (at least 2; if  $|\text{NORBPT}|=9$ ,  
    write all wavefunctions)

IZHXBW:    >0, in HF8, calculate and print all quantities using  
    the (HX) input wavefunctions (primarily to give  
    zeta calculated by the Blume-Watson method;  
    of no great use, as the Blume-Watson method is  
    now used in RCN as well as in HF8)

IPHFWF:    >0, in HF8, print the last  $|\text{IPHFWF}|$  wavefunctions at  
    every mesh point  
              <0, same, except print at only every fourth mesh point  
              ±9, print all wavefunctions

IHF:        =0, signifies an RCN calculation only (hence, do not  
    load HF8)  
              =1, RCN output wavefunctions are for input to HF8  
    (via tape 7, rather than for RCN2 (via tape 2);  
    if  $\text{IREL} > 1$ , RCN calculation of radial integrals  
    is skipped; if  $\text{IREL}=0$  and  $\text{TOLEND} < 1.E-4$ , only  
    ZETA1 is called (to calculate relativistic  
    energy correction for  $E_{av}$  in HF8)  
              =2, carry out a Hartree-Fock calculation within RCN

NPR:        0,      (1) If npr is non-zero, then when niter.ge.npr,  
              expectation values of r for the outermost 10 orbitals are written  
              to the monitor screen. This may show up erratic changes in d or f  
              orbitals due to collapse into the core and expansion back out of  
              the core; this is most likely to occur for neutral or singly  
              ionized elements near the beginning of a transition, rare-earth,  
              or actinide series. The most likely solution is to place small  
              values (e.g., 1030 or even 0208) of ialfmin and ialfmax on the  
              configuration card in question (see below).

- (2) If an orbital fails to converge in scheq, then diagnostic remarks are printed to the monitor screen.
- (3) If the radial mesh is too coarse (emx too small) for accurate calculation and normalization of a continuum function, then diagnostic remarks are printed to the monitor screen.

The significance of the other input quantities is as follows.

IBB 0 sets the outer boundary of the atom at mesh point IBB; do not use this option, as it is not completely debugged.

TOLEND is the maximum permissible value of DELTA (the absolute value of the change in RU) for ending the SCF iteration (see the main program, statements number 530-550 and 700-780).

THRESH is the maximum permissible fractional change in the value of the eigenvalue E to end the eigenvalue iteration (SCHEQ, statements 805 and 205).

MAXIT is the maximum allowable number of SCF iterations; if convergence has not been reached within MAXIT cycles, the calculation is continued for 4 more cycles with diagnostic printout produced via NPR > 0 (RCN, 710-729).

EXF10 is the coefficient of Slater's exchange term for an HFS calculation with no tail cutoff (KUT=1) or with tail cutoff (KUT=0) (RCN 411-417). EXF10=1.5 is Slater's original value and EXF10=1.0 is Kohn and Sham's modified value.

EXFM1, CAO, and CA1 are values of k1, k3, and k2, respectively, for KUT=-1 in an HX calculation [Phys. Rev. 163, 54 (1967), Eqs. (13)-(14) or TASS, Eqs. (7.49)-(7.50)]. Provided IHF=0, EXFM1=0.0 will give a Hartree calculation for KUT=-1, and KUT=-2 gives an HS calculation. (CAO and CA1 are no longer read in from the control card, but simply set to 0.5 and 0.7, respectively, in the code.)

If IREL=0, relativistic terms are omitted from the differential equations (HX or HF); if IREL>0, these terms are included (HXR or HFR). If IREL 2, approximate Breit magnetic and retardation energies will be included, provided the dimensions of QNL are the same as those of PNL. If IREL > 3, some diagnostic printouts will occur.

Other quantities will be discussed later.

(2) Configuration card: This is read at statement 210 of subroutine RCN and contains the following information.

<u>cols</u>	<u>format</u>	<u>variable</u>	<u>significance</u>
1	I1	NHFTRM	Number of LS terms for which HF calculations are to be made
2-5	I4	IZ	Atomic number (fixed point)
6-8	I3	IBB1	For this configuration only, overrides the value IBB read from the control card, provided IBB1 > KO, the storage dimension for the maximum number of orbitals. If

0 IBB1 KO, then the input value is interpreted as a quantity N1SCF, and IBB1 is set to zero. All radial functions with serial number equal to or less than N1SCF are held frozen at their form in the preceding configuration; see examples in Secs. II-J and K.

9-10	I2	NSPECT	1+degree of ionization (1=neutral, 2=singly ionized, 3=doubly ionized, etc.)
11-28	3A6	CONF	BCD configuration label (eg, Ca I 4s 3d), for identification purposes only. (For clarity of RCN2 and RCG output, columns 11-16 should contain the element and ion stage, and the configuration label should be restricted to columns 17-24).
29-32	2I2	IALFMIN	Iteration control variables (normally left blank)
		IALFMAX	--if IALFMIN is non-blank, then so also must be IALFMAX. (Each must consist of two non-blank digits, and represents a value in percent.)
33-35	A3	NLBCD8(1)	Orbital specification (eg, " 4s", "12d", etc)
36-37	A2	WWNL8(1)	Occupation number (0^ or 00 means 0, blank or 1^ or 01 means 1, 2^ or 02 means 2, etc, where ^ signifies a blank)
.	.	.	.
.	.	.	.
.	.	.	.
68-70	A3	NLBCD8(8)	Orbital specification
71-72	A2	WWNL8(8)	Occupation number (default value is 1)
73-74	I2	KUT	For this configuration only, KUT 0 overrides the value of KUT1 from the control card. (See examples in Sec. II-K.)
75-80	F6.5	EE8	Eigenvalue (kinetic energy in rydbergs) of the outermost orbital for a free electron. (EE8 must be greater than 0; the last-punched value of NLBCD8 must be "99s", "99p", "99d", etc, and the corresponding value of WWNL8 must be blank or one.)

The above column-number restrictions for the variables in columns 11 to 80 may be adhered to if desired, but actually a blank-delimited, semi-free-form format is permissible, as follows:

(a) The CONF field begins in column 11 and extends to at least column 16, but terminates at column 28 or whenever three successive blanks occur--whichever happens first.

(b) The IALFMIN/IALFMAX field, if present at all, appears next--two successive non-blank digits if only IALFMAX is present, four successive non-blank digits if IALFMIN and IALFMAX are both present. Floating-point control variables are calculated via

$$\begin{aligned} \text{ALFMIN} &= 0.01 * \text{IALFMIN} \\ \text{ALFMAX} &= 0.01 * \text{IALFMAX} \end{aligned}$$

default values being 0.20 and 1.00, respectively.

(c) The subshell nl values and occupation numbers come next--any number of subshells up to eight, each with format A3,A2 (or A2 and/or A1, if  $n < 10$  and/or occupation number less than 10).

(d) KUT (1 or -1) and/or EE8 (any number of digits, with decimal point) come last, in either order, default values being 0 and 0.0 .

Thus, beginning with column 11, one has almost complete freedom as to the columns in which information is to be typed. For example, for ionized copper plus a free p electron (denoted by using  $n=99$ ) with kinetic energy of 13.6268 Ry, the nominal formats given in the above table would require

```
29 1Cu I d10 13.6p          3d1099p          13.627
```

but actually any one of the following is equally valid:

```
29 1Cu I d10 13.6p          3d1099p          13.627
```

```
29 1Cu I d10 13.6p          3d10 99p          13.6268
```

```
29 1Cu I d10 13.6p 3d10 99p 13.626793
```

This semi-free-form flexibility is provided by reading columns 11-80 with format A70 , and then interpreting this information by means of subroutine ANALYZ (or ANALYZ1, when subroutine DIEL is used).

### C. Calculational Procedure

After reading the control card, the following is done for each configuration card:

(a) If  $IZ > 0$  but columns 11-16 are blank (first configuration card only), the output from IZ completed configurations done on previous runs is skipped over on tape2n, so that results for configurations in the present run will be added on to those done previously.

If  $IZ=0$ , go back and read a new control card. (This feature makes it possible, for example, to make both HF and HFR calculations in a single run.)

If  $IZ < 0$ , write EOF on tape 2 (and on tape7 if IHF 0), and exit.

