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MASTER

PROGRAMS FOR
ATOMIC-STRUCTURE CALCULATIONS

by

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Chemistry Division

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ABSTRACT

Computer programs used for atomic-structure calculations are described and listed. Sample data for each are also presented.

I. INTRODUCTION

Insight into some of the problems associated with the electron-electron interactions within and between the electron configurations of complex atoms may be obtained by studying the results obtained from some approximate atomic model. Such a model is furnished by the nonrelativistic Hartree-Fock (HF) approximation.

The various one- and two-electron interaction integrals of the traditional Slater theory¹ may be estimated provided one has reasonably accurate knowledge of the radial wavefunctions (and hence radial charge distribution). The HF radial wavefunctions used here are those developed within the framework of the central field approximation and are obtained by procedures based on the variation principle and restricted by the usual conditions of integrability and smoothness. The various electrostatic and magnetic interaction and transition integrals may then be computed for any specified configuration (or set of configurations) for any chosen atom or ion. In many cases, comparison is possible with corresponding quantities that have been derived empirically as parameters. In the HF approximation without configuration mixing, the computed quantities correspond to those for a pure configuration, with relativistic and correlation effects omitted, while the empirical quantities have absorbed other effects (such as cumulative effects of weak configuration interaction) which may serve to distort the apparent values of the quantities in question.

Certain quantities are sometimes difficult, if not impossible, to obtain by empirical means. Examples of these are configuration interaction R^k integrals, transition integrals, and the kinetic energy (KE) and one-electron integrals (I_{nl}). These can be estimated by using HF radial functions.

For the study of line intensities, knowledge of the signs, as well as relative magnitudes, of the multipole integrals is of great help in performing detailed analyses. For transition arrays involving mixed configurations, the signs of the R^k integrals are also required. These signs can be obtained by using HF radial functions.

By performing HF calculations for chosen configurations along isoelectronic sequences or for a series of elements of fixed ionization stage, we can investigate regularities (or lack thereof) in detail. Comparison of the HF results for several configurations of a particular ion can reveal, in addition to knowledge of the relative importance of interactions, details of the screening effects caused by electron rearrangement on such quantities as the one-electron integrals and values of the electron density at the nucleus ($|\psi(0)|^2$). Knowledge of the latter are important for the interpretation of isotope and isomer shifts.

This report presents descriptions and source-deck listings of the computer programs (for the ANL CDC-3600) that have been used for such a series of atomic-structure calculations as outlined above.

II. NUMERICAL HARTREE-FOCK (HF) PROGRAM

Since the basic version of this program has been described in detail elsewhere,² we will only give here a few remarks concerning salient features, operational procedures, and notes of changes incorporated. References 1 and 2 are used as a general reference for definitions and notations.

Briefly, the program is a general one which solves the HF equations by an iterative method for a superposition of (up to six) configurations. Solutions may be obtained for average of configuration or for specific terms of a configuration for any open-shell atom or ion. The current program will handle ions of up to 20 orbitals containing s, p, d, and f electrons.

A. Frozen-core Modification

The program has been modified to enable a specified set of outer orbitals to be made self-consistent while the remaining inner orbitals are kept fixed. As input, such frozen-core calculations always require values of the wavefunctions $\bar{P}_i$ and one-electron integrals I_i , obtained from a previous run, for the orbitals to be kept frozen. We have used two alternative modes of operation:

1. Sequential cases--useful for atoms with a small number of orbitals because of run-time considerations. The $\bar{P}_i$'s and I_i 's that form the data for the frozen core are constructed first and are left in the memory as input for following runs.

2. Separate time cases--most useful for heavy-atom calculations. The frozen-core $\bar{P}_i$'s and I_i 's are input as cards which are the output from a previous "core-producing" run.

Input data card 1 now reads:

ATOM, TERM, NWF, NCFG, NF, NG, NR, Z, RHO, H, NO, IORTHO, ITEST, NITT in format (2A6, 5I3, 3F6.0, I6, 3I3).

NITT is the number of wavefunctions to be made self-consistent and must correspond with NITT of card type 8. A nonzero value of NITT causes the $\bar{P}_i$'s and I_i 's either to be taken from the results of a previous run still in the memory, or to be read as card input according to whether the values of IND(I) for the frozen orbitals are +1 or -1. If all wavefunctions NWF are to be made self-consistent, NITT can be equal to zero or NWF.

The subroutine PNCH has been modified to punch the I_i values in one to one, to correspond with those $\bar{P}_i$'s specified to be punched.

After the listing of the HF program (in C below) are two examples of single-configuration input data using the two modes of operation for a frozen-core calculation.

B. Other Changes

ITEST has been added to card 1 in order to handle single orbital cases whose eigenvalues are less than 0.9. If ITEST = 1, then the call to SOLVES in SOLVE is bypassed. This is necessary for such cases, since SOLVES fails for a homogeneous equation; for example, $1s^2$ of H^- and $2p^2$ of HeI would both require ITEST set equal to 1.

Values of the one-electron integrals (I_i) and kinetic energies (KE) are now computed and listed by the subroutine ENERGY. Values of the Slater F^k and G^k integrals are listed in cm^{-1} instead of atomic units. Additional decimal places have been added to the listed total energy and eigenvalues.

To the DATA statements of the subroutine SPIN have been added the coefficients of the V^k and N^k integrals for f-f and d-f type magnetic interactions. These coefficients were omitted from Table I of Blume and Watson³ (also from Ref. 2), but are readily calculated by means of Eq. 18 of Ref. 3.

It was also thought desirable to list in detail the various contributions to the values of the spin-orbit integrals. In addition to the values of $M^O(ab)$, $N^k(ab)$, and $V^k(ab)$ being given, we also list the corresponding values of $M^O(ba)$, $N^k(ba)$, and $V^k(ba)$. The values of this first integral

(with exchanged orbitals) cannot be obtained by symmetry properties. Thus the given values allow us to relate the two different M^k integrals defined by

$$M^k(ab) = \frac{1}{2}[M^k(ab) + M^k(ba)],$$

where the M^k on the left of the equal sign is that defined by Marvin,⁴ and the ones on the right are those defined by Blume and Watson³ and calculated here.

To keep track of computing times such as for multiple run cases, we have added a time check feature to several of the strategic subroutines.

Values of σ , ϵ , and AZ obtained, often with little difficulty, using the Herman and Skillman program are usually sufficient to form good initial estimates for input data. To obtain σ , we must obtain values of $\langle r \rangle$. These may be computed from the Herman and Skillman output⁵ by using a routine such as HFSRPOL described in Section IV.B of this report.

C. Listing of HF Program

A page guide to the subroutines of the HF program precedes the listing of the actual program.

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```

PROGRAM MAIN
C   HARTREE-FOCK SCF ATOMIC STRUCTURE CALCULATION
C   WRITTEN BY DR CHARLOTTE FROESE.
C   MODIFICATIONS (CDC-3600) ARGONNE NATL LAB JUNE 1967
C   SPIN DATA ADDITIONS
C   I(NL) AND KINETIC ENERGY VALUES
C   MODIFIED TO CALCULATE WITH FROZEN CORE
      INTEGER ASTER
      LOGICAL FAIL,RSCAN
      COMMON ATOM,TERM,NWF,Z,RHO,H,NO,D(100),ACC(20),DD(80),E(20,20) ,
1 DUMMY(13472) /TEST/FAIL,RSCAN(20)/SCRAP/DDD(200)
      EQUIVALENCE (IRHO,RHO)
      COMMON /CORE/ IB,EC(20)
      DATA (ASTER = 1H*)
      YTIME = TIMELEFT(TDUMMY)
      PRINT 9998, YTIME
9998 FORMAT(1H0,* INITIAL TIME * E20.8/)
1   FAIL = .FALSE.
11  ET = 0.
      DO 4 I=1,20
      DO 4 J = 1,20
      IF (I .NE. J) E(I,J) = 0.
4   CONTINUE
      CALL DATA(NP)
      READ 2,NSW,NINC,NIT,ID
2   FORMAT(4I3)
      IF (IB.GT. NWF) GO TO 77
      NITT = NWF +1 - IB
      NIT = NITT
77  CONTINUE
      PRINT 22,NINC,NIT,RHO,H,NO
22  FORMAT(/9X,23HCOMPUTATIONAL PROCEDURE //9X,
1 8HTHE LAST 13,22H GROUPS ARE INCOMPLETE/9X,
2 8HTHE LAST 13,29H WILL BE MADE SELF-CONSISTENT. //
3 20X,5HRHO = F12.7/20X,5HH = F12.7/20X,5HNO = 14)
      IB = NWF - NIT + 1
      IRHO = NP
13 PRINT 14,ATOM,TERM
14  FORMAT(1H1,20X,2A6)
      IF (NSW .EQ. 0) GO TO 5
      IL = NWF - NINC
      CALL SCF(IB,IL)
      IF (FAIL) GO TO 8
5   IL = NWF
      DO 7 I=1,4
      CALL SCF(IB,IL)
      IF (FAIL) GO TO 8
      CALL DIAG(ET,DELTA E,ID)
      IF (ABS(DELTA E/ET) .LT. 1.E-6) GO TO 8

```

```

7    CALL ARRAY
    PRINT 9
9    FORMAT(1H1,10X,40HCONFIGURATION INTERACTION NOT CONVERGING )
    YTIME = TIMELEFT(TDUMMY)
    PRINT 9999, YTIME
9999 FORMAT(1H0,* FROM MAIN * E20.8/)
    GO TO 6
8    CALL PRNT
    CALL ENERGY
    CALL RADIUS
    CALL ORTHO
    CALL PNCH
    READ 10,NEXT,ATOM,ZZ,(ACC(I), I=1,NWF)
10   FORMAT(1X,I2,A6,F6.0,20F3.1)
    IF (NEXT .EQ. 0) GO TO 11
    CALL SCALE(ZZ)
    GO TO 13
6    READ 12,NEXT
12   FORMAT(A1)
    IF (NEXT .EQ. ASTER) GO TO 1
    GO TO 6
    END

```

```

SUBROUTINE DATA(NP)
LOGICAL FAIL,RSCAN
COMMON ATOM,TERM,NWF,Z,RHO,H,NO,EL(20),N(20),L(20),S(20),AZ(20),
1    ACC(20),D(60),IND(20),E(20,20),DD(10000),ED,AZD,DDD(3200),NF,
2    NG,CFG(10),KFG(10),IFG(10),NCI(10),JFG(10),NCJ(10),NR,CR(10),
3    KR(10),I1R(10),I2R(10),NCRI(10),J1R(10),J2R(10),NCRJ(10),NCFG,
4    WT(6),QC(20,6)/TEST/FAIL,RSCAN(20)/SCRAP/CONFIG(2),NFG,I1,I2,J1,J2
COMMON/T SOLVE/ ITEST
COMMON /CORE/ IB,EC(20)
DIMENSION EK(20)
EQUIVALENCE (EK(1),IND(1) )
READ 1,ATOM,TERM,NWF,NCFG,NF,NG,NR,Z,RHO,H,NO,IORTHO,ITEST,NITT
1    FORMAT(2A6,5I3,3F6.0,16,3I3)
    IB = NWF - NITT + 1
    IBB = IB - 1
22   CONTINUE
    IF (EOF,60) 70,71
70   CALL EXIT
71   PRINT 2, ATOM, TERM, Z
2    FORMAT(1H1///9X,33HHARTREE-FOCK WAVE FUNCTIONS FOR 2A6.5X,
1    3H(Z= ,F4.0,1X,1H) //27X,13HCONFIGURATION,15X,6HWEIGHT//)
    DO 3 I=1,NCFG
    READ 4,CONFIG,WT(I)
4    FORMAT(2A6,F10.8)
3    PRINT 5,I,CONFIG,WT(I)
5    FORMAT(24X,I2,6X,2A6,F19.8)
    PRINT 6
6    FORMAT(//9X,4HDATA,14X,13HWAVE FUNCTION,4X,17HINITIAL ESTIMATES,

```

```

1  17X36HNUMBER OF ELECTRONS IN CONFIGURATION/28X,2HNL,4X5HSIGMA,
2  6X,5HE(NL),5X6HAZ(NL),4X,3HACC,4X,3HOPT,6X
3  26H1  2  3  4  5  6  //)
  NP = NWF + IORTHO
  DO 9 I=1,NP
    READ 7,EL(I),N(I),L(I),S(I),ED,AZD,ACC(I),IND(I),
1   (QC(I,J),J=1,NCFG)
7   FORMAT(A3,2I3,F6.2,2F9.6,F3.1,I3,6F3.0)
    PRINT 8,I,EL(I),S(I),ED,AZD,ACC(I),IND(I),(QC(I,J), J=1,NCFG)
8   FORMAT(24X,I2,1X,A3,F9.2,F11.4,F11.3,F6.1,I6,4X,6F5.0)
    IF (IND(I) .EQ. 1) GO TO 9
    E(I,I) = ED
    AZ(I) = AZD
9   RSCAN = .TRUE.
    PRINT 10
10  FORMAT(/9X,9HENERGY = 9X,I2HE(AVERAGE) + //)
    NFG = NF + NG
    IF (NFG .EQ. 0) GO TO 13
    DO 20 I=1,NFG
      READ 11,CFG(I),X,KFG(I),IFG(I),NCI(I),JFG(I),NCJ(I)
11  FORMAT(F12.8,A1,I1,1X,2I2,1X,2I2)
      I1 = IFG(I)
      I2 = JFG(I)
20  PRINT 12,CFG(I),NCI(I),NCJ(I),X,KFG(I),EL(I1),EL(I2)
12  FORMAT(26X,F14.8,3H*C(I1,4H)*C(I1,2H) A1,I1,1H(A3,1H,A3,1H))
13  IF (NR .EQ. 0) GO TO 17
      DO 14 I=1,NR
        READ 15,CR(I),KR(I),I1R(I),I2R(I),NCRI(I),J1R(I),J2R(I),NCRJ(I)
15  FORMAT(F12.8,1X,I1,1X,3I2,1X,3I2)
        I1 = I1R(I)
        I2 = I2R(I)
        J1 = J1R(I)
        J2 = J2R(I)
        PRINT 16,CR(I),NCRI(I),NCRJ(I),KR(I),EL(I1),EL(I2),EL(J1),EL(J2)
16  FORMAT(26X,F14.8,3H*C(I1,4H)*C(I1,3H) R,I1,1H(2A3,1H,2A3,1H))
        RSCAN(I1) = .FALSE.
        RSCAN(I2) = .FALSE.
        RSCAN(J1) = .FALSE.
14  RSCAN(J2) = .FALSE.
17  CALL ARRAY
      CALL WAVEFN(NP)
      IF (NITT .EQ. 0) RETURN
      IF (IND(I) .EQ.1 .AND. IB.NE. 1) GO TO 19
      IF ( IB .EQ. 1) RETURN
      READ 18, (EK(I), I=1,IBB)
18  FORMAT (5E16.8)
      RETURN
19  DO 21 I = 1, IBB
21  EK(I) = EC(I)
      RETURN
      END

```

SUBROUTINE ARRAY

COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(100),SUM(20),

1 DD(10422),A(20,20,4),B(20,20,4),NF,NG,CFG(10),KFG(10),IFG(10),

2 NCI(10),JFG(10),NCJ(10),NR,CR(10),KR(10),I1P(10),I2R(10),

3 NCRI(10),J1R(10),J2R(10),NCRJ(10),NCFG,WT(6),QC(20,6)/COEFF/

4 CA(3,3),CB(4,4,4)/SCRAP/C,CC,CON,LI,LJ,NI,NJ,I1,IJ,NL,KL,NFP

DATA (((CA(I,J), I=1,3), J=1,3) = .08,.0317460317,.0205128205,

1 0.0,.0317460317,.013986014,2(0.0),.0179307871), (((CB(I,J,K),

2 I=1,4), J=1,4), K=1,4) = .5,.1666666667,.1,.0714285714,2(.1666666

3667),.0666666667,.0428571429,.1,.0666666667,.1,.0428571429,.071428

45714,2(0.0428571429),.0714285714,5(0.0),.0666666667,.0428571429,

5.0317460317,0.0,.0428571429,.028571428,.019047619,0.0,.0317460317,

62(.019047619),10(0.0),.028571428,.0216450216,2(0.0),.0216450216,

7.012987013,15(0.0),.0166500167)

DO 1 I=1,NWF

SUM(I) = 0.

DO 1 J=1,NWF

DO 1 K=1,4

A(I,J,K) = 0.

B(I,J,K) = 0.

DO 2 K =1,NCFG

C = WT(K)**2

DO 3 I=1,NWF

IF (QC(I,K) .EQ. 0.) GO TO 3

LI = L(I)+1

DO 4 J=1,NWF

IF (QC(J,K) .EQ. 0.) GO TO 4

LJ = L(J)+1

IF (I .NE. J) GO TO 5

CC = C*QC(I,K)*(QC(I,K) - 1.)

A(I,I,1) = A(I,I,1) + CC

IF (LI .EQ. 1) GO TO 4

DO 8 KL = 2,LI

A(I,I,KL) = A(I,I,KL) - CC*CA(LI-1,KL-1)

GO TO 4

CC = C*QC(I,K)*QC(J,K)

A(I,J,1) = A(I,J,1) + CC

DO 9 KL =1,4

B(I,J,KL) = B(I,J,KL) - CC*CB(LI,LJ,KL)

CONTINUE

SUM(I) = SUM(I) + C*QC(I,K)

CONTINUE

IF (NF .EQ. 0) GO TO 10

DO 11 I=1,NF

K = KFG(I)/2 + 1

NI = NCI(I)

NJ = NCJ(I)

CON = CFG(I)*WT(NI)*WT(NJ)

I1 = IFG(I)

IJ = JFG(I)

A(I1,IJ,K) = A(I1,IJ,K) + CON

A(IJ,I1,K) = A(IJ,I1,K) + CON

IF (NG .EQ. 0) GO TO 12

```

NL = NF + NG
NFP = NF + 1
DO 13 I = NFP, NL
  II = IFG(I)
  IJ = JFG(I)
  NI = NCI(I)
  NJ = NCJ(I)
  LI = L(II)
  LJ = L(IJ)
  KL = (KFG(I) - IABS(LI - LJ))/2 + 1
  CON = CFG(I)*WT(NI)*WT(NJ)
  B(II,IJ,KL) = B(II,IJ,KL) + CON
13  B(IJ,II,KL) = B(IJ,II,KL) + CON
12  DO 14 I = 1, NWF
    DO 14 J = 1, NWF
      DO 14 K = 1, 4
        A(I,J,K) = A(I,J,K)/SUM(I)
14  B(I,J,K) = B(I,J,K)/SUM(I)
    RETURN
  END

```