If  $IZ > 0$  and columns 11-16 are not all blank, this is a genuine configuration card, and a calculation is made as follows:

(b) Calculate the number of electrons in the atom from

$$N = IZ + 1 - \text{NSPECT} .$$

Set up the heaviest noble-gas core (ground configuration of He, Ne, Ar, Kr, Xe, Rn, or  $Z=118$ ) having no more than N electrons. Modify or add to this core according to any values of NLBCD8/WWNL8 punched on the configuration card, so as to obtain the final desired configuration, Eq. (1). [Note that any orbital in the noble-gas core modified via NLBCD8/WWNL8 with WWNL8=0 is deleted completely from the final configuration unless it is one of the frozen-core orbitals, in which case the orbital is retained with

zero occupation number.] Estimate a value of the eigenvalue for each orbital (unless EE8 is non-zero, in which case this value is used for the outermost orbital.) [Decoding of WWNL8 (subroutine SETCFG, statements 230-233) and of NLBCD8 (statements 237-242) is done partly via table look-up.]

In setting up each configuration card, it is worth noting that the spectrum number punched in columns 9-10 of the card is used only to find the noble-gas configuration from which to start in setting up the desired final configuration. Fictitious numbers sometimes can be used to simplify the card punching. For example, the following two cards will produce exactly the same results for neutral germanium:

```
32    1Ge I  4p 4d      3d10 4s2 4p 4d
32   -3Ge I  4p 4d      4p 4d
```

The former starts with Ar I  $3p^6$  and adds on 14 more electrons; the latter starts with Kr I  $4p^6$ , changes  $4p^6$  to  $4p^1$ , and adds on  $4d^1$ .

(c) A radial integration mesh is set up in terms of a universal mesh  $X(I)$ , scaled via  $R(I)=C*X(I)$ , where  $C=0.88534138/Z^{1/3}$  (RCN, 290-295).

(d) A suitable starting atomic potential  $RU(I)$  for the current value of  $Z$  is obtained by scaling a universal input potential  $RU0$  (Herman and Skillman's function  $U$  for argon, first configuration only) or the final SCF potential from the preceding configuration (RCN, statements 270-290).

(e) A SCF iteration is carried out by repeatedly (up to MAXIT times): calling SCHEQ to integrate the differential equation to obtain a radial function  $PNL(I,M)$  for each orbital  $M$ ; recalculating the potential  $RU$  from the  $PNL$ ; comparing the  $PNL$  and/or  $RU$  with values from the preceding cycle, and revising as appropriate.

An HX or HF calculation is started by first making an HFS calculation ( $KUT=0$ ) for at least two cycles to obtain approximate wavefunctions (required for the calculation of HX or HF potential functions for use in the differential equation), and then automatically switching to HX or HF ( $KUT=-1$ ) when  $DELTA < TOLKM2$  (RCN, statements 730-735). [To calculate via HFS only, make  $TOLKM2=0$  on the control card; to calculate for two or more values of  $KUT$  in succession (in the order +1, 0, -1, -2), make  $TOLKM2=TOLEND$  on the control card,  $KUT1=1$  (or 0, if  $KUT=1$  is not desired), and  $KUTD=0$  if  $KUT=0$  is not desired (see RCN, statements 990-end).] On other than the first configuration, the initial HFS calculation can be skipped and the HX or HF calculation started immediately by setting  $KUT=-1$  on the configuration card, provided all orbitals in the new configuration are present also (in the same order) in the preceding configuration; for examples, see Sec. II-K.

Stabilization of the SCF iteration is via  $RU$  on early cycles (RCN, statements 600-660), and on the  $PNL$  on later cycles (454-490). The control involves quantities  $ALF(M)$ , recomputed each cycle within the range  $ALFMIN$  to  $ALFMAX$  (normally 0.2 to 1.0). If convergence is not obtained on a run, rerun it with  $ITPOW=1$  or 3 to print values of  $DELTA$  (unless  $IW6 < 0$ , in which case this information is already available on the monitor-screen output). If the SCF iteration seems to be progressing satisfactorily ( $DELTA$  changing more or less monotonically toward zero), but not

satisfying the criterion  $|\text{DELTA}| < \text{TOLEND}$  in MAXIT cycles, MAXIT and/or IALFMIN can be increased on the control card. If the SCF iteration should fail to converge because of oscillatory instabilities (very unlikely), three things can be tried: (1) decrease the values of IALFMIN and IALFMAX read in on the configuration card; (2) increase the value of TOLEND on the control card; (3) in the FORTRAN statement just before statement 708 of RCN, increase the number "5.E-06", which is an upper bound on the fractional change allowed in the tail of each wavefunction.

(f) Using the final SCF radial wavefunctions PNL, various one-electron radial integrals (eg, kinetic energy and electron-nuclear potential energy) are computed, the subroutines POWER, ZETA1, SLI1, and RCN3S are called, and output is written on a BCD output print unit 9 (external name OUT36); also, provided there exists no asterisk anywhere in columns 11-16 of the configuration card, then wavefunctions and other information are written on output file tape2n for use by the computer program RCN2, or (if IHF=1) HFWRTP is called to convert from a linear to a logarithmic mesh and write tape7 for use by program HF8 (see subroutine OUTPT, statements 989-990) .

(g) If the values of TOLKM2, TOLEND, KUT, and KUTD so indicate, additional calculations are automatically made for the same configuration, but with different values of KUT [see under (e) above].

#### D. Input/output units

Data input and printed output are via files 10 and 9 (external names IN36 and OUT36), respectively. In addition, binary file 2 (external name TAPE2N) or 7 is used for output wavefunctions (input to RCN2 or HF8, respectively), and binary file 4 is used for temporary scratch storage. If IW6 < 0, then the progress of the SCF iteration for each configuration is sent to the monitor screen via unit 6.

#### E. Output

The amount of printed output is controlled by the quantities ITPOW, IPTVU, IPTEB, IHF, and NPR punched on the control card, in ways described under "Input," Sec. II-B. If NORBPT > 0, the first two and the last NORBPT radial wavefunctions are printed out. For each function, the value is printed at every fifth mesh point in a two-column format (mesh points 1, 11, 21, 31,        in the first column, and mesh points 6, 16, 26, 36,        in the second column); the radius is printed only at mesh points 1, 11, etc. (If IREL=2 and subroutine EBREIT is in use, then the small-component relativistic function QNL at points 1, 11, 21,        is printed in place of PNL at points 6, 16, 26,        ) If NORBPT > 5, continuum wavefunctions are printed in the above manner, and also at every mesh point in a ten-column format.

Coulomb interaction energies between two electrons, and one-electron and total binding energies (without corrections, and with

relativistic and/or correlation corrections) are printed out on the final page; all values are in rydbergs, except that spin-orbit parameters are given in both rydbergs and  $\text{cm}^{-1}$ .

The final line of each listing (except for timing information) contains the configuration identification CONF, the number of parameters required for an energy-level calculation in the single-configuration approximation, and a list of the parameter values together with an integer code number:

```
0:  Eav = total binding energy, including corrections
      (in rydbergs)
1:  Fk(lilj)      (in units of 1000 cm-1)
2:   i                "
3:  Fk(lilj)      "
4:  Gk(lilj)      "
```

The order of the parameters is the same as that required as input to program RCG.

Finally, provided there is no asterisk in columns 11-16 of the configuration card (columns 1-6 of the element/configuration variable CONF) and IHF=0 or 2, then in subroutine OUTPT (statement 989) most of the important output information is written on file 2. This information includes a configuration serial number ("1" for the first configuration, and automatically made one greater for each succeeding configuration), the atomic number IZ and ionization stage ION (0=neutral), and a number of wavefunctions which for the first configuration of given IZ and ION is determined by NORBPT, and which for later configurations is such as to delete any wavefunctions deleted from the the first configuration. (The purpose here is to delete most inner closed-subshell wavefunctions, which are not needed by RCN2, so as to decrease required disk read/write and storage requirements in RCN2. Note, however, that if inner-subshell excitations are involved in a set of configurations, then it is essential that |NORBPT| be large enough that the inner-subshell orbital in question is written onto unit 2 for all configurations--otherwise RCN2 will put out diagnostic remarks to the effect that orbital so-and-so could not be found, and RCN2 output will be incorrect! To be safe in all cases, one can always use |NORBPT|=9.)

If IHF=1, then wavefunctions and other information required to start a Hartree-Fock calculation via program HF8 are written on unit 7 instead of on unit 2. Most radial integrals are not computed in RCN--only the call of ZETA1 to calculate a relativistic energy correction for carryover to HF8; if IREL > 0, HF8 calculates its own relativistic energy, and time can be saved by using TOLEND equal about 0.05, so that the RCN SCF iteration is not carried out to final convergence.

## F. Hartree-Fock calculations

If  $IHF > 0$ , then a Hartree-Fock (HF) calculation (rather than HFS, HX, or HS) is to be carried out--either through the use of program HF8 ( $IHF=1$ ), or self-contained within program RCN ( $IHF=2$ ).

In either case, it is possible to calculate radial wavefunctions that minimize the energy of a particular LS term instead of the center-of-gravity energy of the configuration, and the added input to RCN is identical in the two cases. This option is called by placing a non-zero value of NHFTRM (number of HF terms) in column one of the configuration card, and following the configuration card by NHFTRM LS-term cards (or sets of cards) containing the following information for the  $i^{\text{th}}$  LS term:

<u>cols</u>	<u>format</u>	<u>variable</u>	<u>significance</u>
1-7	A7	T1HF(I)	Unused identification information (eg, the configuration "pd", "p4 d", etc)
8-10	A3	T2HF(I)	LS term identification (eg, "3P " for $3P$ , etc.)
11-15	I5	NFG	Number of Slater integrals ( $F^k$ and $G^k$ ) involved in the diagonal energy-matrix element for this LS term (excluding $E_{av}$ )
21-29	F9.8	CFG(1,I)	Coefficient $f_k$ or $g_k$ of the $j^{\text{th}}$ $F^k$ or $G^k$ in the matrix element (relative to $E_{av}$ )
30	A1	FG(1,I)	"F" or "G", as appropriate
31	I1	KFG(1,I)	Value of $k$
33-35	A3	IFG(1,I)	Orbital codes; eg, " 3p" and " 3d" for
37-39	A3	JFG(1,I)	$F^2(3p,3d)$ or $G^k(3p,3d)$ .
			For legibility, column 32 may contain a left parenthesis, column 36 a comma, and column 40 a right parenthesis.
41-60			Same as 21-40 for the second $F^k$ or $G^k$
71-80			Same as 21-40 for the third $F^k$ or $G^k$

If more than three Slater integrals are involved in the expression for the energy of this LS term (relative to  $E_{av}$ ), then the remaining coefficients and integral names are punched four to a card in columns 1-20, 21-40, 41-60, and 61-80. (If a HF calculation for the center-of-gravity energy is desired in addition to one or more calculations for specific LS terms, this can be done by faking an LS-term card with  $T2HF=C-G$ ,  $NFG=1$ ,  $CFG(1,I)=0.0$ ,  $IFG$  and  $JFG$  equal any two orbitals of the configuration.) For  $IHF=1$ , none of this information is used in

RCN, but is simply passed on unchanged to program HF8; for IHF=2, this information is used in subroutine HFPOT, and in SLI1 (statements 650-700).

The required values of  $f_k$  and  $g_k$  can in many cases be obtained from tables in J. C. Slater, Quantum Theory of Atomic Structure (McGraw-Hill, New York, 1960), Vol. II, App. 21. Alternatively, they can be computed with the aid of program RCG, using the option ICPC >4 (see RCG writeup, or subroutine PFGD, statements 499-900). This option will write the above information out on file 11, except that the first two characters of IFG and JFG will be the serial numbers of the orbitals in the RCG calculation, and will have to be changed to the appropriate principal quantum numbers before use as input to RCN.

### G. Calculation of continuum functions

A continuum wavefunction is computed when the last orbital defined on the configuration card is singly occupied, has a "principal quantum number" of 99 (ie, has NLBCD8="99s", "99p", "99d", etc), and a positive eigenvalue (kinetic energy) EE8 (in rydbergs) has been included on the card.

In columns 61-65 of the control card, a quantity EMX may be punched with a value approximately equal to the largest value of EE8 contained on any of the configuration cards; if EMX is left zero, RCN will automatically search the input file, and by default set EMX equal to the largest value of EE8 found. The action of EMX > 0 is firstly to set the size (MESH) of the integration mesh to KMSH, the dimension of R, PNL, etc (instead of to 641), and secondly to change the radial integration mesh that is set up: instead of

$$R \quad R(I) - R(I-1)$$

being doubled at mesh points 41, 81, 121, 161, , no further doubling is done after  $R$  becomes  $0.40/(EMX)^{1/2}$ . This ensures that the mesh interval will not become so large but what there will still be about 10 mesh points within each half-wavelength of the continuum function, even at large  $R$ .

It is of course necessary that the dimension of the integration mesh be great enough (hence the use of MESH=1801), or that EMX be small enough, so that sufficiently large radii can be reached for accurate asymptotic normalization--the value of "F" printed via format 97 of SCHEQ should not differ from unity by more than about 0.05 or 0.1 .

Small non-zero values of EMX can also be used to handle large- $n$  bound functions ( $n$  equal about 15 to perhaps 40), which extend to radii too large for the normal 641-point integration mesh. Use of too large a value of  $n$  or an inappropriate value of EMX usually causes eigenvalue-iteration convergence failures or causes execution to bomb on an overflow.

## H. Vinti integrals

If the quantity IVINTI read from column 45 of the control card is non-zero, the subroutine VINTI is called from subroutine RCN just before statement 850:

IVINTI = 0                    no call of subroutine VINTI  
IVINTI > 0                   Vinti integrals calculated and printed  
IVINTI > 1                   some debugging information printed

For any two orbitals  $n_i l_i$  and  $n_j l_j$  with  $l_j = l_i - 1$ , the Vinti integral [J.P. Vinti, Phys.Rev. 56, 1120 (1939)] is defined as

$$J(i,j) = \int_0^{\infty} P_i \frac{dP_j}{dr} - l_i \frac{P_j}{r} dr \quad (4)$$

In a treatment of specific mass shift, this integral is weighted by a factor

$$W_{ij} = \frac{2 l_i w_i w_j}{(4l_i+2)(4l_j+2)} \quad (5)$$

The information printed is

$$J(i,j) \quad J^2(i,j) \quad W_{ij} \times J^2(i,j)$$

for each (i,j), and also the sum

$$\sum_i \sum_j W_{ij} J^2(i,j)$$

## I. Correlation Potential

The quantity CORRF read from columns 66-70 of the control card is used as a multiplying factor for a theoretical approximate correlation potential.

CORRF = 0.0                    effectively deletes the potential  
                                  (equivalent to past versions of RCN)  
  
CORRF = 1.0                    is the theoretically correct value, and is the  
                                  suggested standard for future use  
  
CORRF > 1.0                    exaggerates the correlation potential.

Physically unreal values greater than unity may be needed for negative-ion calculations. For example,

CORRF = 0.0                    is adequate to bind  $Hg^- 5d^9 6s^2 6p^2$  ;  
CORRF = 1.0                    is adequate to bind  $Hg^- 5d^{10} 6s 6p^2$  ,  
                                   $F^- 2p^4 3s^2$ , and  $F^- 2p^4 3p^2$  ;  
CORRF = 1.5                    is needed to (barely) bind  $F^- 2p^4 3s 3p$  ;  
CORRF = 2.0                    is needed to (barely) bind  $Hg^- 5d^{10} 6s^2 6p$  .

It is worth commenting on relationships between the output-listing quantities EE (eigenvalue of the Schroedinger equation), EPSFG (one-electron binding energy calculated from the kinetic energy and the Slater  $F^k$  and  $G^k$  integrals), and EPSFGC (same, except with added perturbation correlation energy correction).

For HF (or HFR) calculations with CORRF=0, EE is equal to EPSFG--this is basically Koopmans' theorem. With CORRF=1, EE is more negative than EPSFG, but is equal to EPSFGC, as is to be expected. With CORRF > 1, EE is more negative even than EPSFGC, and in fact the latter may become positive (in which case SCHEQ may mistakenly treat the radial wavefunction as if it were a continuum function and produce completely incorrect normalization)

As a function of CORRF, the total binding energy of the atom excluding the perturbation correlation correction is a variational minimum for CORRF=0, but the total binding energy including the correlation correction (which is the total energy passed on to RCN2 and RCG) is a variational minimum for CORRF=1. It thus seems appropriate to consider CORRF=1 (rather than CORRF=0) to be the standard value. This results in more-contracted radial wavefunctions and hence in somewhat larger values (usually by only 1 or 2%) of the Slater integrals  $F^k$  and  $G^k$ ; these values are already too large even for CORRF=0, but this can be compensated for by using slightly smaller values of the scale factors in RCN2.

#### J. Frozen-orbital options

If the quantity IBB1 read from columns 6 to 8 of the configuration card is no larger than the dimensional parameter KO (currently KO=20) for storing radial wavefunctions, then this quantity is instead interpreted as N1SCF (and IBB1 set to zero). The first N1SCF orbitals of this configuration are then held fixed at their form in the preceding configuration. If desired, all orbitals can be frozen. For example, with input

```
13 1A1 I      3s2 3p
13 5 1A1 I    3s 3p2 ,
```

all five orbitals of the configuration  $3s3p^2$  (including 1s, 2s, and 2p as well as 3s and 3p) will be held fixed at the form they had in  $3s^23p$ .