```

SUBROUTINE WAVEFN(NP)
COMMON ATOM, TERM, NWF, Z, RHO, H, NO, EL(20), N(20), L(20), S(20), AZ(20),
1  D(80), IND(20), E(20,20), R(200), RR(200), R2(200), P(20,200),
2  Y(20,200), YK(200), YR(200), X(200), ATM(20), TRM(20), ZZ(20)
DIMENSION MAX(20)
EQUIVALENCE (MAX(1), D(21))
DO 1 I = 1, NO
  R(I) = EXP(RHO)/Z
  RR(I) = R(I)*R(I)
  R2(I) = SQRT(R(I))
1  RHO = RHO + H
  RHO = RHO - FLOAT(NO)*H
  DO 9 I = 1, NP
    MAX(I) = NO
    PN = HNORM(N(I), L(I), Z-S(I))
    IF (IND(I)) 7, 8, 9
7  READ 10, ATM(I), TRM(I), M, ZZ(I), (P(I,J), J=1, M)
10  FORMAT(6X, A6, 6X, A6, 11X, I6, F6.0/(7F11.7))
    Z2 = Z/ZZ(I)
    DO 11 J = 1, M
11  P(I,J) = R(I,J)*Z2
    IF (M.EQ. NO) GO TO 24
    MAX(I) = M
    M = M + 1
    DO 13 J = M, NO
13  P(I,J) = 0.
    IF (I - NWF) 24, 24, 9
8  DO 3 J = 1, NO
3  P(I,J) = PN*HWF(N(I), L(I), Z-S(I), R(J))/R2(J)
24  IF (AZ(I) .GT. 0.) GO TO 4
  FN = N(I)

```

```

      AZ(I) = PN*(2.*(Z-.6*S(I))/FN)**(L(I) + 1)
4    CALL YKF(I,I,0)
      DO 2 J= 1,N0
2    Y(I,J) = YK(J)
9    CONTINUE
      PRINT 14
14   FORMAT(1H1,8X18HINITIAL ESTIMATES
1    /10X2HNL,4X5HSIGMA,6X5HE(NL),4X6HAZ(NL),4X13HWAVE FUNCTION //)
      DO 15 I = 1,NWF
      IF (E(I,I) .NE. 0.) GO TO 22
      FN = N(I)
      E(I,I) = ((Z-S(I))/FN)**2 + 2.*S(I)*QUADR(I,I,-1) -E(KIN(I,I))
22  IF (IND(I)) 16,17,18
17  PRINT 19,EL(I),S(I),E(I,I),AZ(I)
19  FORMAT(9X,A3,F9.2,F11.3,F10.3,4X,19HSCREENED HYDROGENIC)
      GO TO 15
16  PRINT 20,EL(I),S(I),E(I,I),AZ(I),ATM(I),TRM(I)
20  FORMAT(9X,A3,F9.2,F11.3,F10.3,4X, 8HSCALED A6 ,A6)
      GO TO 15
18  PRINT 21,EL(I),S(I),E(I,I),AZ(I),ATOM,TERM
21  FORMAT(9X,A3,F9.2,F11.3,F10.3,4X,11HSAME AS FOR A6,A6)
15  CONTINUE
      RETURN
      END

```

```

      FUNCTION HWF(N,L,Z,R)
      FN = N
      M = N+L
      K = N-L-1
      K1=K
      M1=M
      P = 1.
      A = 1.
      B = K1
      C = M1
      X = -2.*Z*R/FN
      IF (K1) 1,2,3
3    DO 4 I = 1,K1
      P = 1. + A/B*P/C*X
      A = A+1.
      B = B-1.
4    C = C-1.
2    HWF = P*EXP (X/2.)*(-X)**(L+1)
      RETURN
1    PRINT 7,N,L,Z,R
7    FORMAT(51H FORBIDDEN COMBINATION OF N AND L IN HWF SUBPROGRAM/
1    4H N = I4.6H L = I4.6H Z = F6.1.6H R = F8.4)
      YTIME = TIMELEFT(TDUMMY)
      PRINT 9999, YTIME
9999 FORMAT(1H0,* FROM HWF * E20.8/)
      STOP
      END

```

```

      FUNCTION HNORM(N,L,Z)
      M = L + L + 1
      A = N + L
      B = M
      T = A
      D = B
      FN = N
      M = M - 1
      IF (M .EQ. 0) GO TO 2
      DO 1 I = 1,M
      A = A - 1.
      B = B - 1.
      T = T*A
1 D = D*B
2 HNORM = SQRT (Z*T)/(FN*D)
      RETURN
      END

```

```

      FUNCTION QUADR(I,J,KK)
      COMMON DD(3),Z,NP,H,NO,EN(40),L(20),DDD(60),MAX(20),DX(460),
1 R(200),RR(400),P(20,200)
      H3 = H/1.5
      K = KK + 2
      DEN = L(I) + L(J) + 1 + K
      FACT = (1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
      D = P(I,1)*P(J,1)*R(1)**K*((1.+Z*R(1)*FACT)/(DEN*H3)+.5)
      M = MAX0 (MAX(I),MAX(J)) - 1
      DO 1 JJ = 2,M,2
      JP = JJ + 1
1 D = D + 2.*P(I,JJ)*P(J,JJ)*R(JJ)**K+P(I,JP)*P(J,JP)*R(JP)**K
      QUADR = D*H3
      RETURN
      END

```

```

SUBROUTINE YKF(I,J,K)
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(60),MAX(20),
1 DD(460),R(200),RR(200),R2(200),P(20,200),Y(20,200),YK(200)
CALL ZK(I,J,K)
C = EXP(-H)
A = 4.*C**(K+1)
AA = A*A/16.
C = 2*K+1
H3 = C*H/3.
F1 = YK(NO)
F2 = YK(NO-1)
DO 9 MM = 3,NO
M = NO -MM+1
F3 = YK(M)
YK(M) = YK(M+2)*AA + H3*(F3 + A*F2 + AA*F1)
F1 = F2
9 F2 = F3
IF (IABS(I-J) + K .NE. 0) GO TO 10
MX = MAX(1)
IF (MX .GE. NO) GO TO 13
MP = MX + 1
DO 14 M = MP,NO
14 YK(M) = 1.
13 A = (1. - YK(MX))/FLOAT (MX)
DO 15 M = 1,MX
FM = M
15 YK(M) = YK(M) + A*FM
10 RETURN
END

```

```

SUBROUTINE ZK(I,J,K)
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(540),R(200),
1 RR(200),R2(200),P(20,200),Y(20,200),YK(200)
DEN = L(I) + L(J) + 3+ K
FACT= (1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
DO 1 JJ = 1,2
1 YK(JJ) = RR(JJ)*P(I,JJ)*P(J,JJ)/DEN*(1.+ Z*R(JJ)*FACT)
C = EXP (-H)
H3 = H/3.
A = C**K
AA = A*A
A = 4.*A
F1 = RR(1)*P(I,1)*P(J,1)
F2 = RR(2)*P(I,2)*P(J,2)
DO 8 M = 3,NO
F3 = RR(M)*P(I,M)*P(J,M)
YK(M) = YK(M-2)*AA + H3*(F3 + A*F2 + AA*F1)
F1 = F2
8 F2 = F3
RETURN
END

```



```

SUBROUTINE SCF(IB,IL)
LOGICAL FAIL
COMMON ATOM,TERM,NWF,Z,DD(143),DPM(20)/TEST/FAIL
CALL GRANGE
PRINT 1
1  FORMAT(///30X,2HED,15X,3HAZD,10X,5HPNORM)
   Z2 = 2.E-7*SQRT(Z*FLOAT(NWF))
   DO 3 J = IB,IL
     CALL SOLVE(J)
     IF (FAIL) GO TO 20
3  CONTINUE
   IC = IL + 3 - IB + ((IL - IB)**2)/8
   DO 6 I = 1,8
     DO 7 II = 1,IC
       D = 0.
       DO 5 J = IB,IL
         IF (D.GT.DPM(J)) GO TO 5
         JJ = J
         D = DPM(J)
5      CONTINUE
         IF (D.LT.Z2) GO TO 11
         CALL SOLVE(JJ)
         IF (FAIL) GO TO 20
7      CONTINUE
         CALL GRANGE
         PRINT 1
11     D = 0.
         DO 8 J = IB,IL
           CALL SOLVE(J)
           IF (FAIL) GO TO 20
8         D = AMAX1(D,DPM(J))
           IF (D.LT.Z2) GO TO 20
6         Z2 = Z2 + Z2
         PRINT 10
10        FORMAT(1H1,20X,30HSCF ITERATIONS NOT CONVERGING )
         YTIME = TIMELEFT(TDUMMY)
         PRINT 9999, YTIME
9999      FORMAT(1H0,* FROM SCF * E20.8/)
         FAIL = .TRUE.
20        RETURN
      END

```

```

SUBROUTINE GRANGE
COMMON ATOM,TERM,NWF,Z,NP,DD(22),N(20),L(20),DDD(60),MAX(20),
1  DPM(20),SUM(20),EK(20),E(20,20),R(600),P(20,200)/SCRAP/D,DI,DJ,
2  IL,QI,QJ,MX,G
COMMON /CORE/IB,EC(20)
IF(NWF .EQ. 1 .OR. IB .EQ. NWF ) GO TO 1
DO 2 I= IB , NWF
  IL = I-1
  DO 3 J=1,IL
    IF (L(I) .NE. L(J)) GO TO 3
    IF (N(I) .EQ. N(J)) GO TO 3
    QI = SUM(I)
    QJ = SUM(J)
    IF (ABS(QI-QJ) .LT. 1.E-6) GO TO 3
    MX = MAX0(MAX(I),MAX(J))
    D = QUADR(I,J,0)
    IF (J.LT.IB) GO TO 10
    DO 11 K = 1,MX
      P(I,K) = P(I,K) - D*P(J,K)
    DI = SQRT(QUADR(I,I,0))
    DO 12 K = 1,MX
      P(I,K) = P(I,K)/DI
    GO TO 13
  10  D = -D/(1./QI + 1./QJ)
    DI = D/QI
    DJ = D/QJ
    DO 4 K=1,MX
      P(J,K) = P(J,K) + DJ*P(I,K)
    4  P(I,K) = P(I,K) + DI*P(J,K)
    DI = SQRT(QUADR(I,I,0))
    DJ = SQRT(QUADR(J,J,0))
    DO 5 K=1,MX
      P(I,K) = P(I,K)/DI
    5  P(J,K) = P(J,K)/DJ
  13  G = (EKIN(J,I) - EKIN(I,J))/(QJ - QI)
    E(I,J) = G*QJ
    E(J,I) = G*QI
  3  CONTINUE
  2  CONTINUE
  PRINT 6
  6  FORMAT(//10X,28HMATRIX OF ENERGY PARAMTERS )
  DO 7 I = 1,NWF
  7  PRINT 8,(E(I,J), J=1,NP)
  8  FORMAT (10X,10F12.6/10X,10F12.6)
  1  RETURN
  END

```

```

FUNCTION EKIN(I,II)
COMMON ATOM,TERM,NWF,Z, NP,H,NO,D(600),R(200),RR(200),R2(200),
1 P(20,200),Y(20,200),YK(200),YR(200),X(200)
CALL XCH(I,2)
CALL POTL(I)
DO 1 J=1,NO
YK(J) = YR(J)
1 YR(J) = P(II,J)
EKIN = 2.*QUADS(I,II,1) + QUAD(II,NO,YR,X)
RETURN
END

```

```

SUBROUTINE SOLVE(I)
LOGICAL FAIL
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),S(20),AZ(20),
1 ACC(20),MAX(20),DPM(20),D(40),E(20,20),R(200),RR(200),R2(200),
2 P(20,200),Y(20,200),YK(200),YR(200),X(200),PDE(200),DD(600),
3 ED,AZD/TEST/FAIL
COMMON/TSOLVE/ITEST
CALL POTL(I)
CALL XCH(I,3)
ED = E(I,I)
AZD = AZ(I)
A1 = 0.
DN1 = 0.
DER1 = 0.
FN = N(I)
FL = L(I)
RJ = (3.*FN*FN - FL*(FL+1.))/(2.*(Z - S(I)))
NJ = ALOG (RJ/R(1))/H - 2.
ETOL = .000001*(Z - S(I))**2
PTOL = .000001*FN
V = YR(1)/R(1)
C = 4.*FL + 6.
CN = (2.*Z/FN)**(L(I) + 1)
CD = (FL+.5)**2
DO 25 J = 1,NO
25 YK(J) = -2.*(Z-YR(J))*R(J) + CD
XX = X(1)/C
XP = X(2)/C
ND = NO - 1
CH= H*H/12.
X1 = X(1)
X2 = X(2)
DO 1 J = 2,ND
X3 = X(J+1)
X(J) = CH*(X1 + 10.*X2 + X3)
X1 = X2
1 X2 = X3
IF (ITEST .EQ. 1) GO TO 99
IF (ED .LT. .9) GO TO 31
99 DO 16 NA = 1,10

```

```

DO 13 NCOUNT = 1,10
  B3 = (      V + V + ED - (Z/FN)**2)/C
  B4 = Z*(FL+1.333333)/((FL+1.)*(FL+2.))
DO 5 J = 1,2
  HW = HWF(N(I),L(I),Z,R(J))/CN
5  PDE(J) = AZD*(HW + R(J)**(L(I)+3)*B3*(1.-R(J)*B4))/P2(J)
  PDE(1) = PDE(1) + XX
  PDE(2) = PDE(2) + XP
  DO 6 J=1,NO
6  YR(J) = (YK(J) + ED*RR(J))*CH
  CALL NMRVS(NJ,DELTA,M,PDE,X)
  PNORM = QUAD(I,M,PDE,PDE)
  Y1 = PDE(NJ-1)
  Y2= PDE(NJ)
  Y3 = PDE(NJ+1)
  DELTA = (Y2 - Y1) + (Y2 - Y3) + 10.*YR(NJ)*Y2 + YR(NJ-1)*Y1 +
1  YR(NJ+1)*Y3 + X(NJ)
  DELTAE = Y2*DELTA/(H*PNORM)
  ED = ED - DELTAE
  IF (ED .LT. 0.) ED = .8*(ED + DELTAE)
  IF (ABS(DELTAE) .LE. ETOL) GO TO 12
13 CONTINUE
  PRINT 22
22  FORMAT(/50H ENERGY ITERATION IN SOLVE ROUTINE NOT CONVERGING )
  FAIL = .TRUE.
  RETURN
12  PN2 = SQRT( PNORM)
  DER2 = (AZD - A1)/(PN1 - PN2)
  IF (DER1 .EQ. 0.) DER1 = DER2
  AZ(I) = AZD + (PN2 - 1.)*(DER1 + DER2)/2.
  IF (AZ(I) .GT. 0.) GO TO 35
  AZ(I) = .8*AZD
  A1 = 0.
  PN1 = 0.
  DER1 = 0.
  GO TO 36
35  A1 = AZD
  PN1 = PN2
  DER1 = DER2
36  AZD = AZ(I)
  IF (ABS(PN2 - 1.) .LE. PTOL) GO TO 51
16 CONTINUE
31  CALL SOLVES(I,XX,XP,V,NJ,M)
  MAX(I) = M
  C=AMAX1(.5,ACC(I))
  AZ(I)=C*AZ(I)+(1. - C)*AZD
  CALL PADJ(I,AMAX1(.5,ACC(I)))
  RETURN
51  MAX(I) = M
  CALL PADJ(I,ACC(I))
  PRINT 14,EL(I),ED,AZD,PN2
14  FORMAT( 20X,A3,2F15.7,F12.7)
  RETURN
  END

```

```

SUBROUTINE SOLVES(I,XY,XP,V,NJ,M)
  DIMENSION ZERO(200),HQ(200)
  LOGICAL FAIL
  COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),W(540),R(200),
1  RR(200),R2(200),DD(8000),YK(200),YR(200),X(200),PDE(200),
2  XX(200),Q1(200),Q2(200),ED,AZD/TEST/FAIL
  EQUIVALENCE (PDE,HQ)
  DATA ((ZERO(I), I=1,200)= 200(0.0))
  FN = N(1)
  FL = L(1)
  C = 4.*FL +6.
  CN = (2.*Z/FN)**(L(1) +1)
  CH = H*H/12.
  DO 26 J = 1,NO
26 YR(J) = (YK(J) + ED*RR(J))*CH
  B3 = (V + V + ED - (Z/FN)**2)/C
  B4 = Z*(FL+1.333333)/((FL+1.)*(FL+2.))
  DO 5 J = 1,2
  HW = HWF(N(1),L(1),Z,R(J))/CN
  5 HQ(J) = AZD*(HW + R(J)**(L(1)+3)*B3*(1.-R(J)*B4))/P2(J)
  CALL NMRVS(NJ,DELH,MH,HQ,ZERO)
  Q1(1) = HQ(1) + XY
  Q1(2) = HQ(2) + XP
  CALL NMRVS(NJ,DEL1,M1,Q1,X)
  AP = -DEL1/DELH
  M = MAX0 (MH,M1)
  DO 7 J = 1,M
  7 Q1(J) = Q1(J) + AP*HQ(J)
  X1 = Q1(1)*RR(1)
  X2 = Q1(2)*RR(2)
  Q2(1) = X1/C
  Q2(2) = X2/C
  DO 8 J = 3,NO
  X3 = Q1(J)*RR(J)
  XX(J-1) = (10.*X2 +(X1+X3))*CH
  X1 = X2
  8 X2 = X3
  CALL NMRVS(NJ,DEL2,M2,Q2,XX)
  AA = -DEL2/DELH
  M = MAX0 (M,M2)
  DO 9 J = 1,M
  9 Q2(J) = Q2(J) + AA*HQ(J)
  A2 = QUAD(1,M,Q1,Q1)
  A3 = QUAD(1,M,Q1,Q2)
  A4 = QUAD(1,M,Q2,Q2)
  D = A3*A3 + A4*(1. - A2)
  IF (D .GE. 0.) GO TO 41
  ED = ED + A3*(1. - SQRT (A2))/A4
  PRINT 62
62 FORMAT(///20X,35HFAILURE IN SOLVES ENERGY ADJUSTMENT )
  YTIME = TIMELEFT(TDUMMY)
  PRINT 9999, YTIME
9999 FORMAT(1H0,*, FROM SOLVES *, E20.8/)
  FAIL = .TRUE.

```

```

RETURN
41 D = SQRT (D)
   BETA1 = (-A3 + D)/A4
   BETA2 = (-A3 -D)/A4
   DE1 = BETA1*A3/(A4*BETA1 + A3)
   DE2 = BETA2*A3/(A4*BETA2 + A3)
   Y1 = Q1(1) + BETA1*Q2(1)
   Y2 = Q1(1) + BETA2*Q2(1)
   BETA = BETA1
   DELTAE = DE1
   IF (Y1 .GT. 0. .AND. Y2 .LE. 0.) GO TO 48
   IF (Y1 .LE. 0. .AND. Y2 .GT. 0.) GO TO 18
   IF (ABS(DE1) .LT. ABS(DE2)) GO TO 48
18  BETA = BETA2
   DELTAE = DE2
48  ED = ED + DELTAE
   YY = AZD*(1. + AP + BETA*AA)
   PN = SQRT (A2+ BETA*(A3+A3+BETA*A4))
   DO 35 J = 1,NO
35  PDE(J) = (Q1(J)+ BETA*Q2(J))/PN
   AZD = YY/PN
   PRINT 31,EL(1),ED,AZD,PN
31  FORMAT(20X,A3,2F15.7,F12.7,1H*)
   RETURN
   END

```

```

SUBROUTINE PADJ(I,C)
COMMON D(6),NO,DD(120),MAX(20),DPM(20),EK(40),E(20,20),R(400),
1  R2(200),P(20,200),Y(20,200),YK(200),YR(400),PDE(200),XX(600),
2  ED,AZD
   MI = NO
   IF (C .EQ. 0.) MI = MAX(I)
   DPM(I) = 0.
   DO 1 J = 1,MI
   DIFF = P(I,J)-PDE(J)
   DPM(I) = AMAX1 (DPM(I),ABS (DIFF)*R2(J))
1  P(I,J) = PDE(J) + C*DIFF
   IF (MI .EQ. NO) GO TO 6
   M = MI + 1
   DO 4 J = M ,NO
4  P(I,J) = 0.
6  IF ( C .EQ. 0.) GO TO 8
   PNORM = SQRT (QUADR(I,1,0))
   DO 10 J=1,MI
10  P(I,J) = P(I,J)/PNORM
8  CALL YKF(I,1,0)
   DO 11 J=1,NO
11  Y(I,J) = YK(J)
   E(I,1) = C*E(I,1) + (1. - C)*ED
   RETURN
   END

```

```

FUNCTION QUAD(I,M,X,Y)
  DIMENSION X(200),Y(200)
  COMMON DD(5),H,NO,EL(20),N(20),L(20),DDD(740),RR(200)
  FL = L(I)
  D = 1.5/(FL+3.)/H
  QUAD = RR(1)*X(1)*Y(1)*(D-.5)
  DO 1 J = 2,M,2
1  QUAD = QUAD + 2.*RR(J)*X(J)*Y(J) + RR(J-1)*X(J-1)*Y(J+1)
  QUAD = QUAD*H/1.5
  RETURN
END

```

```

SUBROUTINE POTL(I)
  COMMON ATOM,TERM,NWF,Z,RHO,H,NO,EL(20),N(20),L(20),D(5140),
1  Y(20,200),YK(200),YR(200),DD(1002),A(20,20,4)
  DO 1 J=1,NO
1  YR(J) = 0.
  LI = L(I)
  DO 2 J=1,NWF
  IF (A(I,J,1).EQ. 0.) GO TO 2
  DO 3 JJ = 1,NO
3  YR(JJ) = A(I,J,1)*Y(J,JJ) + YR(JJ)
4  DO 5 K = 2,4
  C = A(I,J,K)
  IF (C.EQ. 0.) GO TO 5
  CALL YKF(J,J,2*K-2)
  DO 7 JJ=1,NO
7  YR(JJ) = YR(JJ) + C*YK(JJ)
5  CONTINUE
2  CONTINUE
  RETURN
END

```

```

SUBROUTINE XCH(I,IOPT)
LOGICAL FAIL,RSCAN
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(100),SUM(20),
1   EK(20),E(20,20),R(200),RR(200),R2(200),P(20,200),Y(20,200),
2   YK(200),YR(200),X(200),DD(2402),B(20,20,4),DDD(62),NR,CR(10),
3   KR(10),I1R(10),I2R(10),NCRI(10),J1R(10),J2R(10),NCRJ(10),NCFG,
4WT(6)/TEST/FAIL,RSCAN(20)
DO 1 J=1,NO
1  X(J) = 0.
DO 2 J=1,NWF
DO 3 K=1,4
C = B(I,J,K)*2.
IF (C .EQ. 0.) GO TO 3
CALL YKF(I,J,2*(K-1) + 1,ABS(L(I) - L(J)))
DO 6 JJ =1,NO
6  X(JJ) = X(JJ) + C*YK(JJ)*P(J,JJ)
3  CONTINUE
2  CONTINUE
IF (RSCAN(I)) GO TO 4
DO 10 I1=1,NR
N1 = NCRI(I1)
N2 = NCRJ(I1)
C = WT(N1)*WT(N2)*CR(I1)/SUM(I)
DO 11 I2=1,2
DO 12 I1=1,2
IF (I1R(I1) .NE. 1) GO TO 13
CALL YKF(I2R(I1),J2R(I1),KR(I1))
M = J1R(I1)
DO 14 J=1,NO
14  X(J) = X(J) + C*P(M,J)*YK(J)
13  I11 = I1R(I1)
I1R(I1) = I2R(I1)
I2R(I1) = I11
I11 = J1R(I1)
J1R(I1) = J2R(I1)
12  J2R(I1) = I11
I11 = I1R(I1)
I1R(I1) = J1R(I1)
J1R(I1) = I11
I11 = I2R(I1)
I2R(I1) = J2R(I1)
11  J2R(I1) = I11
10  CONTINUE
4  GO TO (15,16,17), IOPT
16  DO 18 J = 1,NO
18  X(J) = X(J)/R(J)
GO TO 15
17  DO 5 J =1,NO
5  X(J) = R(J)*X(J)
DO 7 J = 1,NP
C = E(I,J)
IF (C .EQ. 0. .OR. (J .EQ. 1)) GO TO 7
DO 9 JJ = 1,NO
9  X(JJ) = X(JJ) + C*P(J,JJ)*RR(JJ)

```


15 7 CONTINUE
RETURN
END

```

SUBROUTINE NMRVS(NJ,DELTA,M,PDE,X)
DIMENSION PDE(200),X(200),A(100),D(100)
COMMON ATOM,TERM,NWF,Z,RHO,H,NO,DD(9400),YR(200)/SCRAP/A,D
C = H*H/12.
TOL = .00000001*Z
Y1 = PDE(1)
Y2 = PDE(2)
G1 = YR(1)
G2 = YR(2)
M = NJ + 1
DO 1 I = 3,M
  G3 = YR(I)
  Y3 = (Y2+Y2-Y1 + (10.*G2*Y2 + G1*Y1) + X(I-1)) / (1. - G3)
  PDE(I) = Y3
  Y1 = Y2
  Y2 = Y3
  G1 = G2
1  G2 = G3
  DELTA = Y3
  K = 1
  PDE(M) = -(1. - G1)*Y1 + X(M)
  G = G3
  A(1) = 1. - G
  D(1) = -(2. + 10.*G)
22  RATIO = A(K)/D(K)
  IF (K .GE. 99 .OR. M .EQ. NO) GO TO 20
  K = K + 1
  M = M + 1
  G = YR(M)
  A(K) = 1. - G
  D(K) = -(2. + 10.*G) - A(K)*RATIO
  PDE(M) = -PDE(M-1)*RATIO + X(M)
  IF (ABS (PDE(M)) - TOL) 20,20,22
20  ED = SQRT (G/C)
  CON = EXP (-H*ED)
  PDE(M) = PDE(M)/(D(K) + CON*(1.- YR(M+1)))
  J = M+1
  DO 2 I = J,NO
2  PDE(I) = 0.
  DO 3 J = 2,K
  I = M-J+1
  II = K-J+1
3  PDE(I) = (PDE(I)-A(II+1)*PDE(I+1))/D(II)
  DELTA = DELTA - PDE(I)
  RETURN
END

```

```

SUBROUTINE DIAG(ETOTAL,DELTA E,ID)
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(120),EK(20),
1  E(20,20),DD(13202),NF,NG,CFG(10),KFG(10),IFG(10),NCI(10),
2  JFG(10),NCJ(10),NR,CR(10),KR(10),I1R(10),I2R(10),NCRI(10),
3  J1R(10),J2R(10),ICRJ(10),NCFG,WT(6),QC(20,6)/COEFF/CA(3,3),
4  CB(4,4,4)/SCRAP/ET(6,6),X(6,6),C,CC,CCC,LI,LJ,IM,N1,N2,NFP,NL,
5  NM,IP,JP,RATIO,CONT,ETPREV,ETL
COMMON /CORE/ IB,EC(20)
DO 1 I = 1, NWF
1  EK(I) = -.5*(E(KIN(I,I)) + E(I,I))
DO 2 II=1,NCFG
DO 3 JJ=1,NCFG
3  ET(II,JJ)= 0.
DO 5 I =1,NWF
C = QC(I,II)
IF (C .EQ. 0.) GO TO 5
ET(II,II) = ET(II,II) + C*EK(I) +.5*C*(C-1.)*FK(I,I,0)
LI = L(I)
IF (LI .EQ. 0) GO TO 6
DO 7 K = 1,LI
7  ET(II,II) = ET(II,II) - CA(LI,K)*C*(C-1.)*FK(I,I,2*K)*.5
6  IF (I .EQ. 1) GO TO 5
IM = I-1
LI = LI+1
DO 8 J=1,IM
CC = C*QC(J,II)
IF (CC .EQ. 0.) GO TO 8
ET(II,II) = ET(II,II) + CC*FK(I,J,0)
LJ = L(J)+1
DO 9 K=1,4
CCC = CB(LI,LJ,K)
IF (CCC .EQ. 0.) GO TO 8
9  ET(II,II) = ET(II,II) - CC*CCC*GK(I,J,2*(K-1)+ IABS(LI-LJ))
8 CONTINUE
5 CONTINUE
2 CONTINUE
IF (NF .EQ. 0) GO TO 10
DO 11 I=1,NF
N1 = NCI(I)
N2 = NCJ(I)
CONT = .5*CFG(I) *FK(IFG(I),JFG(I),KFG(I))
ET(N1,N2) = ET(N1,N2) + CONT
11 ET(N2,N1) = ET(N2,N1) + CONT
10 IF (NG .EQ. 0) GO TO 12
NFP = NF+1
NL = NF + NG
DO 13 I=NFP,NL
N1 = NCI(I)
N2 = NCJ(I)
CONT = .5*CFG(I) *GK(IFG(I),JFG(I),KFG(I))
13 ET(N1,N2) = ET(N1,N2) + CONT
ET(N2,N1) = ET(N2,N1) + CONT
12 IF (NR .EQ. 0) GO TO 14
DO 15 I =1,NR

```

```

N1 = NCRI(1)
N2 = NCRJ(1)
CONT = .5*CR(1) *RK(I1R(1),I2R(1),J1R(1),J2R(1),KP(1))
ET(N1,N2) = ET(N1,N2) + CONT
15 ET(N2,N1) = ET(N2,N1) + CONT
14 IF (NCFG .EQ. 1) GO TO 37
IF (ID .GT. 0) GO TO 38
ETPREV = 0.
DO 30 II=1,5
ETL = 0.
DO 16 I=1,NCFG
CONT = 0.
DO 17 J=1,NCFG
17 CONT = CONT + WT(J)*ET(I,J)
16 ETL = ETL + WT(I)*CONT
DO 18 I=1,NCFG
DO 19 J=1,NCFG
19 X(I,J) = ET(I,J)
18 X(I,I) = X(I,I) - ETL
WT(1) = 1.
WT(2) = -X(2,1)/X(2,2)
IF (NCFG .EQ. 2) GO TO 20
NM = NCFG -1
DO 21 I=2,NM
IP = I+1
DO 21 J=IP,NCFG
RATIO = X(J,I)/X(I,I)
DO 23 K=1,NCFG
23 X(J,K) = X(J,K) - RATIO*X(I,K)
21 CONTINUE
WT(NCFG) = -X(NCFG,1)/X(NCFG,NCFG)
DO 24 I = 2,NM
J = NCFG -I+1
JP = J+1
WT(J) = -X(J,1)
DO 25 K = JP,NCFG
25 WT(J) = WT(J) - X(J,K)*WT(K)
24 WT(J) = WT(J)/X(J,J)
DO 26 I=2,NCFG
26 WT(1) = WT(1) + WT(I)**2
WT(1) = 1./SQRT(WT(1))
DO 27 I=2,NCFG
27 WT(I) = WT(I)*WT(1)
IF (ABS((ETPREV-ETL)/ETL) .LT. 1.E-5) GO TO 31
30 ETPREV = ETL
PRINT 40
40 FORMAT(//10X,47HMATRIX DIAGONALIZATION PROCEDURE NOT CONVERGING )
YTIME = TIMELEFT(TDUMMY)
PRINT 9999, YTIME
9999 FORMAT(1H0,* FROM DIAG * E20.8/)
DELTAE = 0.
GO TO 33
31 DELTAE = ETL -ETOTAL
33 ETOTAL = ETL

```

```

PRINT 32,ETOTAL
32  FORMAT(//10X,15HTOTAL ENERGY = F18.8 )
39 PRINT 34
34  FORMAT(/20X,6HWEIGHT,10X,13HENERGY MATRIX )
DO 35 I=1,NCFG
35 PRINT 36,I,WT(I),(ET(I,J), J=1,I)
36  FORMAT(10X,15,F10.5,5X,6F15.6)
RETURN
37  ETOTAL = ET(1,1)
    DELTAE = 0.
    PRINT 32,ETOTAL
    RETURN
38  DELTAE = 0.
    ETOTAL = ET(1,1)
    GO TO 39
END

```

```

FUNCTION FK(I,J,K)
COMMON D(6),NO,DD(5200),Y(20,200),YK(200)
IF (K .NE. 0) GO TO 1
DO 3 JJ=1,NO
3  YK(JJ) = Y(I,JJ)
GO TO 4
1  CALL YKF(I,I,K)
4  FK = QUADS(J,J,1)
RETURN
END

```

```

FUNCTION GK(I,J,K)
CALL YKF(I,J,K)
GK = QUADS(I,J,1)
RETURN
END

```

```

FUNCTION QUADS(I,J,KK)
COMMON DD(3),Z,NP,H,NO,EN(40), L(20),DDD(60),MAX(20),DX(460),
1  R(200),RR(200),R2(200),P(20,200),Y(20,200),YK(200)
DEN = L(I) + L(J) + 3
H3 = H/1.5
CD=1.5*(1.+Z*R(1))*(1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
K = 2 - KK
D = YK(1)*P(I,1)*P(J,1)*R(1)**K*( CD/(DEN*H) +.5)
ND = MAX0 (MAX(I),MAX(J)) - 1
DO 1 M =2,ND,2
MM = M+1
1  D = D + 2.*YK(M)*P(I,M)*P(J,M)*R(M)**K +YK(MM)*P(I,MM)*P(J,MM)*
1  R(MM)**K
QUADS = D*H3
RETURN
END

```

```

FUNCTION RK(I,J,II,JJ,K)
CALL YKF(I,II,K)
RK = QUADS(J,JJ,1)
RETURN
END

```

```

SUBROUTINE PRNT
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),D(100),MAX(20),DPM(20),
1 DD(440),R(200),RR(200),R2(200),P(20,200)/SCRAP/IWF(5),OUT(5)
READ 1,NPAGE
1 FORMAT(13)
DO 2 I = 1,NPAGE
READ 3,NCOL,(IWF(J), J=1,NCOL)
3 FORMAT(6I3)
MX = 0
DO 4 J = 1,NCOL
IJ = IWF(J)
4 MX = MAX0(MX,MAX(IJ))
PRINT 5,ATOM,TERM
5 FORMAT(1H1,9X19HWAVE FUNCTIONS FOR 2A6 //)
DO 7 JJ= 1,NCOL
IJ = IWF(JJ)
7 OUT(JJ) = EL(IJ)
PRINT 8,(OUT(J), J=1,NCOL)
8 FORMAT(17X1HR, 5(15X,A3))
K = 0
KK = 0
DO 6 J = 1,MX
DO 9 JJ= 1,NCOL
IJ = IWF(JJ)
9 OUT(JJ) = P(IJ,J)*R2(J)
K = K + 1
IF (K .LE. 10) GO TO 6
K = 1
KK = KK + 1
IF (KK .LT. 5) GO TO 21
KK = 0
PRINT 23
23 FORMAT(1H1///)
GO TO 6
21 PRINT 18
18 FORMAT(1X)
6 PRINT 10,R(J),(OUT(JJ),JJ=1,NCOL)
10 FORMAT(F20.5,F20.5,4F18.5)
DO 15 J = 1,NCOL
IJ = IWF(J)
15 OUT(J) = DPM(IJ)
PRINT 16,(OUT(J), J=1,NCOL)
16 FORMAT(//10X, 10HDIFFERENCE F20.6,4F18.6)
2 CONTINUE
RETURN
END

```