Also, an orbital with zero occupancy can be retained if its serial number is no greater than N1SCF. For example, with input

```
13 1A1 I      3s2 3p
13 4 1A1 I    3s0 3p3
13 4 1A1 I    3s 3p2 ,
```

the orbitals 1s, 2s, and 2p of  $3p^3$ , and the orbitals 1s, 2s, 2p and 3s of  $3s3p^2$ , will all be the same as the corresponding orbitals of  $3s^23p$ . Further examples are discussed in the following section.

### K. Negative-ion calculations

In principle, if some value of CORRF can be found that will bind the electrons of a negative ion in the HF (or HFR) method, then it should be straightforward to make a calculation. In practice, the procedure can be tricky and may require several trial-and-error attempts. As an example, we consider the following set-up which has been found to work for

$F^- 2p^4 3s^2 + 2p^4 3p^2 - 2p^4 3s 3p$  (with CORRF = 1.5 and IREL = 1).

9		9F	I*	3S	2P4	3S	1S2	2S2	2P4		(a)
9	1	9F	-*	3S2	2P4	3S2	1S2	2S2	2P4		(b)
9		9F	-	3S2	2P4	3S2	1S2	2S2	2P4	-1	(c)
9	1	9F	I*	3S03P	P4	3S0	3P	1S2	2S2	2P4	(d)
9	1	9F	-	3P2	2P4	3S0	3P2	1S2	2S2	2P4	-1 (e)
9	1	9F	-*	3S	3P	P4	3S	3P	1S2	2S2	2P4 -1 (f)
9		9F	-	3S	3P	P4	3S	3P	1S2	2S2	2P4 -1 (g)

In all configurations, NSPECT (column 10) has been taken as 9 so that the code will not set up any noble-gas core to start with (and therefore the 1S2 and 2S2 have to be explicitly provided everywhere). The calculation starts [configuration (a)] with a neutral fluorine case that includes a 3s electron to provide a starting wavefunction for (b) and (c). In (b), a calculation (initially via a couple of HFSL cycles and then changing automatically to HFR) is made for  $F^- 2p^4 3s^2$ , with the 3s orbital fixed at the form obtained in case (a) by including the 1 in column 8. Then in (c), the 3s orbital is allowed to vary freely; by including the variable KUT=-1, the calculation begins immediately via the HFR method, without initially backing up to HFSL, which would have wrecked the convergence.

In (d), we go back to neutral fluorine (and, initially, HFSL) in order to introduce a 3p orbital, holding fixed the  $F^- 3s$  orbital (with zero occupancy) for later use. In (e) we go to  $F^- 3p^2$ , starting immediately with HFR (KUT=-1); it proved to be unnecessary to include here an intermediary calculation analogous to (b), presumably because the 3p electron in (d)--unlike the 3s electron in (a)--does not much penetrate the core, so that the 1s, 2s, and 2p HFR orbitals in (d) already provide adequate starting functions for (e).

In (f) we make a first calculation for  $F^- 2p^4 3s 3p$ , using as starting point the 3s function from (c) and the 3p (and other) functions from (e), but holding 3s fixed while the 3p and other functions are allowed to vary from their forms in  $2p^4 3p^2$ . Finally, in (g) the 3s function is allowed to vary freely to obtain the final  $2p^4 3s 3p$  result. [It proved not to be possible to delete (f), presumably because introduction of the 3s affected the core orbitals too much to allow everything to vary simultaneously].

Several additional remarks are appropriate:

(1) Asterisks have been included within columns 11 to 16 of four of the configuration cards, so that results for only the

three fully relaxed  $F^-$  calculations will be passed on to RCN2 and RCG (see Sec. II-C(f), page 15).

(2) Use of IREL=1 (rather than zero) provides an additional small attractive potential, which helps to bind negative ions; this will of course be more helpful in heavy atoms than in something as light as fluorine.

(3) Numerous attempts were made to make a calculation for  $2p^4 3s 3d$ , none of them successful. This is not surprising: In fluorine, a 3d orbital is essentially hydrogenic, with very little core penetration; the correlation formulation used in RCN depends entirely on wavefunction overlap with other orbitals, so that the correlation potential for 3d is very small. (Physically, 3d may be bound via polarization of the core, but the correlation algorithm used here does not adequately mimic polarization).

(4) Final results should be obtained using a value of CORRF=1 if possible, or if not, then as small a value as will give convergence. If on early attempts a value CORRF=2 (say) is used in order to help ensure success, then an estimate of the smallest possible value of CORRF can be made as follows: For the most weakly bound orbital, note on the final page of the output listing the values of EE (eigenvalue) and ECT (in the column following the column labeled N\*RC). Unit decrease in CORRF will decrease the magnitude of EE by approximately the magnitude of ECT; thus if the magnitude of EE is only about one-third the magnitude of ECT, then it is safe to try a new run in which CORRF is decreased by no more than about one third of a unit--in the present example, from 2.0 to about 1.7.

As an illustration of the sensitivity of Coulomb integrals to the value of CORRF, in the case of  $F^- 2p^4 3p^2$ , decreasing CORRF from 2.3 to 1.0 decreased the 2p-3p Coulomb integrals by about 20%; for  $F^- 2p^4 3s 3p$ , a decrease from 2.3 to 1.5 decreased the inter-subshell integrals by 30 to 50%.

#### L. Dielectronic recombination calculations

RCN input for making dielectronic-recombination calculations in RCG requires knowing the kinetic energies of the free electrons that can be captured into the autoionizing configuration of interest. This requires making preliminary RCN calculations for the autoionizing configuration and for the ion configuration(s) involved to get the kinetic energy (by differencing total binding energies), as well as figuring out by hand the possible value(s) of the angular momentum of the free electron. This hand work can be eliminated and final RCN input constructed automatically by using the subroutine DIEL of RCN36. To do this, the RCN input file IN36 is constructed so as to contain only the exit card with -1 in columns 4-5, and input to DIEL is set up in a separate file named INDIEL (internal file 12). This latter file contains:

- (1) the usual RCN control card;
- (2) a card for the ground configuration of the ion (it being assumed that this is the initial configuration for electron capture), and one for each excited configuration of the ion that the captured atom might autoionize into (a maximum of 5 ion configurations, total);

(3) a card for each of the singly excited configurations that the doubly excited configuration might decay to radiatively so as to produce a system stable against autoionization;

(4) a card for the doubly excited (autoionizing) configuration (program dimensions allow more than one such configuration, but if more than one is used, the RCG output print of individual-level autoionization rates must be interpreted with care and the overall dielectronic-recombination-rate number is incorrect);

(5) the usual "-1" exit card.

Further sets of cards (2)-(5) for other doubly excited configurations may be included if desired, provided that in all sets the radiative-decay configurations have the same parity. (But unlike normal RCN input, all such cards will be utilized--not just the cards in front of the first exit card!) Note also that in this INDIEL file, each configuration card must contain explicitly any orbital (even though full or empty) that is listed as other than the final (outermost) orbital on any other configuration! Also, the value used for NSPECT for the ion configurations (2) must be different from that used for the "atom" configurations (3)-(4).

RCN36 will then first call DIEL to find kinetic energies, determine orbital angular momenta for the free electrons, and set up complete input for the final RCN run--which will then be carried out automatically in the normal way.

#### M. Fractional occupation numbers

A new option (1999) is the possibility of using fractional occupation numbers for the subshells of an atomic "configuration."

Reasons for interest in use of fractional occupancies have been discussed in, for instance, Slater, Mann, Wilson, and Wood, Phys. Rev. 184, 672(1969).

Previously, an input configuration card to program RCN could contain only integral occupation numbers, with no decimal points; for example, for the 3s<sup>2</sup> 3p<sup>2</sup> and 3s 3p<sup>3</sup> configurations of 5-fold ionized potassium, K VI:

```
19      6K VI 3s2 3p2          3s2 3p2
19      6K VI 3s 3p3          3s 3p3
```

Now, fractional occupation numbers are permissible, such as (all for a total of 4 electrons in the n=3 shell):

```
19      6K VI 3s1.8 3p2.2      3s1.8 3p2.2
19      6K VI 3s0.23 3p3.77    3s0.23 3p3.77
19      6K VI 3s.015 p3.985    3s.015 3p3.985
```

The number of characters that may be used for the occupation number is limited to 6. The decimal point can lie in any appropriate point in this number--first, in the middle, or at the end--though this last of course represents an integral occupation number and is therefore no different than if the decimal point is absent.

NOTE 1: If the decimal point lies in the first or second position, a 6-character number will be read and used in the program as having 5 or 4 decimal places, respectively. However, occupation numbers given in the output print file out36 are printed to only three decimal figures in all cases, and it is suggested that the occupation numbers on the input configuration card never use more than three decimal places, as in the last example above.