```

SUBROUTINE ENERGY
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),D(10542),
1  A(20,20,4),B(20,20,4),DD(62),NR,CR(10),KR(10),I1R(10),I2R(10),
2  NCRJ(10),J1R(10),J2R(10),NCRJ(10)/SCRAP/IW(4),OUT(4),H3,ND,KF,
3  I1,I2,J1,J2
  DIMENSION EK(20)
  DIMENSION EKINP(20)
  COMMON /CORE/ IB,EC(20)
  EQUIVALENCE (EK(1), D(121))
  DATA (DU = 1H )
  H3 = H/1.5
  PRINT 1, ATOM, TERM
1  FORMAT(1H1,9X37HVALUES OF F AND G INTEGRALS FOR ATOM A6,7H TERM
1  A6 //)
  ND = NO-1
  DO 2 I = 1,NWF
  EC(I) = EK(I)
  DO 3 J = 1,NWF
  KF = 0
  DO 6 K = 1,4
  IF (A(I,J,K) .EQ. 0.) GO TO 8
  IW(K) = 2*K - 2
  OUT(K) = FK(I,J,IW(K))
  OUT(K)=OUT(K)*219474.6
6  KF = KF+1
8  IF (KF .NE. 0) PRINT 12,(DU,IW(K),EL(I),EL(J),OUT(K), K=1,KF)
12 FORMAT(4(A1,1HF,I1,2H (,A3,1H,A3,4H ) = F10.1,4X))
  MIN = IABS (L(I)-L(J))
  KF = 0
  DO 13 K=1,4
  IF (B(I,J,K) .EQ. 0.) GO TO 15
  IW(K) = MIN + 2*(K-1)
  OUT(K) = GK(I,J,IW(K))
  OUT(K)=OUT(K)*219474.6
13 KF = KF+1
15 IF (KF .NE. 0) PRINT 19,(DU,IW(K),EL(I),EL(J),OUT(K), K=1,KF)
19 FORMAT(4(A1,1HG,I1,2H (A3,1H,A3,4H ) = F10.1,4X))
18 CONTINUE
3  CONTINUE
2  CONTINUE
  PRINT 99, ATOM, TERM, Z
99  FORMAT (1H1, /24X5HATOM A6,3X5HTERM A6,5X3H(Z= ,F4.0,1X,1H) )
  PRINT 26
26  FORMAT (//,9X,43HONE ELECTRON INTEGRALS AND KINETIC ENERGIES//
1  , 15X, 2HNL,6X5HI(NL), 11X,2HKE/)
  DO 27 I =1, NWF
  EKINP(I) = EK(I) +Z*QU/DR(I,1,-1)
  PRINT 28,EL(I), EK(I), EKINP(I)
28  FORMAT (14X, A3, 2F14.6)
27  CONTINUE
  IF (NR .EQ. 0) GO TO 20
  PRINT 21
21  FORMAT(//9X21HVALUES OF R INTEGRALS //)
  DO 22 I = 1,NR

```

```

      I1 = I1R(I)
      I2 = I2R(I)
      J1 = J1R(I)
      J2 = J2R(I)
      OUT(1) = RK(I1,I2,J1,J2,KR(I))
22 PRINT 23,KR(I),EL(I1),EL(I2),EL(J1),EL(J2),OUT(1)
23   FORMAT(21X,1HR,I1,2H (,2A3,1H, 2A3,4H ) = F10.6 )
20 RETURN
   END

```

```

SUBROUTINE RADIUS
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),S(20),AZ(20),
1D(100),E(20,20)/SCRAP/F3(20),RM,RMM,RH,SC,RMMM,RMMMM,OC(20,6)
COMMON /CORE/ IB,EC(20)
PRINT 1,ATOM,TERM ,Z
1   FORMAT(1H1,24X5HATOM A6,3X5HTERM A6,5X3H(Z=,F4.0,1X,1H) //,68X
   1 13HMEAN VALUE OF/
   2 15X,2HNL,7X5HE(NL),9X6HAZ(NL),6X5HSIGMA,7X1HR,12X4HR**2,
   3 10X6H1/R**3,10X4HR**4)
   PUNCH 3,ATOM,TERM
3   FORMAT(10X,5HATOM ,A6,3X,5HTERM ,A6)
   DO 2 I = 1,NWF
   RM = QUADR(I,I,1)
   RMM = QUADR(I,I,2)
   RMMM=QUADR(I,I,4)
   RH = 3*N(I)*N(I) - L(I)*(L(I) + 1)
   SC = 7 - .5*RH/RM
   RH = 3*N(I)*N(I) - L(I)*(L(I) + 1)
   SC = 7 - .5*RH/RM
   S(I) = SC
   R3(I) = 0.
   IF (L(I) .NE. 0) R3(I) = QUADR(I,I,-3)
   PRINT 4,EL(I),E(I,I),AZ(I),SC,RM,RMM,R3(I),RMMM
4   FORMAT(14X,A3,F15.7,F14.6,F9.3,2F14.6,F14.4,F14.6)
2   CONTINUE
   NIT = NWF +1- IB
   PRINT 5, NIT
5   FORMAT (/20X,8HTHE LAST 13, 3X,20HMADE SELF CONSISTENT )
   CALL SPIN
   RETURN
   END

```

SUBROUTINE SPIN

COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),DD(13885),NCFG,

1 WT(6),QC(20,6)/SCRAP/R3(20),SS(3),QI,QJ,LI,LJ,SP,C,CC

DIMENSION CV(3,4,6), CN(3,4,7)

DATA(CV=-1.0,0.0,0.0, 0.0,-.2,0.0, .2,0.0,-.08571428,0.0,.085714286,0.0,

1 0.0,-.6,0.0, -.6,0.0,-.17142857, 0.0,-.08571428,0.0,.257142857,0.0,

2 -0.02857142857,

3 0.0,0.0,-.42857143, 0.0,-.34285714,0.0, -.51428571,0.0,-.085714285,

4 0.0,-.057142857,0.0,

5 0.0,0.0,0.0, 0.0,0.0,-.23809523, 0.0,-.28571428,0.0, -.476190476,0.0,

6 -0.0649350649,

7 0.0,0.0,0.0, 0.0,0.0,0.0, 0.0,0.0,-.19480519, 0.0,-.259740259,0.0,

8 0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,-0.174825175)

DATA(CN=2.0,0.0,0.0, 0.0,.8,0.0, .8,0.0, .514285714, 0.0,.514285714,0.0,

1 0.0,.1,8,0.0, -1.0,0.0,.85714285, 0.0,-.6,0.0, 1.28571428,0.0,

2 -0.4285714285,

3 -1.0,0.0,1.7142857, 0.0,-.14285714,0.0, -1.6857143,0.0,-.25714285,

4 0.0,-.714285714,0.0,0.0,-1.2,0.0,0.0,-.04761905,0.0,-.17142857,0.0,

5 -2.4761905,0.0,-0.142857142,

6 0.0,0.0,-1.28571428, 0.0,-.34285714,0.0, .51428571,0.0,.033766233,

7 0.0,-.3688311688,0.0,0.0,0.0,0.0,-.47619047,0.0,0.0,.9523809524,

8 0.0,-0.06493506492,

9 0.0,0.0,0.0, 0.0,0.0,0.0, 0.0,0.0,-.19480519, 0.0, .2597402597,0.0)

DATA (B = 4H

PRINT 1

1 FORMAT(//22X,41HDETAILS OF MAGNETIC INTERACTION INTEGRALS /)

DO 2 K = 1,NCFG

DO 7 I = 1,NWF

QI = QC(I,K)

LI = L(I)

IF (QI .EQ. FLOAT(4*LI+2) .OR. LI .EQ. 0) GO TO 7

SP = Z*R3(I)*5.843574

SPO=SP

PRINT 50, EL(I),SPO

50 FORMAT(///20X, 10HORIG ZETA(A3,4H) = F10.2 /)

DO 4 J = 1,NWF

QJ = QC(J,K)

IF (QJ .EQ. 0. .OR. I .EQ. J) GO TO 4

LJ = L(J)

C=QJ

SPI=SP

SP = SP - 2.*C*SM(I,J,0)

SPDIF=SPI-SP

SMP=SM(I,J,0)*1.

SMQ=SM(J,I,0)

PRINT 51,EL(I),EL(J),SP,SPI,SPDIF,SMP,SMQ

51 FORMAT(/20X,8HZETA C (A3,1H,A3,4H) = 3X, 2F10.3,3F10.5,/))

DO 5 KK=1,6

CC = CV(LI,LJ+1,KK)

SPO=SP

IF (CC .NE. 0.) SP = SP - C*CC*V(I,J,KK-1)

KKK=KK-1

IF(SP.EQ.SPO) GO TO 5

SVP= V(I,J,KK-1)


```

SVQ=V(J,I,KK-1)
PRINT 52, KKK, EL(I), EL(J), SP, SVP, SVQ
52  FORMAT(20X, 7HZETAC-V 1X, I2, 1H(A3, 1H, A3, 4H) = F10.2, 20X, 2F10.5)
5  CONTINUE
DO 6 KK = 1, 7
CC = CN(LI, LJ+1, KK)
SPO=SP
IF (CC .NE. 0.) SP = SP - C*CC*SN(I, J, KK-2)
KKK=KK-2
IF (SP.EQ.SPO) GO TO 6
SNP= SN(I, J, KK-2)
SNQ=SN(J, I, KK-2)
PRINT 53, KKK, EL(I), EL(J), SP, SNP, SNQ
53  FORMAT(20X, 8HZETACV-N , I2, 1H(A3, 1H, A3, 4H) = F10.2, 20X, 2F10.5)
6  CONTINUE
4  CONTINUE
SS(1) = SM(I, I, 0)
C = QC(I, K)
IF (C .EQ. 1.) GO TO 9
C=C+C-3.
SP = SP - C*SS(1)
SSP=SS(1)
SSQ=SN(I, I, 0)
PRINT 54, EL(I), SP, SSP, SSQ
54  FORMAT(20X, 11HZETACVN-SSP , 1H(A3, 3H, M0, 4H) = F10.2, 5X, 2F10.5/)
GO TO (3, 11, 12), LI
11  SS(2) = SM(I, I, 2)
SP = SP + .85714286*SS(2)
SSP=SS(2)
SSQ=SN(I, I, 2)
PRINT 55, EL(I), SP, SSP, SSQ
55  FORMAT(20X, 11HZETACVN-SSD , 1H(A3, 3H, M2, 4H) = F10.2, 5X, 2F10.5/)
GO TO 3
12  SS(2) = SM(I, I, 2)
SS(3) = SM(I, I, 4)
SP = SP + SS(2) + .45454545*SS(3)
SSP1=SS(2)
SSP2=SS(3)
SSQ1=SN(I, I, 2)
SSQ2=SN(I, I, 4)
PRINT 56, EL(I), SP, SSP1, SSQ1, SSP2, SSQ2
56  FORMAT(20X, 11HZETACVN-SSF , 1H(A3, 3H, M4, 4H) = F10.2, 5X, 4F10.5/)
GO TO 3
9  PRINT 10, K, EL(I), SP
10  FORMAT (20X, I4, 6H ZETA(A3, 4H)= F10.2. )
GO TO 7
3  PRINT 14, K, EL(I), SP, (B, EL(I), EL(I), SS(II), II=1, LI)
14  FORMAT(20X, I4, 6H ZETA(A3, 4H) = F10.2, 4X, A4, 3HM0(A3, 1H, A3, 4H) = F6.3
1  , A4/55X, 3HM2(A3, 1H, A3, 4H) = F6.3
2  , A4/55X, 3HM4(A3, 1H, A3, 4H) = F6.3)
7  CONTINUE
2  CONTINUE
RETURN
END

```

```
FUNCTION SM(I,J,K)
CALL ZK(J,J,K)
SM = QUADS(I,I,3)*2.921787
RETURN
END
```

```
FUNCTION SN(I,J,K)
CALL ZK(I,J,K)
SN = QUADS(I,J,3)*2.921787
RETURN
END
```

```
FUNCTION V(I,J,K)
CALL DYK(I,J,K)
V = QUADS(I,J,2)
CALL DYK(J,I,K)
V = (V - QUADS(I,J,2))*2.921787
RETURN
END
```

```

SUBROUTINE DYK(I,J,H)
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),D(540),R(200),
1 RR(200),R2(200),P(20,200),Y(20,200),YK(200)/SCRAP/R3(30),DEN,
2 C,H3,A,AA,FACT,F1,F2,F3,ND
DEN = L(I)+ L(J)+ 2 + K
DO 1 JJ =1,2
1 YK(JJ) = FLOAT (L(J))*P(I,JJ)*P(J,JJ)*R(JJ)/DEN
C = EXP (-H)
H3 = H/3.
A = C**K
AA = A*A
A = 4.*A
FACT = FLOAT (L(J))
F1 = FACT*P(I,1)*P(J,1)*R(1)
F2 = FACT*P(I,2)*P(J,2)*R(2)
ND = NO-1
DO 8 M =3,ND
F3 =.5*P(I,M)*((P(J,M+1)-P(J,M-1))/H - P(J,M))*R(M)
YK(M) = YK(M-2)*AA + H3*(F3+ A*F2 + AA*F1)
F1 = F2
8 F2 = F3
A = A*(C)**3
AA = A*A/16.
C = .2*K+3
H3 = C*H3
YK(NO)= YK(ND)
F1 = YK(NO)
F2 = F1
DO 9 MM = 3,NO
M = NO -MM+1
F3 =YK(M)
YK(M) = YK(M+2)*AA + H3*(F3 +A*F2 + AA*F1)
F1 = F2
9 F2 = F3
RETURN
END

```

```

SUBROUTINE ORTHO
COMMON ATOM,TERM,NWF,D(4),EL(20),N(20),L(20)
PRINT 1,ATOM,TERM
1  FORMAT(1H1,9X,33HORTHOGONALITY INTEGRALS FOR ATOM A6,6H TERM A6//
1  20X, 4H(NL),3X,4H(NL),7X,8HINTEGRAL //)
    DO 2 I = 2,NWF
        JF = I - 1
        DO 3 J = 1,JF
            IF (L(I) .NE. L(J)) GO TO 3
            T = QUADR(I,J,0)
            PRINT 7,EL(I),EL(J),T
7  FORMAT(21X,A3,4X,A3,F15.8)
3  CONTINUE
2  CONTINUE
    YTIME = TIMELEFT(TDUMMY)
    PRINT 9999, YTIME
9999 FORMAT(1H0,* FROM ORTHO * E20.8/)
    RETURN
END

```

```

SUBROUTINE PNCH
COMMON ATOM,TERM,NWF,Z,NP,H,N0,EL(20),D(100),MAX(20),DD(1060),
1  P(20,200)/SCRAP/IW(20)
DIMENSION EK(20),EKPNC(20)
EQUIVALENCE (EK(1),DD(41))
READ 1,NPNCH,(IW(K), K=1,NPNCH)
1  FORMAT(21I3)
    IF (NPNCH .EQ. 0) GO TO 2
    DO 6 IJ = 1,NPNCH
        I = IW(IJ)
        MX = MAX(I)
        PUNCH 4,ATOM,TERM,EL(I),MX,Z
4  FORMAT(6H ATOM ,A6,6H TERM ,A6,8HELECTRON,A3,16,F6.0)
6  PUNCH 5,(P(I,J), J=1,MX)
5  FORMAT(7F11.7)
    I = 1
    DO 9 K=1,NPNCH
        KK = IW(K)
        EKPNC(I) = EK(KK)
        I = I + 1
9  CONTINUE
    PUNCH 25, (EKPNC(I), I = 1,NPNCH )
25  FORMAT (5F16.8)
2  RETURN
END

```

```

SUBROUTINE SCALE(ZZ)
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),S(20),AZ(20),
1 ACC(20),MAX(20),D(60),E(20,20),R(200),RR(200),R2(200),P(20,200)
2 ,Y(20,200),YK(200),RS(200),PS(200)/SCRAP/RATIO,SR,SC,SS,K,F0,
3 F1,F2,F3
RATIO = Z/ZZ
SR = SQRT (RATIO)
DO 1 J = 1,NO
R(J) = R(J)*RATIO
RR(J) = R(J)*R(J)
1 R2(J) = R2(J)*SR
DO 2 I = 1,NWF
SC = (ZZ-S(I))/(Z-S(I))
SS = SC*RATIO
DO 3 J = 1,NO
RS(J) = R(J)/SS
3 PS(J) = P(I,J)*SC
K = 3
ND = NO - 1
DO 4 J = 1,NO
5 IF (K .EQ. ND) GO TO 7
IF (RS(K) .GT. R(J)) GO TO 6
K = K + 1
GO TO 5
6 THETA = ALOG(R(J)/RS(K-1))/H
F0 = PS(K-2)
F1 = PS(K-1)
F2 = PS(K)
F3 = PS(K+1)
P(I,J) = .5*(F1+F2) + (THETA -.5)*(F2 - F1) + .25*(THETA-1.)*THETA
1 *(F0 - F1 - F2 + F3)
GO TO 4
7 P(I,J) = 0.
4 CONTINUE
PNORM = SQRT(QUADR(I,1,0))
DO 10 J = 1,NO
10 P(I,J) = P(I,J)/PNORM
CALL YKF(I,1,0)
DO 11 J = 1,NO
11 Y(I,J) = YK(J)
MAX(I) = K
E(I,1) = E(I,1)*SC**2
SC = (ZZ - .5*S(I))/(Z - .5*S(I))
SR = SQRT (SC)
2 AZ(I) = AZ(I)*SC**(L(I)+1)*SR
Z = ZZ
RETURN
END

```

D. Sample Data for HF Program

1. This first sample is an example of a sequential-type frozen-core run.

First, the solutions for the configuration $1s^2 2s^2$ of B II are calculated using the usual procedure of constructing initial estimates from the screening numbers. These $1s$ and $2s$ functions are then taken as initial estimates for the second case, although the $1s$ and $2s$ functions are kept fixed while making the $2p$ self-consistent. Next, these solutions are left in the memory to calculate the third case, in which the $2s$ and $2p$ orbitals are made self-consistent in the field of the frozen $1s^2$ core. Finally, for comparison purposes, we obtain a solution for $1s^2 2s^2 p$ of B I, allowing all three orbitals to vary. (Total run time: 1min 14 sec.)