NOTE 2: As usual, the length of the configuration label (the characters starting with "K VI" and ending before the [at least] three blank spaces) can be no more than 18 characters; the principal quantum number "3" for the 3p subshell has been omitted in the last example above to stay within this limit.

NOTE 3: For a configuration containing fractional occupancies, no output file is written on the binary output file tape2n used for input to program RCN2, as such cases are inappropriate for RCN2 and RCG calculations. Both the old- and new-style configuration cards can be intermixed in a single RCN calculation, but in such a case, RCN2 may not work properly.

In addition to the above fractional-occupation feature, further modifications have been made to RCN:

(1) If npr is non-zero, then when niter.ge.npr the former output of diagnostic potentials and radial wavefunctions has been removed and replaced by a write to the monitor screen of expectation values of r for the outermost 10 orbitals. This may show up erratic changes in d or f orbitals due to collapse into the core and expansion back out of the core; this is most likely to occur for neutral or singly ionized elements near the beginning of a transition, rare-earth, or actinide series. The most likely solution is to place small values (e.g., 1030 or even 0208) of ialfmin and ialfmax on the configuration card in question.

(2) If an orbital fails to converge in scheq, then diagnostic remarks are printed to the monitor screen.

(3) If the radial mesh is too coarse (emx too small) for accurate calculation and normalization of a continuum function, then diagnostic remarks are printed to the monitor screen.

#### N. Storage requirements

Memory storage requirements for 20 orbitals and an integration mesh of 561 points (adequate for n up to about 10) or 1801 points (needed for continuum functions or large n) is, on the CRAY-1, about as follows (number of 64-bit words, octal):

	<u>561</u>		<u>1801</u>	
	<u>no QNL</u>	<u>QNL</u>	<u>no QNL</u>	<u>QNL</u>
FORTTRAN code (2 to 4 instrs. per word)	27K	27K	27K	27K
Utility/library	46K	46K	46K	46K
Data storage	61K	106K	221K	327K
	<u>        </u>	<u>        </u>	<u>        </u>	<u>        </u>
Total (excluding I/O buffers)	156K	203K	316K	424K

On a Macintosh, the minimum RAM for execution is about 2.5 Mbytes with QNL and 1801-point mesh.

Storage requirements can be reduced in various ways, depending on the kinds of calculations one is interested in. The parameter KO can be reduced if one is interested only in atoms involving fewer than 20 orbitals, and KMSH can be reduced to, say, 521 if one is not interested in continuum or large-n bound orbitals. If the option IREL=2 is not desired (and, in fact, the Breit magnetic and retardation corrections seem to provide no increase in accuracy even for very high Z), then KMSHQ and KOQ can each be reduced to 1 and routines EBREIT, BRTINT, and S3J can be discarded. If RCN is used only to provide input to HF8 (IHF=1), the subroutines POWER, SLI1, RCN3S, S3JOSQ, FCTR, and all routines from HFPOT on may be discarded. If IHF=1 and IREL>0, then subroutine ZETA1 may be discarded as well.

Of course, 2 or 3 Mbytes is no limitation on modern desktop and laptop computers!

#### O. Conversion to other computers

Conversion problems to other computers having a FORTRAN 77 compiler should be minor except for the following:

The SCF iteration must be carried out to very tight tolerance if one wishes to compute meaningful excitation energies by differencing values of  $E_{av}$  for two configurations, because many significant figures are lost in this difference (about 6 or 7 significant figures for an actinide). This means that most calculations must be done with a precision of 9 or more significant figures. On machines using 60- or 64-bit basic floating-point word lengths, this is no problem. On VAX or IBM 32-bit machines (about 7 significant figures), it is necessary to compile using 64-bit floating-point numbers--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. This means using basically double-precision floating-point numbers. To simplify converting back and forth between CRAY and VAX-type machines, the following program modifications have been incorporated, as mentioned earlier:

(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 VAX-type 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 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 the 32-bit-machine case it will automatically be converted to double precision.

### III. PROGRAM RCN2

#### A. Outline

This is a FORTRAN 77 program for the CRAY-1 or CDC CYBER 205 computer, or for VAX, Sun, IBM RISC, or Macintosh and similar computers. It reads information from the output disk unit 2 of RCN or HF8, calculates configuration-interaction radial Coulomb integrals  $R^k$  and electric dipole and quadrupole reduced matrix elements

$$P^{(k)}_{ll'} = \frac{1}{2} |P^{(k)}_{ll'}| \quad (k=1 \text{ or } 2)$$

or analogous matrix elements of spherical Bessel functions, scales all energy-level-structure parameters  $F^k$ ,  $G^k$ ,  $R^k$ , and  $\rho$ , and writes on unit 11 a complete file of input data for making energy-level and spectrum calculations via program RCG. [Note: For HF wavefunctions, RCN2 output is useful mainly for center-of-gravity (not LS-term-dependent) calculations; nominally, RCG assumes c-g results exclusively.]

The program consists of a main program and nine subroutines.

MAIN reads control cards and calls various subroutines accordingly.

OVER computes an overlap integral between two specified radial wavefunctions from the same or from different configurations.

ZETA2 computes single-configuration or configuration-interaction spin-orbit parameters [using the simple central-field formula (3)]. The former are computed by ZETA1 of RCN, and the latter are usually so small as to be negligible, so in practice this subroutine is almost never used.

DIP computes electric dipole and quadrupole integrals  $P^{(k)}_{ll'}$  or matrix elements of spherical Bessel functions.

SLI2 computes configuration-interaction radial integrals  $R^k(l_1l_2, l_3l_4)$ .

G5INP is a master program that calls SLI2 and DIP as appropriate, and prepares the input file for RCG. (Note: The name "G5INP" refers to the preparation of input for RCG Mod5, which is now a misnomer since the current version of RCG is Mod 11.)

S3J calculates the 3-j symbol

$$\begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array}$$

S3J0SQ calculates values of

$$\begin{array}{ccc} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{array}^2$$

FCTRL calculates the factorial of an argument A for use by S3J and S3J0SQ.

SBESS evaluates the spherical Bessel function of specified order for a given radius and wavenumber.

## B. Input

Input consists of radial wavefunctions and other information written on unit 2 (in a file named TAPE2N) by program RCN or by program HF8, and of one control card for each calculation being made. The control card is read as a string of 80 BCD characters at statement 200 of MAIN, and then is decoded according to a format appropriate to subroutines other than G5INP. The first three characters (columns 1-3 on the control card) specify the subroutine to be called and columns 11-20 (format 2I5) specify the serial numbers of the two configurations from which wavefunctions are to be selected; the orbitals themselves are specified in columns 21-30 [format 2(2X,A3) for OVER, ZETA2, and DIP] or columns 21-40 [format 4(2X,A3) for SLI2]. The program RCN2 usually is no longer used to call the subroutines OVER, DIP, and SLI2 directly, but only via G5INP. Hence we shall not describe these options further, but consider only the case in which the first 3 characters of the data card are "G5I".

In this case, control is transferred to subroutine G5INP, which decodes the control card according to a new format (statement 100):

<u>cols</u>	<u>format</u>	<u>variable</u>	<u>normal value</u>
1-5	A3,2X	-----	g5inp
6-7	A2	NCK	blank (or as desired for RCG input)
8	I1	IOVFACT	0
9-10	I2	NOCET	blank (or 1 to produce input for RCE)
11	I1	NSCONF(3,1)	0 (or as desired for RCG input)
12-13	I2	NSCONF(3,2)	0 (or as desired for RCG input)
14-20	F7.4	EAV11	0.0 (or as desired for RCG input)
21	I1	IABG	0 (or as desired for RCG input)
22-49	3A8,A4	OPTION	blank (or as desired for RCG input)
50	I1	IQUAD	0 (non-zero for E2 spectra)
51-60	5I2	IFACT	9999999999, 8099808080, 9399939393, etc
61-65	A5	DMIN	blank (or as desired for RCG input)
66-70	A5	IPRINT	blank (or as desired for RCG input)
71	A1	IENGYD	blank (or as desired for RCG input)
72	A1	ISPECC	blank (or as desired for RCG input)
73	I1	ICON	2
74	I1	ISLI	2
75	I1	IDIP	9 (0 for plane-wave-Born calcns., 5, 7, or 8 for photoionization calcns.)
76-80	F5.0	ALF	blank (0.0)

IOVFACT if non-zero multiplies  $R^k$  values or radial multipole integrals or both by the product of overlap integrals for all spectator electrons for the subshells included in the RCN2 output, according as IOVFACT is 1, 2, or greater than 2, respectively.

NOCSET is normally zero, but if not (normally +1), the RCG input file OUT2ING will be set up to provide input files for RCE.