```
B II      AV.    2  1      5.   -3.0 .0625   140      2
1S2/2S2      1.0
1S  1  0 0.397      2
2S  2  0 1.965      2
  0  0  2
  1
  2  1  2
  2  1  2
```

```
*
B I       AV.    3  1      5.   -3.0 .0625   140      1
2P       1.0
1S  1  0 0.397      1  2
2S  2  0 1.965      1  2
2P  2  1 2.732      1
  0  1  1
  1
  3  1  2  3
  3  1  2  3
```

```
*
B I       AV.    3  1      5.   -3.0 .0625   140      2
2P       1.0
1S  1  0 0.397      1  2
2S  2  0 1.965      1  2
2P  2  1 2.732      1  1
  0  1  2
  1
  3  1  2  3
  3  1  2  3
```

```
*
B I       AV.    3  1      5.   -3.0 .0625   140
2P       1.0
1S  1  0 0.397      1  2
2S  2  0 1.965      1  2
2P  2  1 2.732      1  1
  0  1  3
  1
  3  1  2  3
  2  2  3
```

*

2. This second sample is an example of a separate-time frozen-core run.

First the solutions of a previous "core-producing" run are obtained and the selected core $\bar{P}_i$'s and I_i 's are obtained by means of the PNCH option. In this example, the first nine orbitals ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$) of the La II $5d^2$ solution were chosen as the core, thus enabling various other rearrangements of electrons among the orbitals beyond the 4d to be made self-consistent in the field of this core. For the example here, the solutions for La II $6s6p$ are obtained by making the outermost four orbitals self-consistent. Note that only the first 15 and last 7 cards of this example input have to be punched manually since those for the $\bar{P}_i$'s and I_i 's correspond to the punched output of the "core-producing" run. (Total run time: ~4 min.)

LA II	AV.	13	1	57.	-3.0	.0625	174	4
6S/6P		1.0						
1S	1	0	0.71		-1	2		
2S	2	0	4.45		-1	2		
2P	2	1	5.58		-1	6		
3S	3	0	11.84		-1	2		
3P	3	1	13.79		-1	6		
3D	3	2	16.6		-1	10		
4S	4	0	21.96		-1	2		
4P	4	1	24.51		-1	6		
4D	4	2	29.71	8.5	-1	10		
5S	5	0	35.29	2.75		2		
5P	5	1	38.48	1.55	.4	6		
6S	6	0.45		0.838	8.55	.4	1	
6P	6	145.	0.607		112.2	.4	1	
ATOM LA II	TERM	AV.	ELECTRON	1S	104	57		
23.9728096	24.6545199	25.3503688	26.0601157	26.7834524	27.5199963	28.2692833		
29.0307598	29.8037745	30.5875699	31.3812730	32.1838853	32.9942731	33.8111565		
34.6330988	35.4584950	36.2855605	37.1123193	37.9365925	38.7559869	39.5678837		
40.3694282	41.1575198	41.9288038	42.6796638	43.4062173	44.1043117	44.7695253		
45.3971703	45.9822997	46.5197204	47.0040098	47.4295397	47.7905071	48.0809720		
48.2949046	48.4262409	48.4689486	48.4171033	48.2649753	48.0071274	47.6385232		
47.1546461	46.5516264	45.8263778	44.9767379	44.0016123	42.9011186	41.6767249		
40.3313788	38.8696211	37.2976777	35.6235259	33.8569130	32.0093500	30.0940439		
28.1257780	26.1207323	24.0962418	22.0704934	20.0621640	18.0900072	16.1724000		
14.3268637	12.5695792	10.9149172	9.3750096	7.9593855	6.6746967	5.5245528		
4.5094818	3.6270239	2.8719575	2.2366463	1.7114884	1.2854365	0.9465572		
0.6825881	0.4814585	0.3317389	0.2229953	0.1460338	0.0930314	0.0575605		
0.0345245	0.0200267	0.0111963	0.0059982	0.0030457	0.0014315	0.0005859		
0.0001658	-0.0000272	-0.0001034	-0.0001221	-0.0001142	-0.0000955	-0.0000741		
-0.0000537	-0.0000362	-0.0000221	-0.0000114	-0.0000039	0.0000006			
ATOM LA II	TERM	AV.	ELECTRON	2S	108	57		
7.8208289	8.0429088	8.2695389	8.5006301	8.7360697	8.9757188	9.2194095		
9.4669423	9.7180826	9.9725577	10.2300532	10.4902092	10.7526162	11.0168110		
11.2822720	11.5484148	11.8145870	12.0800631	12.3440395	12.6056286	12.8638535		
13.1176427	13.3658240	13.6071194	13.8401397	14.0633797	14.2752136	14.4738913		
14.6575350	14.8241377	14.9715616	15.0975398	15.1996783	15.2754609	15.3222565		
15.3373298	15.3178545	15.2609314	15.1636101	15.0229161	14.8358828	14.5995894		
14.3112056	13.9680422	13.5676085	13.1076779	12.5863585	12.0021724	11.3541398		
10.6418690	9.8656501	9.0263515	8.1265159	7.1684540	6.1563321	5.0952499		
3.9915030	2.8526267	1.6874139	0.5059020	-0.6806770	-1.8599894	-3.0187400		
-4.1428647	-5.2177762	-6.2286653	-7.1608534	-8.0001909	-8.7334933	-9.3490000		
-9.8368396	-10.1894808	-10.4021433	-10.4731456	-10.4041593	-10.2003502	-9.8703706		
-9.4262087	-8.8828649	-8.2578670	-7.5706350	-6.8417219	-6.0919681	-5.3416204		
-4.6094725	-3.9120889	-3.2631700	-2.6731089	-2.1487716	-1.6935154	-1.3074318		
-0.9877832	-0.7295806	-0.5262391	-0.3702464	-0.2537831	-0.1692480	-0.1096584		
-0.0689124	-0.0419192	-0.0246159	-0.0138980	-0.0074934	-0.0038097	-0.0017787		
-0.0007153	-0.0002012	0.0000012						

ATOM LA II	TERM	AV.	ELECTRON 2P	124	57		
0.1090664	0.1195941	0.1311244	0.1437506	0.1575741	0.1727055	0.1892647	
0.2073825	0.2272004	0.2488725	0.2725655	0.2984600	0.3267517	0.3576519	
0.3913890	0.4282090	0.4683773	0.5121790	0.5599203	0.6119297	0.6685585	
0.7301819	0.7971996	0.8700368	0.9491439	1.0349973	1.1280988	1.2289752	
1.3381774	1.4562787	1.5838729	1.7215714	1.8699992	2.0297904	2.2015828	
2.3860101	2.5836943	2.7952351	3.0211986	3.2621040	3.5184076	3.7904858	
4.0786151	4.3829502	4.7035000	5.0401012	5.3923899	5.7597720	6.1413914	
6.5360981	6.9424161	7.3585118	7.7821646	8.2107406	8.6411714	9.0699391	
9.4930703	9.9061409	10.3042937	10.6822719	11.0344703	11.3550061	11.6378111	
11.8767473	12.0657438	12.1989567	12.2709480	12.2768804	12.2127231	12.0754596	
11.8632908	11.5758212	11.2142171	10.7813267	10.2817384	9.7217878	9.1094817	
8.4543446	7.7671811	7.0597595	6.3444233	5.6336491	4.9395692	4.2734907	
3.6454406	3.0637700	2.5348501	2.0628837	1.6498494	1.2955825	0.9979832	
0.7533300	0.5566682	0.4022341	0.2838761	0.1954402	0.1310886	0.0855390	
0.0542145	0.0333106	0.0197908	0.0113273	0.0062064	0.0032171	0.0015383	
0.0006359	0.0001767	-0.0000389	-0.0001260	-0.0001485	-0.0001409	-0.0001210	
-0.0000980	-0.0000760	-0.0000569	-0.0000413	-0.0000291	-0.0000199	-0.0000131	
-0.0000083	-0.0000050	-0.0000029	-0.0000015	-0.0000006			
ATOM LA II	TERM	AV.	ELECTRON 3S	139	57		
3.5352246	3.6355899	3.7380079	3.8424377	3.9488275	4.0571137	4.1672193	
4.2790528	4.3925069	4.5074564	4.6237575	4.7412452	4.8597319	4.9790051	
5.0988256	5.2189255	5.3390051	5.4587313	5.5777349	5.6956077	5.8119002	
5.9261189	6.0377237	6.1461250	6.2506813	6.3506971	6.4454199	6.5340389	
6.6156833	6.6894205	6.7542564	6.8091348	6.8529384	6.8844911	6.9025607	
6.9058636	6.8930708	6.8628159	6.8137055	6.7443309	6.6532839	6.5391744	
6.4006516	6.2364286	6.0453106	5.8262270	5.5782669	5.3007193	4.9931164	
4.6552806	4.2873749	3.8899553	3.4640250	3.0110885	2.5332053	2.0330395	
1.5139049	0.9798016	0.4354418	-0.1137390	-0.6615882	-1.2012649	-1.7252940	
-2.2256488	-2.6938669	-3.1212004	-3.4988024	-3.8179489	-4.0702955	-4.2481638	
-4.3448508	-4.3549530	-4.2746923	-4.1022296	-3.8379483	-3.4846901	-3.0479211	
-2.5358095	-1.9591949	-1.3314340	-0.6681102	0.0133959	0.6944725	1.3559614	
1.9789380	2.5455443	3.0398296	3.4485406	3.7618034	3.9736427	4.0822908	
4.0902553	4.0041326	3.8341715	3.5936144	3.2978606	2.9635086	2.6073477	
2.2453767	1.8919234	1.5589388	1.2555216	0.9877062	0.7585204	0.5682847	
0.4150974	0.2954311	0.2047582	0.1381320	0.0906675	0.0578918	0.0359563	
0.0217271	0.0127768	0.0073134	0.0040722	0.0021998	0.0011441	0.0005621	
0.0002485	0.0000844	0.0000024	-0.0000349	-0.0000484	-0.0000495	-0.0000448	
-0.0000378	-0.0000303	-0.0000235	-0.0000177	-0.0000130	-0.0000093	-0.0000065	
-0.0000044	-0.0000030	-0.0000019	-0.0000012	-0.0000008	-0.0000005		
ATOM LA II	TERM	AV.	ELECTRON 3P	125	57		
0.0516146	0.0565965	0.0620529	0.0680278	0.0745692	0.0817294	0.0895652	
0.0981383	0.1075158	0.1177704	0.1289810	0.1412330	0.1546188	0.1692383	
0.1851993	0.2026182	0.2216201	0.2423397	0.2649214	0.2895201	0.3163015	
0.3454422	0.3771304	0.4115660	0.4489608	0.4895380	0.5335330	0.5811921	
0.6327725	0.6885412	0.7487738	0.8137531	0.8837668	0.9591054	1.0400585	
1.1269118	1.2199417	1.3194105	1.4255600	1.5386042	1.6587208	1.7860416	
1.9206419	2.0625279	2.2116236	2.3677557	2.5306377	2.6998523	2.8748331	
3.0548454	3.2389665	3.4260660	3.6147865	3.8035255	3.9904197	4.1733321	
4.3498431	4.5172479	4.6725606	4.8125269	4.9336474	5.0322133	5.1043553	
5.1461077	5.1534897	5.1226022	5.0497430	4.9315370	4.7650815	4.5481023	
4.2791175	3.9576022	3.5841474	3.1606059	2.6902140	2.1776786	1.6292212	
1.0525643	0.4568538	-0.1474936	-0.7490201	-1.3355380	-1.8945148	-2.4135238	
-2.8807413	-3.2854664	-3.6186325	-3.8732776	-4.0449367	-4.1319242	-4.1354790	
-4.0597549	-3.9116481	-3.7004663	-3.4374575	-3.1352216	-2.8070444	-2.4661939	
-2.1252294	-1.7953734	-1.4859967	-1.2042587	-0.9549329	-0.7404262	-0.5609816	
-0.4150274	-0.2996234	-0.2109438	-0.1447414	-0.0967457	-0.0629675	-0.0398990	
-0.0246151	-0.0147916	-0.0086648	-0.0049537	-0.0027675	-0.0015120	-0.0008071	
-0.0004187	-0.0002084	-0.0000963	-0.0000381	-0.0000094	0.0000022		
ATOM LA II	TERM	AV.	ELECTRON 3D	139.	57		
0.0001421	0.0001660	0.0001938	0.0002263	0.0002643	0.0003085	0.0003602	
0.0004205	0.0004908	0.0005727	0.0006684	0.0007798	0.0009098	0.0010612	
0.0012377	0.0014434	0.0016829	0.0019618	0.0022866	0.0026645	0.0031043	
0.0036159	0.0042107	0.0049022	0.0057057	0.0066391	0.0077227	0.0089804	
0.0104392	0.0121307	0.0140907	0.0163607	0.0189881	0.0220273	0.0255402	
0.0295978	0.0342811	0.0396819	0.0459047	0.0530679	0.0613056	0.0707688	
0.0816277	0.0940733	0.1083191	0.1246035	0.1431915	0.1643763	0.1884813	
0.2158614	0.2469037	0.2820288	0.3215900	0.3663725	0.4165916	0.4728892	
0.5358291	0.6059900	0.6839571	0.7703105	0.8656116	0.9703864	1.0851054	

1.2101609	1.3458409	1.4923000	1.6495278	1.8173154	1.9952208	2.1825343
2.3782448	2.5810103	2.7891324	3.0005390	3.2127762	3.4230139	3.6280651
3.8244236	4.0083216	4.1758080	4.3228483	4.4454452	4.5397785	4.6023571
4.6301804	4.6208987	4.5729628	4.4857545	4.3596854	4.1962560	3.9980704
3.7687952	3.5130672	3.2363496	2.9447403	2.6447383	2.3429804	2.0459579
1.7597313	1.4896606	1.2401719	1.0145825	0.8150000	0.6423080	0.4962397
0.3755281	0.2781164	0.2014000	0.1424746	0.0983629	0.0662039	0.0433912
0.0276599	0.0171254	0.0102824	0.0059755	0.0033522	0.0018080	0.0009307
0.0004508	0.0001990	0.0000730	0.0000139	-0.0000111	-0.0000195	-0.0000205
-0.0000183	-0.0000152	-0.0000121	-0.0000094	-0.0000072	-0.0000054	-0.0000041
-0.0000030	-0.0000023	-0.0000017	-0.0000013	-0.0000010	-0.0000007	
ATOM LA II TERM AV. ELECTRON 4S 143 57						
1.6625190	1.7097159	1.7578777	1.8069851	1.8570137	1.9079334	1.9597080
2.0122943	2.0656416	2.1196910	2.1743746	2.2296145	2.2853223	2.3413978
2.3977282	2.4541869	2.5106327	2.5669083	2.6228394	2.6782335	2.7328782
2.7865407	2.8389658	2.8898751	2.9389655	2.9859083	3.0303479	3.0719009
3.1101556	3.1446709	3.1749764	3.2005721	3.2209290	3.2354901	3.2436716
3.2448650	3.2384401	3.2237486	3.2001293	3.1669131	3.1234311	3.0690227
3.0030454	2.9248871	2.8339792	2.7298122	2.6119526	2.4800625	2.3339204
2.1734438	1.9987144	1.8100029	1.6077962	1.3928241	1.1660857	0.9288746
0.6828018	0.4298144	0.1722099	-0.0873569	-0.3458759	-0.5999937	-0.8460386
-1.0800604	-1.2978862	-1.4951944	-1.6676073	-1.8108033	-1.9206473	-1.9933391
-2.0255754	-2.0147226	-1.9589936	-1.8576228	-1.7110291	-1.5209578	-1.2905908
-1.0246116	-0.7292157	-0.4120535	-0.0820981	0.2505694	0.5750582	0.8800468
1.1542307	1.3868246	1.5680919	1.6898732	1.7460799	1.7331165	1.6502007
1.4995506	1.2864182	1.0189563	0.7079150	0.3661719	0.0081126	-0.3511121
-0.6964155	-1.0136370	-1.2903769	-1.5167311	-1.6858575	-1.7943143	-1.8421318
-1.8326142	-1.7718890	-1.6682655	-1.5314726	-1.3718597	-1.1996342	-1.0242017
-0.8536514	-0.6944116	-0.5510830	-0.4264409	-0.3215820	-0.2361852	-0.1688438
-0.1174251	-0.0794162	-0.0522226	-0.0333964	-0.0207860	-0.0126120	-0.0074816
-0.0043591	-0.0025111	-0.0014426	-0.0008347	-0.0004909	-0.0002951	-0.0001813
-0.0001134	-0.0000715	-0.0000452	-0.0000283	-0.0000175	-0.0000107	-0.0000064
-0.0000037	-0.0000021	-0.0000011				
ATOM LA II TERM AV. ELECTRON 4P 143 57						
0.0237509	0.0260434	0.0285541	0.0313035	0.0343136	0.0376083	0.0412140
0.0451589	0.0494739	0.0541925	0.0593510	0.0649887	0.0711480	0.0778749
0.0852191	0.0932340	0.1019772	0.1115106	0.1219007	0.1332187	0.1455407
0.1589480	0.1735270	0.1893696	0.2065731	0.2252402	0.2454787	0.2674019
0.2911277	0.3167786	0.3444808	0.3743640	0.4065597	0.4412006	0.4784190
0.5183447	0.5611035	0.6068139	0.6555847	0.7075115	0.7626722	0.8211232
0.8828938	0.9479807	1.0163411	1.0878865	1.1624740	1.2398990	1.3198856
1.4020781	1.4860309	1.5711995	1.6569310	1.7424555	1.8268779	1.9091723
1.9881771	2.0625936	2.1309880	2.1917974	2.2433410	2.2838374	2.3114286
2.3242120	2.3202803	2.2977707	2.2549226	2.1901447	2.1020896	1.9897354
1.8524727	1.6901931	1.5033775	1.2931780	1.0614910	0.8110127	0.5452746
0.2686491	-0.0136787	-0.2957792	-0.5710922	-0.8325873	-1.0729727	-1.2849478
-1.4614933	-1.5961873	-1.6835324	-1.7192752	-1.7006986	-1.6268660	-1.4987982
-1.3195666	-1.0942917	-0.8300363	-0.5355934	-0.2211673	0.1020434	0.4223484
0.7281341	1.0084650	1.2536805	1.4559367	1.6096456	1.7117634	1.7618961
1.7622084	1.7171493	1.6330195	1.5174350	1.3787404	1.2254262	1.0655976
0.9065313	0.7543418	0.6137724	0.4881098	0.3792171	0.2876682	0.2129599
0.1537738	0.1082538	0.0742701	0.0496464	0.0323332	0.0205214	0.0127018
0.0076769	0.0045401	0.0026355	0.0015079	0.0008547	0.0004828	0.0002734
0.0001558	0.0000896	0.0000520	0.0000304	0.0000179	0.0000106	0.0000063
0.0000037	0.0000022	0.0000012				
ATOM LA II TERM AV. ELECTRON 4D 150 57						
0.0000643	0.0000751	0.0000877	0.0001024	0.0001195	0.0001396	0.0001629
0.0001902	0.0002220	0.0002591	0.0003023	0.0003528	0.0004115	0.0004801
0.0005599	0.0006529	0.0007612	0.0008874	0.0010343	0.0012053	0.0014042
0.0016356	0.0019046	0.0022174	0.0025809	0.0030030	0.0034931	0.0040619
0.0047218	0.0054867	0.0063732	0.0073998	0.0085880	0.0099623	0.0115508
0.0133855	0.0155030	0.0179448	0.0207580	0.0239961	0.0277195	0.0319964
0.0369034	0.0425266	0.0489622	0.0563174	0.0647113	0.0742754	0.0851549
0.0975085	0.1115093	0.1273449	0.1452166	0.1653397	0.1879416	0.2132601
0.2415412	0.2730352	0.3079923	0.3466568	0.3892599	0.4360113	0.4870887
0.5426261	0.6027005	0.6673164	0.7363896	0.8097292	0.8870191	0.9677995
1.0514479	1.1371624	1.2239470	1.3106001	1.3957081	1.4776460	1.5545852
1.6245110	1.6852521	1.7345209	1.7699682	1.7892503	1.7901092	1.7704628
1.7285038	1.6628022	1.5724073	1.4569428	1.3166903	1.1526551	0.9666094