Any punches in columns 6-7, 22-49, and 61-72 are unused in RCN2, and are simply transferred unchanged to the same columns of the RCG input control card; likewise, punches in columns 11, 12-13, and 21 are transferred unchanged to columns 15 and 19-21. (See the description of this control card in Sec. IV(4)(A) of the RCG program writeup). For a modification of these remarks when column 33 contains a number greater than 4, see Sec. IV-F of this writeup (page 34).

EAV11 is the value desired for the center-of gravity energy  $E_{av}$  of the first configuration (in units of  $1000 \text{ cm}^{-1}$ ). It merely shifts the energy scale of all energy levels calculated by RCG.

If IABG > 0, it is a signal that the effective-operator parameters  $\alpha$ ,  $\beta$ ,  $\gamma$  are to be included in the RCG calculation. Values of these parameters cannot easily be computed theoretically; hence, RCN2 simply leaves room at the proper places on the single-configuration parameters cards of the RCG input file, where empirical parameter values can be inserted by hand (except that the number ALF punched in columns 76-80 of the G5INP control card will be punched for  $\alpha$ ).

IQUAD (column 50) causes electric-quadrupole radial integrals to be computed for configurations of the first, second, or both parities according as IQUAD=1, 2, or 3, respectively; the value of IQUAD is also transferred unchanged to column 50 of the RCG control card.

All this provides a means of controlling within RCN2 the various RCG options in a chained RCN/RCN2/RCG or RCN/HF8/RCN2/RCG run.

The values of IFACT(5) are converted to floating point and divided by 100 to provide scale factors FACT(5); if IFACT=01 or 99, FACT is set to 0.001 or 1.00, respectively. The values of FACT(5) are fudge factors to be applied to the theoretical values of the parameters  $F^k(l_i, l_i)$ ,  $F^k(l_i, l_j)$ ,  $G^k(l_i, l_j)$ , and  $R^k(l_i l_j, l_i l_j)$ , respectively, to give scaled-down parameters for input to RCG. It is known empirically that computed energy-level intervals will agree better with experiment if the Coulomb parameter values are 5 to 30% smaller than theoretical. Values of FACT of 0.85, 0.95, 0.85, 0.85, 0.85 are assumed by the code if zeroes are read in. Values of 0.90, 1.00, 0.90, 0.90, 0.90 are about right for HF calculations on about 5- or 10-fold ionized atoms. The first and the last three values should be more like 0.80 for most neutral atoms (except about 0.70 for lanthanides and actinides), and should be 0.92 to 0.95 for very highly ionized atoms. (All values should be about 0.05 smaller if HX calculations are used instead of HF.)

ICON = 1 the RCG-input control and config. cards are not punched  
 > 1 the number of subshells set up on the configuration cards is limited to no more than ICON if possible  
ISLI = 0 print maximum SLI2 output  
 = 1 omit page restore and most printout  
 = 2 omit all but final punched card image (except that parameter values are printed unscaled as well as scaled)  
 = 3 omit all printout  
  
IDIP = 1 do not punch dipole cards  
 = 5 configuration-interaction radial matrix elements between a bound and a continuum configuration are set to zero if the two configurations have the same total energy; otherwise, as for IDIP=9  
 = 6 configuration-interaction matrix elements involving a continuum electron are set to zero except for core bound-bound interactions in the case of two continuum configurations for which the free electrons have the same angular momenta and kinetic energies  
 = 7 values of  $R^k$  and dipole integrals in Rydberg series will be modified appropriately for pseudo-discrete calculations. [Each Rydberg-series configuration is given an effective-energy-width weighting factor  $E$ , which is unity for successive- $n$  discrete configurations, greater than one for non-successive- $n$  discrete configurations, and an effective width in rydbergs for continuum configurations.  $R^k$  values are weighted by the square root of  $1 \times 2$ , and discrete-continuum dipole integrals are weighted by the square root of  $E_2$ --see the RCG writeup, Sec. XI(B).]  
 = 8 modifications will automatically be made for simple photoionization calculations in RCG. [The value of NSCONF(3,2) on the RCG control card is set to -8, and all  $R^k$  involving a continuum configuration are set to zero--see the RCG writeup, Sec. XI(A)]  
 = 9 values of  $E_{av}$ ,  $R^k$ , and dipole integrals involving continuum functions will be modified appropriately for perturbation calculation of autoionization transition probabilities in program RCG. [The continuum  $E_{av}$  are changed to large negative values, and the continuum-continuum  $R^k$  and discrete-continuum dipole integrals are set to zero--see the RCG writeup, Sec. XII]. The value IDIP=9 can be used as a universal value for runs not involving continuum configurations.

### C. Calculational procedure

In order for G5INP to properly prepare input decks for RCG, it is necessary that the pertinent configurations be arranged on unit 2 in a specific order, and hence that the input configuration cards for RCN also be arranged in this order:

(a) All configurations of given IZ and ION that are to be included in one RCG calculation must be arranged in succession. Usually the lowest-energy configuration is chosen as the first one; all configurations of this same parity follow, and then come all configurations of the opposite parity (if any). Within a given parity, all configurations that are members of a single Rydberg series (eg,  $3p^53d$ ,  $3p^54d$ ,  $3p^55d$ , ...) should preferably be placed in succession. Each input configuration card for RCN should be punched so that all orbitals (other than the outer, most-weakly-bound, singly occupied orbital) are arranged in order of increasing  $n$ , and for given  $n$  in order of increasing  $l$ ; if orbitals are not arranged this way, G5INP attempts to rearrange things so, but the code is not bug-proof. [Note the exception to this order in the negative-ion example of Sec. II-K, necessitated by the fact that only the "inner" (ie, first-listed) orbitals can be held frozen.]

(b) In multi-configuration runs involving excitations out of inner subshells, RCN2 may incorrectly give zero for certain radial dipole integrals unless the configurations are arranged in such an order that the different  $nl$  values of the outermost excited electron first appear in the same order in each parity; for example, if the even parity configurations are

$2s^22p^2$   
 $2s^22p3p$   
 $2s2p^23s$   
 $2s2p^23d$

(outer electrons in the order  $3p$ ,  $3s$ ,  $3d$ ), then for the second parity the order should be

$2s2p^23p$   
 $2s^22p3s$   
 $2s^22p3d$  .

If the first-parity configuration  $2s2p^23s$  is omitted, then the second-parity order should be

$2s2p^23p$   
 $2s^22p3d$   
 $2s^22p3s$  .

This caveat can probably be ignored if ICON on the G5INP control card is set to two.

(c) G5INP will process sets of configurations in groups such that each group ends when (a) G5INP has already found two parities for a given ion and encounters on unit 2 the first parity again, or (b) it encounters a different element or ionization stage. For example, if A, B, C, D, and E represent five sets of consecutive configurations, all configurations of a given set belonging to the same ion and parity, and of the following sort (ION = degree of ionization):

<u>set</u>	<u>Z</u>	<u>ION</u>	<u>parity</u>
A	12	9	even
B	12	9	odd
C	12	9	even
D	14	9	even or odd
E	14	7	even or odd

then A and B will be processed together (including calculation of radial dipole integrals), but C, D, and E will each be processed individually. If for some reason one had desired that A and B also be processed individually (or that the set C be processed as two separate subsets), this could have been accomplished by separating A and B (or the two subsets of C) by, say, the set E or by some single dummy configuration with Z 12 and/or ION 9.

The calculational procedure is as follows:

(1) Disk unit 2 ("tape2n") is searched to find a group of consecutive configurations of the type described above--all having the same Z and same ION, and of at most two non-interleaved parities. (With current dimensions, the maximum number of configurations in any one group is 90.)

(2) The configurations of the first parity are copied onto disk unit 31, and those of the second parity (if any) are copied onto unit 32. (This is done to reduce disk search times after rewinding in the case of configuration sets D, E, far from the beginning of the file on disk unit 2.)

(3) All subshells  $1^w$  that are full ( $w=4l+2$ ) in all configurations of the group are ignored. The remaining subshells in the various configurations are ascertained, and arranged according to the requirements of RCG.

(4) The RCG control card is "punched" (ie, written on file 11--external name "out2ine"); this card contains the total number of subshells and the number of configurations of each parity [NSCONF(2,K)], among other things.

(5) The  $l$  and  $w$  values are punched for each configuration. [The configuration label and total binding energy (in units of  $1000 \text{ cm}^{-1}$ ) are also punched, though this information is not used by RCG.]

(6) The single-configuration parameter values VPAR supplied by RCN (via disk 2) are rearranged if necessary [see the remark in Sec. C(a) above], scaled by the factors FACT, and punched. [First parity only]

(7) Parameter values  $R^k$  for all possible configuration interactions are computed with the aid of calls to SLI2, and punched. [First parity]

(8) If the value of IQUAD so indicates, values of the electric quadrupole reduced matrix element  $\mathbf{P}^{(2)}_{11}$ , [or of the appropriate spherical Bessel function, if IGEN (column 33 of the G5INP control card) = 5] are computed via calls to DIP and punched. [First parity]

(9) If configurations of both parities are present, (6)-(8) are repeated for the second parity, and then values of the electric dipole reduced matrix element [or of the spherical Bessel function] are computed via calls to DIP and punched.

(10) A card with "-99999999." in columns 21-30 is punched to provide the "end" card for an RCG calculation. (If the value of NCMAX is non-zero, a similar card with fives instead of nines is punched first.)

(11) Disk unit 2 is searched to see if there exist additional configurations. If so, items (2)-(10) are repeated for each remaining group of configurations. [If the new group of configurations is identical with the preceding set so far as the  $l_j w_j$  are concerned, then ICTC=1 is punched in column 78 of the RCG control card and step (5) above omitted, so that RCG will not waste time repeating the calculation of quantum numbers and angular matrix elements--see the RCG writeup, SEC. IV(4)(A).]

(12) When unit 2 has been exhausted, a return is made to the main program, and a new RCN2 control card is read and processed. (This feature could, for example, be used to run RCG with two different sets of scale factors by including two G5INP control cards.) A final "control card" containing a negative number in columns 8-10 results in an exit from RCN2 (after writing to file 11 an RCG exit card--a card with a negative number in columns 1-5).

Note: The identification labeling that RCN2 provides on the configuration-interaction-parameter cards consists of whatever appears in columns 17-25 of the two RCN configuration-definition cards involved. For maximum legibility, it is suggested that these latter cards contain (insofar as possible) the element and ion stage in columns 11-16 and the configuration label in columns 17-25 (or, even better, in columns 17-24, because of some eight-character limitations in labeling in RCE)

#### D. Input/output units

Data input and output are via units 10 and 9 (external names IN2 and OUT2), respectively. In addition, disk unit 2 (external name TAPE2N) is used for input wavefunctions from RCN or HF8, and unit 11 (external name OUT2ING) is used for the output file that will be the input file for RCG. Disk units 31 and 32 are used for scratch storage in the manner described earlier, and unit 8 is used to store CI strengths for use in program RCG.

#### E. Output

Output includes the ASCII file OUT2ING on unit 11 ready to be used directly as input to program RCG. Such a file may be used without change (except for the name change to ING11) or it may be modified by hand in various obvious ways. For example, the print options in columns 66-70 of the RCG control card may be modified; if one wishes to add or delete calculation of magnetic dipole spectra, that can be done simply by changing column 49 appropriately; if configurations of both parity were included in the RCN/RCN2 run but one wishes to include only the first parity in the RCG calculation, it is only necessary to insert zeroes in

columns 16-20 of the control card, and delete all configuration-definition and parameter-value cards for the second parity, and remove all electric dipole cards; if one wishes to make the RCG calculation in the JJ- rather than LS-coupling representation, column 5 of the control card can be changed from 1 to 2; etc.

Parameter values in file OUT2ING are always in kK (units of  $1000 \text{ cm}^{-1}$ ). Decimal points are usually omitted to provide an extra column to obtain an additional significant figure; values are read in RCG (subroutine ENERGY) with a format such that the implied decimal point lies between columns 5 and 6 of the 10-digit parameter field. (Note: The tenth digit is not actually part of the parameter value, but is rather a code number that indicates the type of parameter--see Sec. X of the RCG writeup.)

In addition to the file 11 output, all information in this file is also printed via the output file 9 (OUT2), as is some additional detail regarding the calculation of the  $R^k$  and the  $P^{(k)}_{11}$ .

#### F. Plane-wave-Born calculations in RCG

Input for plane-wave-Born collision-strength calculations via program RCG is prepared when column 33 of the G5INP control card of RCN2 is greater than 4. In this case, certain columns of the control card are interpreted differently from the manner indicated in Sec. IV-B:

cols	format	variable	normal value
23-25	I3	NBIGKS	41 or blank (default=41)
26-27	I2	NENRGS	blank (default=21)
33	I1	IGEN	9 (or as desired for RCG input)
34	I1	IRNQ	(default=0)
35	I1	IRXQ	(default=IRNQ)
36	I1	IRND	(default=1)
37	I1	IRXD	(default=IRND)
50	I1	IQUAD	
73	I1	ICON	0
75	I1	IDIP	0

After interpretation of the above information, columns 22-29 are in effect reset to blanks, and then columns 22-50 transferred directly on to the RCG control card just as when column 33 is less than 5; ICON and IDIP are also ultimately reset to zero.

The amount of printed output in RCG for IGEN 5 is smaller the larger the value of IGEN; the value IGEN=9 is recommended. The effect within RCN2 is the same for any value IGEN 5, and is to cause matrix elements

$$1 |j_t(Kr) c^{(t)}|_l'$$

of the spherical Bessel function  $j_t(Kr)$  to be computed in DIP instead of the electric multipole reduced matrix elements

$$1 |r^t c^{(t)}|_l' ;$$

see TASS, Secs. 18-12 and 18-13 for details. Calculations will be made for

$$t = \text{IRNQ}, \text{IRNQ}+2, \dots, \text{IRXQ}$$

in the case of parity-conserving excitations (called for by IQUAD 0 in the usual fashion), and/or for

$$t = \text{IRND}, \text{IRND}+2, \dots, \text{IRXD}$$

in the case of parity-changing excitations, at NBIGKS different values of the momentum transfer K. The values of IRNQ and IRXQ must be even integers covering the range of values of t needed for all parity-conserving excitations included in the present calculation, as specified by NCK(1) [default=1 when IGEN 5] and NCK(2); similarly, ICND and IRXD are odd integers covering the range needed for all parity-changing excitations. [Note: For intra-configuration excitations, calculations are made (incorrectly in some cases, just as for electric quadrupole radiative transitions) for a given partially filled subshell only if there exists no other less-tightly-bound, non-s, partially occupied orbital.]

The values of K are equally spaced on a logarithmic scale, covering an energy-transfer range from  $10^{-3}$  Ry to  $4.4 \cdot \text{XMAX} \cdot \text{ENMAX}$ , where ENMAX is the difference between the highest and lowest values of  $E_{av}$  [or is the value of VPAR(2) if there is only one configuration present]. Values of collision strength are to be computed in RCG at NERGS values of  $X E / (E)$  on a logarithmic mesh from XMIN to XMAX, where E is the kinetic energy of the impacting electron, E is the excitation energy, and

	1.01	if ICON=0
	1.1	if ICON=1
XMIN =	ICON	if ICON=2 to 8
	10	if ICON=9
	100	if IDIP=0
	20	if IDIP=1
XMAX =	100*IDIP	if IDIP=2 to 8
	1000	if IDIP=9

#### G. Photoionization and autoionization calculations in RCG

Calculation of photoionization cross sections can be carried out in RCG in various ways. The value of IDIP in column 75 of the RCN2 G5INP control card needs to be chosen appropriate to the method to be used in RCG. In one method (appropriate only if all configuration interactions involving continuum configurations may be neglected), IDIP should be eight. In another method (in which all interactions are to be retained, with no necessity for handwork in the preparation of input to RCG), IDIP should be equal to seven; the kinetic energies of the free electron in the various continuum configurations then need to be chosen judiciously, and RCN2 will modify the various  $R^k$  and radial multipole integrals in

a manner appropriate to the energy spacings between successive configurations of each Rydberg series.

If detailed autoionization calculations (by perturbation methods) are to be made in RCG, then IDIP should be nine. In this case, RCN2 will modify  $E_{av}$  for continuum configurations to appropriate large negative values, and will set to zero all continuum-continuum  $R^k$  and all radial multipole integrals involving a continuum configuration.

See Sec. IVB above--for further details, see the RCG program writeup.

#### H. Configuration-interaction strength estimates

[January 2005] An addition to RCN2 has been made to compute for each pair of interacting configurations a quantity *cistrength*, added to columns 81-90 of each CI parameter card in the output file *out2ing*. This quantity is here defined to be

$$\text{cistrength} = 4.0 * \text{sum of the squares of all } R_k \text{ for both configs.} \\ / [(\Delta E_{av}) * (\text{sum of all } F_k, G_k, \text{zeta for both configs})].$$

(The coefficient 4.0 has been chosen empirically on the basis of some simple cases such that, for example, *cistrength*=0.01 corresponds to CI energy perturbations equal to about one percent of the energy spread within either configuration.)

The values of *cistrength* are also written on a file "tape.ci" (unit 8) to be read by RCG. If values are less than an optional variable "cicriterion" in that program, then the corresponding CIs are excluded from all calculations in RCG.