```

0.7611090 0.5394802 0.3057734 0.0646835 -0.1785686 -0.4183901 -0.6490093
-0.8647011 -1.0600381 -1.2301538 -1.3709972 -1.4795583 -1.5540395 -1.5939532
-1.6001342 -1.5746621 -1.5207125 -1.4423344 -1.3441951 -1.2313071 -1.1087581
-0.9814624 -0.8539441 -0.7301612 -0.6133777 -0.5060844 -0.4099745 -0.3259684
-0.2542860 -0.1945546 -0.1459421 -0.1072985 -0.0772941 -0.0545409 -0.0376909
-0.0255068 -0.0169053 -0.0109776 -0.0069895 -0.0043695 -0.0026878 -0.0016320
-0.0009824 -0.0005897 -0.0003555 -0.0002169 -0.0001350 -0.0000862 -0.0000566
-0.0000382 -0.0000264 -0.0000185 -0.0000131 -0.0000093 -0.0000065 -0.0000045
-0.0000031 -0.0000020 -0.0000012
-1.62431800+003 -4.03487498+002 -4.02887272+002 -1.71603156+002 -1.69673936+002
-1.66960044+002 -8.42262421+001 -8.11328956+001 -7.42557921+001 -3.83903492+001
0 2 4
3
5 1 2 3 4 5
5 6 7 8 9 10
3 11 12 13
2 12 13

```

*

III. R^k INTEGRALS PROGRAM

RKMAIN is a program that computes values of

$$R^k(i,j,l,m) = \int_0^\infty \int_0^\infty P_i(r_1) P_j(r_2) P_l(r_1) P_m(r_2) \frac{r_1^k}{r_2^{k+1}} dr_1 dr_2,$$

where $P_i(r)$ are the card output from HF on the usual logarithmic radial mesh.

A. Data Input

1. Card 1. NWF, ATOM, TERM, Z, NRK in Format (I3, 2A6, F3.0, I3).
2. Card 2. N(I), L(I) for I = 1, NWF in Format (20I3) NWF ≤ 20; therefore one or two cards of type 2 may be required.
3. NWF decks of type 3: TRM(I), EL(I), M, (P(I,J), J=1,M) in Format (18X,A6,8X,A3,I6/(7F11.7)).

These are decks of $\bar{P}_i$ card output from HF.

4. NRK cards of type 4: I, J, L, M, K in Format (5I3).

Multiple runs may be stacked sequentially.

The output contains, in addition to the R^k values in cm^{-1} , an indication of the amount of cancellation that has occurred in forming the integral. This cancellation factor is defined here as the ratio of the true R^k value to that of a pseudo "absolute" R^k value calculated using the modulus of each $\bar{P}_i$. Thus, for a cancellation factor of 0.9, say, only 10% of the integral has disappeared, whereas a factor of 0.1 means that 90% has disappeared and hence the R^k value is far more sensitive to small changes in the $\bar{P}_i$'s.

B. Listing of R^k Program

```

PROGRAM RKMAIN
C ROUTINE FOR CALCULATING RK INTEGRALS
C CDC 3600 VERSION ANL 1966,
C CANCELLATION FACTORS A LA BOB COWAN INCLUDED
COMMON ATOM,TERM,NWF,Z,RHO,H,NO,EL(20),N(20),L(20),S(20),AZ(20),
1D(20),MAX(20),DD(40),IND(20),E(20,20),R(200),RR(200),R2(200),
2 P(20,200), INP, DUM(4200), AP(20,200)
DIMENSION TRM(20)
1 READ (5,2) NWF, ATOM, TERM, Z, NRK
2 FORMAT (I3,2A6,F3.0,I3)
IF(EOF,60) 20,21
20 CALL EXIT
21 WRITE (6,3) ATOM, TERM
3 FORMAT(1H1,10X,17HRK INTEGRALS FOR 2A6/39X,2HRK,16X,
1 7HMOD RK ,12X,12HCANCELLATION/)
H=.0625
NO = 200
RHO = -3.0
DO 4 J=1,200
R(J)=EXP(RHO)/Z
RR(J)= R(J)*R(J)
R2(J)= SQRT (R(J))
4 RHO = RHO + H
READ (5,5) (N(I), L(I), I=1,NWF)
5 FORMAT (20I3)
DO 8 I=1,NWF
READ (5,7) TRM(I),EL(I),M, (P(I,J),J=1,M)
7 FORMAT(18X,A6,8X,A3,16/(7F11.7))
MAX(I)= M
8 CONTINUE
DO 12 I = 1, NWF
DO 13 J = 1,M
AP(I,J) = ABS(P(I,J))
13 CONTINUE
12 CONTINUE
DO 10 KK= 1,NRK
READ (5,5) I,J,II,JJ, K
ANS= RK(I,J,II,JJ,K)
ANS = 219474.62*ANS
INP =1
CANS = RK(I,J,II,JJ,K)
CANS = 219474.62*CANS
INP = 0
CANF = ANS/CANS
10 WRITE(6,11) K,EL(I),EL(J),EL(II),EL(JJ),ANS,CANS,CANF
11 FORMAT (11X,1HR,11,1H( 2A3,1H,2A3,4H) = 3F20.8)
GO TO 1
END

```

```

FUNCTION RK(I,J,II,JJ,K)
CALL YKF(I,II,K)
RK = QUADS(J,JJ,1)
RETURN
END

```

```

SUBROUTINE ZK(I,J,K)
COMMON ATOM,TERM,NWF,Z,NP,H,NO,EL(20),N(20),L(20),D(540),R(200),
1 RR(200),R2(200),P(20,200),INP,Y(20,200),YK(200),AP(20,200)
DEN = L(I) + L(J) + 3 + K
FACT = (1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
IF (INP.EQ.1) GO TO 9
DO 1 JJ = 1,2
1 YK(JJ) = RR(JJ)*P(I,JJ)*P(J,JJ)/DEN*(1.+ Z*R(JJ)*FACT)
C = EXP(-H)
H3 = H/3.
A = C**K
AA = A*A
A = 4.*A
F1 = RR(1)*P(I,1)*P(J,1)
F2 = RR(2)*P(I,2)*P(J,2)
DO 8 M = 3,NO
F3 = RR(M)*P(I,M)*P(J,M)
YK(M) = YK(M-2)*AA + H3*(F3 + A*F2 + AA*F1)
F1 = F2
8 F2 = F3
GO TO 10
9 DO 11 JJ = 1,2
11 YK(JJ) = RR(JJ)*AP(I,JJ)*AP(J,JJ)/DEN*(1.+Z*R(JJ)*FACT)
C = EXP(-H)
H3 = H/3.
A = C**K
AA = A*A
A = 4.*A
F1 = RR(1)*AP(I,1)*AP(J,1)
F2 = RR(2)*AP(I,2)*AP(J,2)
DO 13 M = 3, NO
F3 = RR(M)*AP(I,M)*AP(J,M)
YK(M) = YK(M-2)*AA + H3*(F3 + A*F2 + AA*F1)
F1 = F2
13 F2 = F3
10 CONTINUE
RETURN
END

```

```

SUBROUTINE YKF(I,J,K)
COMMON ATOM,TERM,NWF,Z, NP,H,NO,EL(20),N(20),L(20),D(60),MAX(20),
1 DD(460),R(200),RR(200),R2(200),P(20,200),INP,Y(20,200),YK(200),
2 AP(20,200)
CALL ZK(I,J,K)
C = EXP(-H)
A = 4.*C**(K+1) $ AA= A*A/16.
C = 2*K+1
H3 = C*H/3.
F1 = YK(NO) $ F2 =YK(NO-1)
DO 9 MM = 3,NO
M = NO -MM+1
F3 = YK(M)
YK(M) = YK(M+2)*AA + H3*(F3 + A*F2 + AA*F1)
F1 = F2
9 F2 = F3
IF (IABS(I-J) + K .NE. 0) GO TO 10
MX = MAX(I)
IF (MX .GE. NO) GO TO 13
MP = MX + 1
DO 14 M = MP,NO
14 YK(M) = 1.
13 A = (1. - YK(MX))/FLOAT (MX)
DO 15 M = 1,MX
FM = M
15 YK(M) = YK(M) + A*FM
10 RETURN
END

```

```

FUNCTION QUADS(I,J,KK)
COMMON DD(3),Z,NP,H,NO,EN(40), L(20),DDD(60),MAX(20),DX(460),
1 R(200),RR(200),R2(200),P(20,200),INP,Y(20,200),YK(200),AP(20,200)
DEN = L(I) + L(J) + 3
H3 = H/1.5
CD=1.5*(1.+Z*R(1))*(1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
K = 2 - KK
D = YK(1)*P(I,1)*P(J,1)*R(1)**K*( CD/(DEN*H) +.5)
ND = MAX0 (MAX(I),MAX(J)) - 1
IF (INP .EQ. 1) GO TO 2
DO 1 M =2,ND,2
MM = M+1
1 D = D + 2.*YK(M)*P(I,M)*P(J,M)*R(M)**K +YK(MM)*P(I,MM)*P(J,MM)*
1 R(MM)**K
GO TO 4
2 D =YK(1)*AP(I,1)*AP(J,1)*R(1)**K*(CD/(DEN*H)+.5)
DO 3 M= 2,ND,2
MM = M+1
3 D=D+2.*YK(M)*AP(I,M)*AP(J,M)*R(M)**K+YK(MM)*AP(I,MM)*AP(J,MM)
1 * R(MM)**K
4 CONTINUE
QUADS = D*H3
RETURN
END

```


0.3086420	0.2860188	0.2615462	0.2352776	0.2072944	0.1777094	0.1466696
0.1143581	0.0809967	0.0468468	0.0122105	-0.0225700	-0.0571135	-0.0910023
-0.1237863	-0.1549887	-0.1841128	-0.2106513	-0.2340963	-0.2539523	-0.2697488
-0.2810555	-0.2874976	-0.2887710	-0.2846579	-0.2750412	-0.2599176	-0.2394080
-0.2137661	-0.1833834	-0.1487702	-0.1106528	-0.0697657	-0.0270394	0.0165180
0.0598236	0.1017484	0.1411508	0.1769144	0.2079881	0.2334276	0.2524356
0.2643973	0.2689101	0.2658030	0.2551452	0.2372429	0.2126236	0.1820099
0.1462852	0.1064535	0.0635979	0.0188391	-0.0267024	-0.0719388	-0.1158425
-0.1574673	-0.1959649	-0.2305976	-0.2607480	-0.2859266	-0.3057782	-0.3200874
-0.3287816	-0.3319321	-0.3297521	-0.3225901	-0.3109185	-0.2953171	-0.2764516
-0.2550473	-0.2318603	-0.2076469	-0.1831335	-0.1589884	-0.1357985	-0.1140501
-0.0941177	-0.0762586	-0.0606146	-0.0472201	-0.0360157	-0.0268649	-0.0195742
-0.0139132	-0.0096342	-0.0064897	-0.0042460	-0.0026939	-0.0016547	-0.0009823
-0.0005626	-0.0003103	-0.0001645	-0.0000837	-0.0000408	-0.0000190	-0.0000085
-0.0000036	-0.0000014	-0.0000005	0.0000000	0.0000000	0.0000000	
ATOM SC I	TERM	AV.	ELECTRON 4P	158	21	
0.0020020	0.0021952	0.0024069	0.0026386	0.0028924	0.0031701	0.0034741
0.0038067	0.0041704	0.0045683	0.0050032	0.0054785	0.0059978	0.0065650
0.0071843	0.0078602	0.0085976	0.0094017	0.0102781	0.0112328	0.0122724
0.0134036	0.0146340	0.0159712	0.0174235	0.0189997	0.0207090	0.0225612
0.0245663	0.0267348	0.0290778	0.0316065	0.0343323	0.0372671	0.0404225
0.0438103	0.0474419	0.0513285	0.0554806	0.0599077	0.0646185	0.0696200
0.0749174	0.0805136	0.0864090	0.0926007	0.0990819	0.1058417	0.1128642
0.1201278	0.1276046	0.1352599	0.1430513	0.1509280	0.1588304	0.1666895
0.1744265	0.1819525	0.1891684	0.1959653	0.2022247	0.2078193	0.2126144
0.2164692	0.2192390	0.2207777	0.2209406	0.2195879	0.2165889	0.2118256
0.2051978	0.1966273	0.1860628	0.1734846	0.1589087	0.1423906	0.1240292
0.1039686	0.0824000	0.0595627	0.0357430	0.0112721	-0.0134768	-0.0380948
-0.0621436	-0.0851655	-0.1066942	-0.1262681	-0.1434447	-0.1578167	-0.1690269
-0.1767834	-0.1808724	-0.1811676	-0.1776361	-0.1703397	-0.1594313	-0.1451473
-0.1277966	-0.1077466	-0.0854087	-0.0612239	-0.0356486	-0.0091440	0.0178334
0.0448389	0.0714438	0.0972394	0.1218392	0.1448817	0.1660329	0.1849907
0.2014886	0.2153018	0.2262523	0.2342146	0.2391208	0.2409643	0.2398021
0.2357553	0.2290075	0.2198009	0.2084302	0.1952350	0.1805897	0.1648920
0.1485502	0.1319695	0.1155381	0.0996132	0.0845092	0.0704866	0.0577443
0.0464152	0.0365656	0.0281980	0.0212584	0.0156460	0.0112249	0.0078374
0.0053165	0.0034974	0.0022268	0.0013694	0.0008115	0.0004624	0.0002526
0.0001320	0.0000658	0.0000312	0.0000140	0.0000059	0.0000024	0.0000009
0.0000000	-0.0000000	-0.0000000	-0.0000000			
ATOM SC I	TERM	AV.	ELECTRON 3D	151	21	
0.0000104	0.0000121	0.0000142	0.0000166	0.0000193	0.0000226	0.0000264
0.0000308	0.0000359	0.0000419	0.0000489	0.0000571	0.0000666	0.0000777
0.0000906	0.0001057	0.0001232	0.0001436	0.0001674	0.0001951	0.0002273
0.0002647	0.0003083	0.0003590	0.0004178	0.0004862	0.0005656	0.0006577
0.0007646	0.0008886	0.0010323	0.0011988	0.0013915	0.0016145	0.0018723
0.0021702	0.0025142	0.0029111	0.0033686	0.0038956	0.0045021	0.0051993
0.0060001	0.0069188	0.0079715	0.0091765	0.0105538	0.0121262	0.0139186
0.0159586	0.0182770	0.0209072	0.0238858	0.0272527	0.0310509	0.0353268
0.0401299	0.0455125	0.0515297	0.0582391	0.0656999	0.0739722	0.0831168
0.0931934	0.1042600	0.1163713	0.1295772	0.1439213	0.1594390	0.1761558
0.1940853	0.2132273	0.2335660	0.2550678	0.2776802	0.3013295	0.3259194
0.3513298	0.3774153	0.4040039	0.4308971	0.4578686	0.4846649	0.5110066
0.5365903	0.5610921	0.5841729	0.6054851	0.6246816	0.6414262	0.6554048
0.6663385	0.6739950	0.6782003	0.6788466	0.6758989	0.6693964	0.6594510
0.6462417	0.6300054	0.6110255	0.5896193	0.5661247	0.5408876	0.5142512
0.4865471	0.4580887	0.4291672	0.4000497	0.3709794	0.3421764	0.3138406
0.2861536	0.2592812	0.2333754	0.2085749	0.1850057	0.1627799	0.1419942
0.1227274	0.1050383	0.0889632	0.0745141	0.0616775	0.0504146	0.0406623
0.0323358	0.0253315	0.0195314	0.0148077	0.0110278	0.0080589	0.0057726
0.0040482	0.0027761	0.0018594	0.0012147	0.0007731	0.0004788	0.0002882
0.0001684	0.0000954	0.0000524	0.0000278	0.0000143	0.0000071	0.0000034
0.0000016	0.0000007	0.0000000	0.0000000			
ATOM SC I	TERM	AV.	ELECTRON 4P	160	21	
0.0014929	0.0016370	0.0017949	0.0019677	0.0021569	0.0023640	0.0025907
0.0028387	0.0031100	0.0034066	0.0037310	0.0040854	0.0044727	0.0048957
0.0053575	0.0058615	0.0064114	0.0070110	0.0076646	0.0083766	0.0091518
0.0099954	0.0109129	0.0119101	0.0129931	0.0141685	0.0154432	0.0168244
0.0183197	0.0199368	0.0216841	0.0235698	0.0256025	0.0277911	0.0301442
0.0326706	0.0353788	0.0382772	0.0413736	0.0446752	0.0481883	0.0519183

0.0558689	0.0600424	0.0644391	0.0690568	0.0738906	0.0789322	0.0841698
0.0895875	0.0951643	0.1008745	0.1066865	0.1125625	0.1184580	0.1243218
0.1300951	0.1357118	0.1410981	0.1461728	0.1508479	0.1550285	0.1586144
0.1615008	0.1635800	0.1647432	0.1648830	0.1638953	0.1616827	0.1581578
0.1532457	0.1468885	0.1390480	0.1297094	0.1188845	0.1066144	0.0929722
0.0780643	0.0620324	0.0450528	0.0273370	0.0091291	-0.0092963	-0.0276383
-0.0455753	-0.0627714	-0.0788855	-0.0935803	-0.1065331	-0.1174477	-0.1260649
-0.1321741	-0.1356217	-0.1363179	-0.1342411	-0.1294379	-0.1220198	-0.1121573
-0.1000709	-0.0860197	-0.0702905	-0.0531855	-0.0350121	-0.0160740	0.0033358
0.0229396	0.0424774	0.0617076	0.0804064	0.0983661	0.1153936	0.1313083
0.1459411	0.1591336	0.1707388	0.1806226	0.1886655	0.1947667	0.1988471
0.2008540	0.2007658	0.1985957	0.1943963	0.1882618	0.1803301	0.1707825
0.1598416	0.1477669	0.1348476	0.1213935	0.1077236	0.0941536	0.0809825
0.0684795	0.0568720	0.0463370	0.0369943	0.0289050	0.0220726	0.0164495
0.0119453	0.0084388	0.0057895	0.0038500	0.0024768	0.0015381	0.0009200
0.0005287	0.0002912	0.0001533	0.0000769	0.0000367	0.0000165	0.0000070
0.0000028	0.0000011	0.0000004	-0.0000000	-0.0000000	-0.0000000	-0.0000000
1	3	1	3	2		
4	5	4	5	2		
2	3	5	4	1		
2	3	4	5	2		
1	2	4	4	2		

IV. MULTIPOLE INTEGRALS

Two programs are given in this section, each using a different type of radial mesh, to calculate multipole integrals defined as

$$(i|r^k|j) = \int_0^\infty P_i(r)P_j(r)r^k dr.$$

A. Logarithmic Mesh

HFRPOL computes multipole integrals for wavefunctions using a logarithmic radial mesh such as those output by the HF program.

1. Data Input

- a. Card 1. NWF, NK, ATOM, Z in Format (2I3, A6, F3.0).
- b. Card 2. NWF values of L(I) in Format (20I3).
- c. NWF decks of card type 3: EL(I), M, (P(I,J), J=1,M) in Format (32X, A3, I6/(7F 11.7)).

These are decks of $\bar{P}_i$ card output from HF.

- d. NK cards of type 4: I, J, K in Format (3I3).

Multiple runs may be stacked sequentially.

The output contains values of multipole integrals, together with pseudo "absolute" values calculated using the modulus of each $\bar{P}_i$ and cancellation factors defined as the ratio of these.

2. Listing of HFRPOL

```

PROGRAM HFRPOL
DIMENSION R(200),P(20,200),L(20),EL(20),MAX(20),AP(20,200)
COMMON R,P,L,EL,MAX,H3,Z,AP
H = .0625
RHO = -3.0
H3 = H/1.5
1 READ 2,NWF,NK,ATOM,Z
2 FORMAT(2I3,A6,F3.0)
  IF (EOF,60) 30,31
30 CALL EXIT
31 PRINT 13,ATOM,Z
13 FORMAT(1H1,*INTEGRALS FOR*,2X,A6,2X,* ATOMIC NUMBER*,F5.0//)
DO 48 I=1,200
  R(I) = EXP(RHO)/Z
48  RHO = RHO + H
  RHO = -3.0
  READ 49, (L(I),I=1,NWF)
49  FORMAT(20I3)
DO 8 I = 1,NWF
  READ 7, EL(I),M,(P(I,J), J=1,M)
7  FORMAT( 32X,A3,I6/(7F11.7))
8  MAX(I) = M
DO 50 I=1,NWF
  M = MAX(I)
DO 51 J=1,M
  AP(I,J) = ABS(P(I,J))
51  CONTINUE
50  CONTINUE
DO 10 I = 1,NK
  READ 5,II,JJ,M
5  FORMAT(3I3)
  ANS = QUADR(II,JJ,M)
  ABANS = ABQDR(II,JJ,M)
  CANS = ANS/ABANS
10  PRINT 12,EL(II),EL(JJ),M,ANS, ABANS, CANS
12  FORMAT(1H0, 70X,3HABS, 6X, *CANCELLATION*,/
1    5X,*THE INTEGRAL OF P(*A3,6H) * P(A3,8H) * R**(12,
2  5H) = , 3F14.6 /)
  GO TO 1
END

```

```

FUNCTION QUADR(I,J,KK)
DIMENSION R(200),P(20,200),L(20),EL(20),MAX(20)
COMMON R,P,L,EL,MAX,H3,Z ,AP
K = KK + 2
DEN = L(I) + L(J) + 1 + K
FACT= (1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
D = P(I,1)*P(J,1)*R(1)**K*( (1.+Z*R(1)*FACT)/(DEN*H3)+.5)
M = MIN0(MAX(I),MAX(J))
DO 1 JJ = 2,M,2
  JP = JJ + 1
1 D = D + 2.*P(I,JJ)*P(J,JJ)*R(JJ)**K+P(I,JP)*P(J,JP)*R(JP)**K
QUADR = D*H3
RETURN
END

```

```

FUNCTION ABQDR(I,J,KK)
DIMENSION R(200),P(20,200),L(20),EL(20),MAX(20),AP(20,200)
COMMON R,P,L,EL,MAX,H3,Z ,AP
K = KK + 2
DEN = L(I) + L(J) + 1 + K
FACT= (1./FLOAT(L(I)+1)+1./FLOAT(L(J)+1))/(DEN+1.)
D=AP(I,1)*AP(J,1)*R(1)**K*((1.+Z*R(1)*FACT)/(DEN*H3)+.5)
M = MIN0(MAX(I),MAX(J))
DO 1 JJ = 2,M,2
  JP = JJ + 1
1 D=D+2.*AP(I,JJ)*AP(J,JJ)*R(JJ)**K+AP(I,JP)*AP(J,JP)*R(JP)**K
ABQDR = D*H3
RETURN
END

```

3. Sample Data for HFRPOL

For the example given here, three sets of $\bar{P}_i$'s will be read in. The first set is a 5p function obtained from the solution of the configuration $4f^6$ of Eu IV. The second and third sets are the 5p and 6p functions obtained from the solution of the core-excited configuration $5p^5 4f^6 6p$ of Eu IV.

The output specified will calculate

$$\left. \begin{array}{l} (5p|r^2|6p) \\ (5p|r^{-3}|6p) \end{array} \right\} \text{the 5p being that from the } 4f^6 \text{ solution,}$$

and

$$\left. \begin{array}{l} (5p|r^2|6p) \\ (5p|r^{-3}|6p) \end{array} \right\} \text{the 5p being that from the } 5p^5 4f^6 6p \text{ solution.}$$

Note that only the first two and last four cards of this example input have to be punched manually.

3 4 EU IV 63

1 1 1

ATOM EU IV	TERM	AV.	ELECTRON 5P	151	63		
0.0101395	0.0111181	0.0121900	0.0133637	0.0146487	0.0160553	0.0175945	
0.0192786	0.0211207	0.0231351	0.0253372	0.0277439	0.0303733	0.0332449	
0.0363801	0.0398015	0.0435339	0.0476035	0.0520388	0.0568701	0.0621300	
0.0678530	0.0740762	0.0808385	0.0881817	0.0961493	0.1047874	0.1141444	
0.1242703	0.1352174	0.1470394	0.1597915	0.1735296	0.1883101	0.2041891	
0.2212216	0.2394609	0.2589569	0.2797553	0.3018961	0.3254116	0.3503244	
0.3766457	0.4043721	0.4334833	0.4639390	0.4956752	0.5286010	0.5625945	
0.5974990	0.6331189	0.6692153	0.7055021	0.7416424	0.7772448	0.8118609	
0.8449834	0.8760454	0.9044215	0.9294304	0.9503400	0.9663752	0.9767289	
0.9805761	0.9770921	0.9654744	0.9449692	0.9149012	0.8747077	0.8239756	
0.7624808	0.6902284	0.6074929	0.5148559	0.4132384	0.3039266	0.1885866	
0.0692665	-0.0516190	-0.1713222	-0.2868183	-0.3948842	-0.4921999	-0.5754725	
-0.6415778	-0.6877152	-0.7115693	-0.7114672	-0.6865237	-0.6367632	-0.5632072	
-0.4679203	-0.3540047	-0.2255393	-0.0874595	0.0546240	0.1946626	0.3264574	
0.4439819	0.5417214	0.6150036	0.6602906	0.6754043	0.6596613	0.6139032	
0.5404186	0.4427698	0.3255442	0.1940565	0.0540322	-0.0887056	-0.2285267	
-0.3602488	-0.4793520	-0.5821451	-0.6658841	-0.7288365	-0.7702924	-0.7905204	
-0.7906743	-0.7726542	-0.7389413	-0.6924130	-0.6361566	-0.5732932	-0.5068220	
-0.4394908	-0.3736964	-0.3114153	-0.2541649	-0.2029921	-0.1584893	-0.1208335	
-0.0898447	-0.0650596	-0.0458126	-0.0313184	-0.0207484	-0.0132958	-0.0082243	
-0.0048999	-0.0028052	-0.0015394	-0.0008075	-0.0004038	-0.0001919	-0.0000864	
-0.0000367	-0.0000147	-0.0000055	-0.0000019				

ATOM EU IV	TERM	AV.	ELECTRON 5P	150	63		
0.0105063	0.0115204	0.0126311	0.0138472	0.0151787	0.0166362	0.0182311	
0.0199762	0.0218849	0.0239722	0.0262540	0.0287478	0.0314723	0.0344479	
0.0376964	0.0412417	0.0451091	0.0493260	0.0539217	0.0589279	0.0643781	
0.0703082	0.0767565	0.0837636	0.0913724	0.0996283	0.1085790	0.1182745	
0.1287668	0.1401100	0.1523598	0.1655733	0.1798085	0.1951238	0.2115773	
0.2292262	0.2481254	0.2683268	0.2898778	0.3128197	0.3371860	0.3630003	
0.3902739	0.4190035	0.4491681	0.4807257	0.5136102	0.5477272	0.5829507	
0.6191181	0.6560267	0.6934290	0.7310286	0.7684763	0.8053667	0.8412350	
0.8755557	0.9077412	0.9371436	0.9630567	0.9847222	1.0013369	1.0120643	
1.0160497	1.0124385	1.0003993	0.9791508	0.9479935	0.9063443	0.8537752	
0.7900540	0.7151860	0.6294560	0.5334665	0.4281720	0.3149054	0.1953933	
0.0717579	-0.0534983	-0.1775283	-0.2971975	-0.4091662	-0.5099943	-0.5962696	
-0.6647549	-0.7125489	-0.7372524	-0.7371329	-0.7112741	-0.6597021	-0.5834769	
-0.4847394	-0.3667059	-0.2336049	-0.0905522	0.0566367	0.2016929	0.3381920	
0.4598892	0.5610708	0.6368971	0.6837052	0.6992432	0.6828102	0.6352874	
0.5590586	0.4578301	0.3363731	0.2002155	0.0553132	-0.0922742	-0.2366851	
-0.3725207	-0.4950678	-0.6004736	-0.6858704	-0.7494467	-0.7904634	-0.8092134	
-0.8069306	-0.7856509	-0.7480418	-0.6972089	-0.6364970	-0.5692959	-0.4988647	
-0.4281793	-0.3598130	-0.2958500	-0.2378369	-0.1867714	-0.1431270	-0.1069103	
-0.0777431	-0.0549612	-0.0377189	-0.0250880	-0.0161439	-0.0100309	-0.0060049	
-0.0034549	-0.0019048	-0.0010028	-0.0005018	-0.0002370	-0.0001046	-0.0000424	
-0.0000152	-0.0000044	-0.0000008					

ATOM EU IV	TERM	AV.	ELECTRON 6P	161	63		
0.0040485	0.0044393	0.0048672	0.0053359	0.0058489	0.0064106	0.0070251	
0.0076976	0.0084331	0.0092374	0.0101167	0.0110776	0.0121274	0.0132741	
0.0145259	0.0158920	0.0173822	0.0190071	0.0207781	0.0227071	0.0248073	
0.0270923	0.0295771	0.0322772	0.0352091	0.0383904	0.0418394	0.0455754	
0.0496185	0.0539894	0.0587096	0.0638011	0.0692864	0.0751878	0.0815278	
0.0883283	0.0956107	0.1033947	0.1116987	0.1205386	0.1299272	0.1398737	
0.1503823	0.1614518	0.1730740	0.1852327	0.1979023	0.2110465	0.2246165	
0.2385497	0.2527677	0.2671752	0.2816577	0.2960805	0.3102871	0.3240983	
0.3373113	0.3496994	0.3610126	0.3709784	0.3793043	0.3856804	0.3897840	
0.3912853	0.3898547	0.3851714	0.3769344	0.3648738	0.3487651	0.3284436	
0.3038206	0.2748991	0.2417903	0.2047282	0.1640834	0.1203728	0.0742659	
0.0265853	-0.0216990	-0.0694833	-0.1155528	-0.1586129	-0.1973306	-0.2303838	
-0.2565188	-0.2746131	-0.2837402	-0.2832340	-0.2727473	-0.2523017	-0.2232366	
-0.1836632	-0.1375931	-0.0857839	-0.0302556	0.0266958	0.0825952	0.1349063	
0.1811647	0.2191183	0.2468648	0.2629748	0.2665872	0.2574695	0.2360335	
0.2033091	0.1608766	0.1107684	0.0553500	-0.0028092	-0.0610658	-0.1168251	
-0.1676537	-0.2113782	-0.2461696	-0.2706095	-0.2837388	-0.2850839	-0.2746610	
-0.2529583	-0.2208973	-0.1797779	-0.1312128	-0.0770555	-0.0193261	0.0398620	
0.0983745	0.1541286	0.2051672	0.2497342	0.2863517	0.3138934	0.3316498	
0.3393776	0.3373222	0.3262102	0.3072052	0.2818272	0.2518404	0.2191196	
0.1855075	0.1526793	0.1220298	0.0945951	0.0710172	0.0515532	0.0361225	
0.0243833	0.0158230	0.0098488	0.0058656	0.0033338	0.0018032	0.0009253	
0.0004491	0.0002054	0.0000882	0.0000354	0.0000132	0.0000046	0.0000015	

1 3 2

1 3 -3

2 3 2

2 3 -3

B. Linear Mesh

HFSRPOL computes multipole integrals for wavefunctions using a Herman and Skillman type radial mesh.⁵ Also, if $I = J$, it computes the screening number σ .

1. Data Input

- a. Card 1. NWF, NK, Z in Format (2I5, F5.0).
- b. Card 2. Any suitable title in Format (9A8).
- c. NWF decks of type 3: N(I), L(I), M, (P(I,J),J=1,M) in Format (1X, I2, I1, 31X, I5/(6F 13.7)).

These are decks of P_i card output from Herman and Skillman program.

- d. NK cards of type 4: I, J, K in Format (3I5).

Multiple runs may be stacked sequentially.

2. Listing of HFSRPOL

```
PROGRAM HFSRPOL
```

```
DIMENSION PNL(25,521),R(521),RS(521),N(25),L(25),NPTS(25),
```

```
1HEAD(9),A(6)
```

```
DATA (A = 1HS,1HP,1HD,1HF,1HG,1HH)
```

```
1000 READ 100,NORBITS,NINTGRLS,Z,HEAD
```

```
100 FORMAT(2I5,F5.0/9A8)
```

```
IF (EOF,60) 20,21
```

```
20 CALL EXIT
```

```
21 PRINT 200,HEAD
```

```
200 FORMAT(1H1,9A8//)
```

```
LIMIT = 0.0
```

```
DO 1 I = 1,NORBITS
```

```
READ 101,N(I),L(I),NPT,(PNL(I,J), J=1,NPT)
```

```
101 FORMAT(1X,I2,I1,31X,I5/(6F13.7))
```

```
NPTS(I) = NPT
```

```
1 LIMIT = MAX0(LIMIT,NPTS(I))
```

C
C
C

```
GENERATE R ARRAY
```

```
RINCR = 0.88534138 * Z**(-1./3.) * 0.0025
```

```
H = 0.5 * RINCR
```

```
R(1) = 0.0
```

```
NBLKS = LIMIT/40
```

```
MIN = -38
```

```

DO 3 INDX = 1,NBLKS
MIN = MIN + 40
MAX = MIN + 39
H = 2. * H
DO 3 K = MIN,MAX
3 R(K) = R(K-1) + H

C
C   COMPUTE INTEGRALS
C
DO 4 INDX = 1,NINTGRLS
READ 102,I1,I2,NXP
102 FORMAT(3I5)
LIMIT = MIN0(NPTS(I1),NPTS(I2))
IF (NXP .EQ. 1) GO TO 6
IF (NXP .EQ. 0) GO TO 13
DO 5 J = 1,LIMIT
RS(J) = R(J)
5 R(J) = R(J)**NXP
GO TO 6
13 DO 12 J = 1,LIMIT
RS(J) = R(J)
12 R(J) = 1.0
6 NBLKS = LIMIT/40
J = -4
H = 0.5 * RINCR
RINT = 0.0
DO 7 I1 = 1,NBLKS
H = 2.0 * H
SUM = 0.0
DO 8 NC = 1,8
J = J + 5
8 SUM = SUM + 19.*(R(J)*PNL(I1,J)*PNL(I2,J) + R(J+5)*PNL(I1,J+5)*
1PNL(I2,J+5)) + 75.*(R(J+1)*PNL(I1,J+1)*PNL(I2,J+1) + R(J+4)*
2PNL(I1,J+4)*PNL(I2,J+4)) + 50.*(R(J+2)*PNL(I1,J+2)*PNL(I2,J+2) +
3R(J+3)*PNL(I1,J+3)*PNL(I2,J+3))
7 RINT = RINT + H*SUM
RINT = 5.*RINT/288.

C
IF (NXP .EQ. 1) GO TO 10
DO 9 JJ = 1,LIMIT
9 R(JJ) = RS(JJ)
10 IF (I1 .NE. I2) GO TO 11
RH = 0.5 * (3.*N(I1)*N(I1) - L(I1)*L(I1) - L(I1))
SIGMA = Z - RH/RINT
KK = L(I1) + 1
PRINT 201,N(I1),A(KK),NXP,RINT,SIGMA
201 FORMAT(1H0,5X,*INTEGRAL OF P(*I2,A1,12H) **2 * R**(.I2,*) IS *,
1F16.7/10X,*SIGMA IS *,F16.7/)
GO TO 4
11 K1 = L(I1) + 1
K2 = L(I2) + 1
PRINT 202,N(I1),A(K1),N(I2),A(K2),NXP,RINT
202 FORMAT(1H0,5X,*INTEGRAL OF P(*I2,A1,6H) * P(I2,A1,8H) * R**(.I2,*)
1 IS *,F16.7/)
4 CONTINUE
GO TO 1000
END

```

3. Sample Data for HFSRPOL

The two sets of P_i 's to be read in are the 5f and 6d functions obtained from the $5f6d^2$ configuration of Th II.

The output specified will calculate

$(5f|r|5f)$ and σ_{5f} ,

$(5f|r|6d)$,

and

$(6d|r|6d)$ and σ_{6d} .

Note that only the first two and last four cards of this example input have to be punched manually.