#### I. Storage requirements

Storage requirements for up to 90 configurations of given IZ and ION, 20 orbitals per configuration (so far as the information written on unit 2 is concerned), and 561 or 1801 mesh points are, for the CRAY-1, about as follows (number of 64-bit words, octal):

FORTTRAN code (2 to 4 instructions/word)	16K	16K
Utility/library	46K	46K
Data storage	<u>130K</u>	<u>234K</u>
Total (excluding I/O buffer)	214K	320K

On a Macintosh or PC, execution requires a minimum RAM of about 2 Mbytes.

## J. Conversion to other computers

Conversion problems to other computers should be minor, in the same manner discussed for program RCN36 (Sec. II-N). Except for the calculation of values of  $E_{av}$ , double-precision calculations are probably not really necessary, but floating-point variables have to be defined consistently with RCN because of the binary information passed from RCN to RCN2 via TAPE2N.)

If plane-wave-Born calculations are of no interest, subroutine SBESS can be deleted and the dimension KBGKS reduced to unity, thus reducing data storage requirements by about 14K octal words.

## IV. PROGRAM USAGE AND EXAMPLE

### A. Execution

An RCN/RCN2 calculational session might go as follows:

- (1) Assuming that the RCN and RCN2 executable files, and sample IN36 and IN2 input files, are available:
- (2) Edit any desired changes into the RCN control card (eg, change the desired values of IREL, CORRF, IW6, etc.).
- (3) Following the control card, type in the desired configuration cards, followed by an exit card (-1 in columns 4-5).
- (4) Make any desired changes in the RCN2 G5INP control card.
- (5) Execute RCN and then RCN2.
- (6) The output print files are named out36 and out2. The name of the RCN2 output file OUT2ING can be changed to ING11, ready for use as input to an RCG calculation.

### B. Program availability

The source programs are available by anonymous ftp: The three source files (SUN versions) and nine different sample input data files have been placed on the Web in a public ftp directory  
aphysics/pub/cowan  
on the Los Alamos t4 network, and can be accessed by anyone having a suitable Web browser in the following way:

As URL, use <http://t4.lanl.gov>, and follow links to my programs; or alternatively, go directly to

<ftp://aphysics/pub/cowan>

Download the Readme file, the source programs rcn.f, rcn2.f, and rcg.f, and sample input files as desired.

For use on a CRAY, VAX or Macintosh, PC, or IBM, in each of the three programs modify the timing routine SUBROUTINE SECONDS by commenting out the SUN section and uncommenting the appropriate section.

For a first RCG calculation, use ing11k (renamed ing11) as input in order to calculate binary files TAPE72, TAPE73, and TAPE74 for subsequent RCG calculations; this input file contains all cfp decks that can be used in RCG with the dimensions provided. The file CFP includes additional cfp decks (for f5, f6, f7, f8, f9, and f10),

but these can be used in RCG only if numerous dimensions are increased appropriately, as described by comment cards in the RCG source program, lines 174 to 204.

C. Sample input files

Sample RCN36 and RCN2 input files follow:

Sample RCN input file, in36

```

333 9      2   10  0.2    5.e-08    1.e-11-2    190    1.0 0.65  0.0  0.0  -6
   1      1H I   1s      1s
  19      6K VI  3s2 3p2    3s2 3p2
  19      6K VI  3p4      3p4
  19      6K VI  3p 3d     3s2 3p 3d
  -1
  29      1Cu I  1s2 4s      1s2 3d10 4s
  29      1Cu I  1s 4s .1p   1s 3d10 4s 99p 0.1
  29      1Cu I  1s 4s 1.p   1s 3d10 4s 99p 1.0
  -1
  10      1Ne I  2p6      2p6
  10      1Ne I  2p5 3d     2p5 3d
  10      1Ne I  2p5 4d     2p5 4d
  10      1Ne I  2p5 6d     2p5 6d
  10      1Ne I  2p5 8d     2p5 8d
  10      1Ne I  2p5 .1d    2p5 99d 0.1
  10      1Ne I  2p5 .2d    2p5 99d 0.2
  10      1Ne I  2p5 1.d    2p5 99d 1.0
  10      1Ne I  2p5 2.d    2p5 99d 2.0
  -1

```

The above control card is for long output print (for debugging purposes, for example); for normal output, use

```

2   9      2   10  0.2    5.e-08    1.e-11-2    190    1.0 0.65  0.0  0.0  -6

```

Sample RCN2 input file, in2

```

g5inp      000 0.0000      01      9099909090 0.00      07229
  -1

```

(The "1" on the control card deletes printing in RCG of eigenvectors in the JJ-coupling representation, and the scale factors of "90" are appropriate for 5- to 10-fold ionized atoms.)

## D. Command-file methods

As an alternative to launching each program one at a time, one can use a command file to run each program in turn, with the input files contained within the command file.

### D1. UNIX command file for running RCN/RCN2/RCG

A sample command file for running a three-configuration problem in 5-fold ionized potassium on UNIX machines, including execution of RCG as well as of RCN and RCN2, is the following:

```
#!/bin/csh -f
rm in36 in2 inputg ing11
cat << eod36 > in36
2 -9 2 10 0.2 5.e-08 1.e-11-2 090 1.0 0.65 0.0 0.0 -6
19 6K VI 3s2 3p2 3s2 3p2
19 6K VI 3p4 3p4
19 6K VI 3p 3d 3s2 3p 3d
-1
1 1H I 1s 1s
29 1Cu I 1s2 4s 1s2 3d10 4s
29 1Cu I 1s 4s .1p 1s 3d10 4s 99p 0.1
29 1Cu I 1s 4s 1.p 1s 3d10 4s 99p 1.0
-1
eod36
rcn36.out
cat << eod2 > in2
g5inp 000 0.0000 00 9099909090 0.00 07229
-1
eod2
rcn2.out
cat << eodg > inputg
3 10e-350e05 000005 10. 0 5.0 2.0 1.0 0.5 0.2
0 0000000000 1000.0000
eodg
cat inputg out2ing >> ing11
rcg11.out
cat in36 out36 in2 out2 ing11 outg11 >> out$1
```

Let us suppose that this command file is named "cosmos", for example. Any desired input changes can be edited by hand into this file, and then the command

```
chmod 777 cosmos
```

will probably have to be given before it can be executed. If it is launched by the command

```
cosmos .KVI
```

then the final combined output file will be named

```
out.KVI
```

D2. UNIX command file for a dielectronic-recombination run, using the DIEL feature:

```
#!/bin/csh -f
rm indiel in36 in2 inputg ing11
cat << eoddiel > indiel
2 -9 2 10 0.2 5.e-08 1.e-11-2 090 1.0 0.65 0.0 0.0 -6
 34 26Se+25 s2 p5 2s2 2p5
 34 25se+24 s2 p5 9i 2s2 2p5 9i
 34 25se+24 sp6 9i 2s 2p6 9i
-1
eoddiel
cat << eod36 > in36
-1
eod36
rcn36.out
cat << eod2 > in2
g5inp 000 0.0000 00 9099909090 0.00 07229
-1
eod2
rcn2.out
cat << eodg > inputg
 3 10e-350e05 000005 10. 0 5.0 2.0 1.0 0.5 0.2
 0 0000000000 1000.0000
eodg
cat inputg out2ing >> ing11
rcg11.out
cat in36 out36 in2 out2 ing11 outg11 >> out$1
```

D3. Command file for VMS operating systems analogous to D1:

```
$create in36.dat
2 -9 2 10 0.2 5.e-08 1.e-11-2 090 1.0 0.65 0.0 0.0 -6
19 6K VI 3s2 3p2 3s2 3p2
19 6K VI 3p4 3p4
19 6K VI 3p 3d 3s2 3p 3d
-1
1 1H I 1s 1s
29 1Cu I 1s2 4s 1s2 3d10 4s
29 1Cu I 1s 4s .1p 1s 3d10 4s 99p 0.1
29 1Cu I 1s 4s 1.p 1s 3d10 4s 99p 1.0
-1
$run rcn36.exe
$create in2.dat
g5inp 000 0.0000 00 9099909090 0.00 07229
-1
$run rcn2.exe
$create inputg.dat
3 10e-350e05 000005 10. 0 5.0 2.0 1.0 0.5 0.2
0 0000000000 1000.0000
$copy inputg.dat,out2ing.dat ing11.dat
$run rcg11.exe
$copy in36.dat,out36.dat,in2.dat,out2.dat,ing11.dat,outg11.dat 'P1'.dat
```

If this file is named "cosmos.com"  
and launched via

@cosmos KVI

then the combined output file will be named KVI.dat