```

  2      3  90.
TH II  5F/6D2  SCREENING  ++ DIPOLE INTEGRAL
531      3      -1.2060613      1  401      11558.3189623      90
0.0000000  0.0000000  0.0000000  0.0000001  0.0000002  0.0000004
0.0000008  0.0000015  0.0000026  0.0000041  0.0000062  0.0000089
0.0000125  0.0000170  0.0000226  0.0000295  0.0000378  0.0000477
0.0000593  0.0000728  0.0000884  0.0001063  0.0001267  0.0001497
0.0001756  0.0002045  0.0002367  0.0002723  0.0003116  0.0003548
0.0004020  0.0004535  0.0005095  0.0005701  0.0006357  0.0007063
0.0007822  0.0008637  0.0009508  0.0010439  0.0011430  0.0013605
0.0016048  0.0018775  0.0021801  0.0025141  0.0028808  0.0032817
0.0037180  0.0041912  0.0047024  0.0052527  0.0058434  0.0064754
0.0071498  0.0078675  0.0086294  0.0094363  0.0102889  0.0111881
0.0121344  0.0131283  0.0141706  0.0152615  0.0164016  0.0175912
0.0188305  0.0201199  0.0214596  0.0228496  0.0242900  0.0257810
0.0273224  0.0289143  0.0305566  0.0322490  0.0339914  0.0357836
0.0376253  0.0395161  0.0414558  0.0434800  0.0454800  0.0474943
0.0586764  0.0634346  0.0683639  0.0734582  0.0787117  0.0841176
0.0896695  0.0953602  0.1011827  0.1071296  0.1131934  0.1193665
0.1256414  0.1320101  0.1384649  0.1449980  0.1516016  0.1582679
0.1649891  0.1717574  0.1785652  0.1854050  0.1922693  0.1991507
0.2060419  0.2129358  0.2198255  0.2267040  0.2335647  0.2404010
0.2472066  0.2539753  0.2607009  0.2673777  0.2740000  0.2805623
0.2870592  0.2998366  0.3122934  0.3243936  0.3361045  0.3473958
0.3582405  0.3686141  0.3784949  0.3878640  0.3967046  0.4050026
0.4127462  0.4199256  0.4265331  0.4325629  0.4380112  0.4428756
0.4471555  0.4508516  0.4539661  0.4565023  0.4584647  0.4598590
0.4606917  0.4609703  0.4607030  0.4598988  0.4585673  0.4567189
0.4543643  0.4515148  0.4481820  0.4443779  0.4401148  0.4354054
0.4302624  0.4246988  0.4187276  0.4123619  0.4056150  0.3910304
0.3750792  0.3578658  0.3394928  0.3200607  0.2996670  0.2784061
0.2563692  0.2336438  0.2103137  0.1864588  0.1621553  0.1374755
0.1124878  0.0872571  0.0618444  0.0363070  0.0106989  -0.0149296
-0.0405313  -0.0660624  -0.0914819  -0.1167521  -0.1418379  -0.1667069
-0.1913296  -0.2156786  -0.2397289  -0.2634578  -0.2868446  -0.3098705
-0.3325188  -0.3547741  -0.3766231  -0.3980538  -0.4190554  -0.4396190
-0.4597364  -0.4794011  -0.4986073  -0.5156270  -0.5307705  -0.5440266
-0.6353963  -0.6648914  -0.6925329  -0.7183499  -0.7423781  -0.7646592
-0.7852395  -0.8041689  -0.8215008  -0.8372905  -0.8515952  -0.8644730
-0.8759829  -0.8861838  -0.8951346  -0.9028937  -0.9095187  -0.9150662

```

-0.9195916	-0.9231490	-0.9257912	-0.9275693	-0.9285326	-0.9287292	
-0.9282048	-0.9270040	-0.9251692	-0.9227411	-0.9197588	-0.9162593	
-0.9122782	-0.9078493	-0.9030046	-0.8977746	-0.8921891	-0.8862726	
-0.8800538	-0.8668031	-0.8526153	-0.8376497	-0.8220477	-0.8059341	
-0.7894193	-0.7726006	-0.7555641	-0.7383853	-0.7211308	-0.7038592	
-0.6866221	-0.6694644	-0.6524257	-0.6355403	-0.6188381	-0.6023451	
-0.5860834	-0.5700720	-0.5543269	-0.5388617	-0.5236873	-0.5088128	
-0.4942452	-0.4799900	-0.4660510	-0.4524308	-0.4391308	-0.4261512	
-0.4134914	-0.4011500	-0.3891247	-0.3774128	-0.3660108	-0.3549150	
-0.3441210	-0.3336242	-0.3234198	-0.3135025	-0.3038671	-0.2854195	
-0.2680314	-0.2516561	-0.2362466	-0.2217560	-0.2081391	-0.1953477	
-0.1833411	-0.1720758	-0.1615110	-0.1516076	-0.1423293	-0.1336375	
-0.1255014	-0.1178879	-0.1107664	-0.1041043	-0.0978607	-0.0920282	
-0.0865569	-0.0814272	-0.0766162	-0.0721022	-0.0678651	-0.0638867	
-0.0601497	-0.0566385	-0.0533384	-0.0502339	-0.0473185	-0.0445745	
-0.0419930	-0.0395639	-0.0372777	-0.0351257	-0.0330998	-0.0311922	
-0.0293957	-0.0277037	-0.0261100	-0.0231942	-0.0206057	-0.0183070	
-0.0162652	-0.0144512	-0.0128393	-0.0114069	-0.0101338	-0.0090022	
-0.0079965	-0.0071025	-0.0063079	-0.0056017	-0.0049740	-0.0044162	
-0.0039204	-0.0034799	-0.0030886	-0.0027409	-0.0024320	-0.0021576	
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-0.0002164	-0.0001694	-0.0001325	-0.0001036	-0.0000810	-0.0000633	
-0.0000494	-0.0000386	-0.0000301	-0.0000235	-0.0000183	-0.0000143	
-0.0000111	-0.0000087	-0.0000067	-0.0000052	-0.0000041	-0.0000032	
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-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	
621	2	-0.7408393	2	441	2996.6994403	90
0.0000000	0.0000004	0.0000028	0.0000093	0.0000218	0.0000419	
0.0000714	0.0001117	0.0001642	0.0002304	0.0003114	0.0004085	
0.0005225	0.0006546	0.0008057	0.0009764	0.0011677	0.0013802	
0.0016144	0.0018710	0.0021504	0.0024531	0.0027794	0.0031296	
0.0035041	0.0039029	0.0043263	0.0047744	0.0052474	0.0057451	
0.0062677	0.0068151	0.0073871	0.0079838	0.0086050	0.0092505	
0.0099201	0.0106136	0.0113307	0.0120712	0.0128348	0.0144299	
0.0161132	0.0178816	0.0197319	0.0216604	0.0236635	0.0257372	
0.0278775	0.0300802	0.0323412	0.0346560	0.0370204	0.0394299	
0.0418802	0.0443667	0.0468851	0.0494310	0.0520001	0.0545881	
0.0571907	0.0598037	0.0624230	0.0650446	0.0676644	0.0702789	
0.0728838	0.0754758	0.0780512	0.0806066	0.0831386	0.0856438	
0.0881192	0.0905618	0.0929685	0.0953367	0.0976635	0.0999464	
0.1021829	0.1043707	0.1065075	0.1106198	0.1145038	0.1181456	
0.1215328	0.1246547	0.1275019	0.1300668	0.1323432	0.1343261	
0.1360119	0.1373982	0.1384838	0.1392685	0.1397531	0.1399394	
0.1398301	0.1394286	0.1387391	0.1377666	0.1365166	0.1349952	
0.1332089	0.1311650	0.1288708	0.1263344	0.1235638	0.1205676	
0.1173545	0.1139334	0.1103134	0.1065038	0.1025139	0.0983531	
0.0940309	0.0895567	0.0849400	0.0801902	0.0753167	0.0703288	
0.0652358	0.0547707	0.0439928	0.0329713	0.0217727	0.0104607	
-0.0009045	-0.0122654	-0.0235685	-0.0347633	-0.0458030	-0.0566443	
-0.0672473	-0.0775755	-0.0875957	-0.0972779	-0.1065954	-0.1155244	
-0.1240439	-0.1321358	-0.1397845	-0.1469771	-0.1537020	-0.1599533	
-0.1657221	-0.1710048	-0.1757989	-0.1801035	-0.1839193	-0.1872485	
-0.1900946	-0.1924623	-0.1943577	-0.1957875	-0.1967597	-0.1972830	
-0.1973670	-0.1970216	-0.1962578	-0.1950867	-0.1935201	-0.1892492	
-0.1835458	-0.1765137	-0.1682590	-0.1588884	-0.1485080	-0.1372227	
-0.1251350	-0.1123448	-0.0983487	-0.0850394	-0.0707060	-0.0560331	
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0.1350574	0.1480230	0.1605659	0.1726645	0.1842997	0.1954551	
0.2061167	0.2162729	0.2259141	0.2350327	0.2436230	0.2516809	
0.2592042	0.2661919	0.2726444	0.2839521	0.2921547	0.3002950	
0.3054295	0.3086249	0.3099569	0.3095077	0.3073647	0.3036189	

0.2983634	0.2916927	0.2837014	0.2744834	0.2641316	0.2527368
0.2403875	0.2271698	0.2131663	0.1984569	0.1831179	0.1672220
0.1508386	0.1340334	0.1168685	0.0994026	0.0816909	0.0637850
0.0457334	0.0275813	0.0093709	-0.0088588	-0.0270714	-0.0452334
-0.0633139	-0.0812844	-0.0991187	-0.1167930	-0.1342854	-0.1515761
-0.1686470	-0.2020660	-0.2344313	-0.2656541	-0.2956658	-0.3244148
-0.3518645	-0.3779912	-0.4027823	-0.4262346	-0.4483532	-0.4691502
-0.4886435	-0.5068561	-0.5238152	-0.5395512	-0.5540975	-0.5674897
-0.5797651	-0.5909622	-0.6011204	-0.6102798	-0.6184807	-0.6257632
-0.6321674	-0.6377330	-0.6424991	-0.6465042	-0.6497858	-0.6523806
-0.6543247	-0.6556526	-0.6563982	-0.6565941	-0.6562720	-0.6554622
-0.6541943	-0.6524964	-0.6503958	-0.6479185	-0.6450895	-0.6384716
-0.6307214	-0.6220032	-0.6124661	-0.6022460	-0.5914655	-0.5802357
-0.5686564	-0.5568175	-0.5447996	-0.5326750	-0.5205077	-0.5083546
-0.4962666	-0.4842884	-0.4724581	-0.4607941	-0.4492992	-0.4379752
-0.4268238	-0.4158467	-0.4050455	-0.3944218	-0.3839771	-0.3737127
-0.3636298	-0.3537292	-0.3440119	-0.3344785	-0.3251293	-0.3159647
-0.3069847	-0.2981892	-0.2895778	-0.2811500	-0.2729051	-0.2648423
-0.2569605	-0.2492586	-0.2417351	-0.2272178	-0.2133950	-0.2002514
-0.1877700	-0.1759325	-0.1647194	-0.1541100	-0.1440833	-0.1346177
-0.1256910	-0.1172811	-0.1093653	-0.1019231	-0.0949310	-0.0883681
-0.0822132	-0.0764456	-0.0710452	-0.0659925	-0.0612686	-0.0568553
-0.0527349	-0.0488906	-0.0453062	-0.0419663	-0.0388560	-0.0359612
-0.0332686	-0.0307655	-0.0284397	-0.0262798	-0.0242751	-0.0224152
-0.0206905	-0.0190920	-0.0176111	-0.0162397	-0.0149704	-0.0137959
-0.0127097	-0.0107775	-0.0091285	-0.0077234	-0.0065276	-0.0055114
-0.0046489	-0.0039177	-0.0032985	-0.0027748	-0.0023323	-0.0019587
-0.0016438	-0.0013784	-0.0011551	-0.0009672	-0.0008094	-0.0006769
-0.0005657	-0.0004725	-0.0003944	-0.0003290	-0.0002743	-0.0002286
-0.0001904	-0.0001585	-0.0001319	-0.0001097	-0.0000912	-0.0000758
-0.0000629	-0.0000522	-0.0000433	-0.0000360	-0.0000298	-0.0000247
-0.0000205	-0.0000170	-0.0000140	-0.0000116	-0.0000096	-0.0000066
-0.0000045	-0.0000031	-0.0000021	-0.0000014	-0.0000010	-0.0000007
-0.0000004	-0.0000003	-0.0000002	-0.0000001	-0.0000001	-0.0000001
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000	-0.0000000
1	1	1			
1	2	1			
2	2	1			

V. CENTRAL POTENTIAL

A. Discussion

It is sometimes of interest to study the details of the so-called central potential. Therefore, we have written an optional subroutine (CPOTL) which may be used in conjunction with the HF program to give such details.

This subroutine lists, as functions of r , the following:

1. CENPOT 1, the central potential, for an electron in the specified orbital i, defined as

$$\frac{2}{r}[z - Y_i(r) - X_i(r)],$$

where $X_i(r)$ are the usual exchange terms plus contributions due to inclusion of the off-diagonal ϵ_{ij} terms.

2. EFF CENPOT 1, the effective central potential, defined as

$$\text{CENPOT 1} = \frac{\ell_i(\ell_i + 1)}{r^2}.$$

3. RPOT 1, the effective central potential multiplied by r .

4. CENPOT 2, as for item 1 above, except that $X_i(r)$ is defined so as not to include the effects of ϵ_{ij} .

5. EFF CENPOT 2, as for item 2 above, except that $X_i(r)$ is defined so as not to include the effects of ϵ_{ij} .

6. RPOT 2, as for item 3 above, except that $X_i(r)$ is defined so as not to include the effects of ϵ_{ij} .

7. CORE, the total charge distribution, defined as

$$\sum_i \int_0^r P_i^2(r) q_i dr,$$

where q_i is the occupation number of the i th orbital.

8. ZNL, Slater's effective Z for wavefunction, defined as

$$Z_{pi} = Z - \int_0^{r_i} \sum_{j \neq i} P_j^2 dr_j - \int_{r_i}^{\infty} \sum_{j \neq i} P_j^2 \frac{r_i}{r_j} dr_j. \quad (\text{Ref. 1, §9.7})$$

This subroutine is used by inserting the statement CALL CPOTL immediately after the statement CALL PRNT in HF MAIN and adding before the PNCH control card (i.e., card of type 11 in Ref. 2) an extra data card which contains NCORE and K in FORMAT (2I3). NCORE is an integer defining the number of orbitals required to define the core, and K is an index of the first orbital for which a detailed printout of the CPOTL option is required. For example, in the case of $\text{ScI } 1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$, NCORE = 6 will give the charge density due to all six orbitals and K = 5 will give details of the central potential, etc., for just the 3p and 3d orbitals (i.e., the fifth and sixth).

B. Listing of Subroutine CPOTL

```

SUBROUTINE CPOTL
  LOGICAL FAIL, RSCAN
  COMMON ATOM, TERM, NWF, Z, NP, H, NO, EL(20), N(20), L(20), D(100), SUM(20),
1   EK(20), E(20,20), R(200), RR(200), R2(200), P(20,200), Y(20,200),
2   YK(200), YR(200), X(200), DD(2402), B(20,20,4), DDD(62), NR, CR(10),
3   KR(10), I1R(10), I2R(10), NCRI(10), J1R(10), J2R(10), NCRJ(10), NCFG,
4   WT(6), QC(20,6)/TEST/FAIL, RSCAN(20)
  DIMENSION MAX(20)
  EQUIVALENCE ( MAX(1), D(61) )
  DIMENSION VNL1(200), VNL2(200), VLL1(200), EVNL1(200), EVNL2(200),
1 VLL2(200), TC(200), ZC(200)
  READ 56, NCORE, K
56  FORMAT (2I3)
  PTOL = 2.E-7*SQRT(Z)
  DO 6 I = K, NWF
  PRINT 55
55  FORMAT(1H1, /2X47HVALUES OF CENTRAL AND EFFECTIVE POTENTIAL VS R /)
  PRINT 7, EL(I)
7   FORMAT( 4XA3/5X1HR10X8HCENPOT 1, 6X12HEFF CENPOT 16X8HCENPOT 2 3X,
112HEFF CENPOT 2, 6X8H RPOT 1 3X12H RPOT 2, 10X4HCORE11X3HZNL)
  CALL POTL(I)
  CALL XCH(I,3)
  M = MAX(I)
  DO 1 JJ = 1, M
  IF(JJ.LT. 40) GO TO 57
  IF(ABS(P(I,JJ)*R2(JJ)).LE. PTOL) GO TO 14
57  CONTINUE
  VNL1( JJ) = (2.*(Z-YR(JJ))-(X(JJ) )/P(I,JJ))/R(JJ)
  VLL1( JJ) = VNL1( JJ)*R(JJ)
  EVNL1( JJ) = VNL1( JJ)-((L(I)*(L(I)+1))/R(JJ)*R(JJ))
  VNL1(JJ) = -VNL1(JJ)
  VLL1(JJ) = -VLL1(JJ)
  EVNL1(JJ) = -EVNL1(JJ)
1  CONTINUE
14  M=JJ -1
  CALL XCH(I,1)
  DO 11 JJ = 1, M
11  X(JJ) = R(JJ)*X(JJ)
  DO 2 JJ = 1, M
  VNL2( JJ) = (2.*(Z-YR(JJ))-(X(JJ)/P(I,JJ)))/R(JJ)
  VLL2( JJ) = VNL2( JJ)*R(JJ)
  EVNL2( JJ) = VNL2( JJ)-((L(I)*(L(I)+1))/R(JJ)*R(JJ))
  VNL2(JJ) = -VNL2(JJ)
  VLL2(JJ) = -VLL2(JJ)
  EVNL2(JJ) = -EVNL2(JJ)
2  CONTINUE
  DO 8 JJ = 1, M
  ZC(JJ) = Z
  TC(JJ) = 0
  DO 9 K = 1, NCORE
  TC(JJ) = TC(JJ) + ((P(K,JJ)*R2(JJ))**2)*QC(K,1)
9  CONTINUE
  ZC(JJ) = Z
  DO 13 K = 1, NWF
  C = QC(K,1)
  IF(K.EQ. 1) C=C-1.
13  ZC(JJ) = ZC(JJ) -C*Y(K,JJ)
8  CONTINUE
  DO 5 JJ = 1, M
  PRINT 4, R(JJ), VNL1(JJ), EVNL1(JJ), VNL2(JJ), EVNL2(JJ), VLL1(JJ),
1 VLL2(JJ), TC(JJ), ZC(JJ)
4  FORMAT (F11.5, 8F15.5)
5  CONTINUE
6  CONTINUE
  RETURN
  END

```

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