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PROGRAMS FOR ATOMIC-STRUCTURE CALCULATIONS

by

C. Froese Fischer and M. Wilson

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C. Froese Fischer* and M. Wilson

Chemistry Division

January 1968

*Department of Mathematics and Computing Centre,
University of British Columbia, Vancouver 8, B.C.

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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 theory[1] 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 ($I_{n\ell}$). 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 $\overline{P}_i$ 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 $\overline{P}_i$'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 $\overline{P}_i$'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 $\overline{P}_i$'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 $\overline{P}_i$'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 Watson[3] (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

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

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 Watson[3] 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 output[5] 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.

	Page		Page
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XCH	24		

```
      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) ,
     1DUMMY(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 I3,22H GROUPS ARE INCOMPLETE/9X,
     2 8HTHE LAST I3,29H WILL BE MADE SELF-CONSISTENT  //
     3 20X,5HRHO = F12.7/20X,5HH   = F12.7/20X,5HNO  = I4)
      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,DELTAE,ID)
      IF (ABS(DELTAE/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,
       4WT(6),QC(20,6)/TEST/FAIL,RSCAN(20)/SCRAP/CONFIG(2),NFG,I1,I2,J1,J2
        COMMON/TSOLVE/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,I6,3I3)
        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),5X6HA7(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,12HE(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(1) .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,II,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.
    1 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
    8 A(I,I,KL) = A(I,I,KL) - CC*CA(LI-1,KL-1)
      GO TO 4
    5 CC = C*QC(I,K)*QC(J,K)
      A(I,J,1) = A(I,J,1) + CC
      DO 9 KL =1,4
    9 B(I,J,KL) = B(I,J,KL) - CC*CB(LI,LJ,KL)
    4 CONTINUE
    3 SUM(I) = SUM(I) + C*QC(I,K)
    2 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)
      II = IFG(I)
      IJ = JFG(I)
      A(II,IJ,K) = A(II,IJ,K) + CON
   11 A(IJ,II,K) = A(IJ,II,K) + CON
   10 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,NO
    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) -EKIN(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(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
```

```
      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
11    P(I,K) = P(I,K) - D*P(J,K)
      DI = SQRT(QUADR(I,I,0))
      DO 12 K = 1,MX
12    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.
       PN1 = 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))/R2(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(I)
       FL = L(I)
       C = 4.*FL +6.
       CN = (2.*Z/FN)**(L(I) +1)
      CH = H*H/12.
      DO 26 J = 1,NO
   26 YR(J) = (YK(J) + ED*RR(J))*CH
    3  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 HQ(J)    = AZD*(HW + R(J)**(L(I)+3)*B3*(1.-R(J)*B4))/R2(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(I,M,Q1,Q1)
       A3 = QUAD(I,M,Q1,Q2)
      A4 = QUAD(I,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(I),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,I,0))
       DO 10 J=1,MI
   10  P(I,J) = P(I,J)/PNORM
8     CALL YKF(I,I,0)
       DO 11 J=1,NO
   11  Y(I,J) = YK(J)
      E(I,I) = C*E(I,I) + (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) + IABS(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 II=1,NR
      N1 = NCRI(II)
      N2 = NCRJ(II)
      C = WT(N1)*WT(N2)*CR(II)/SUM(I)
      DO 11 I2=1,2
      DO 12 I1=1,2
      IF (I1R(II) .NE. I) GO TO 13
      CALL YKF(I2R(II),J2R(II),KR(II))
      M = J1R(II)
      DO 14 J=1,NO
14    X(J) = X(J) + C*P(M,J)*YK(J)
13    III = I1R(II)
      I1R(II)= I2R(II)
      I2R(II)= III
      III = J1R(II)
      J1R(II) = J2R(II)
12    J2R(II) = III
      III = I1R(II)
      I1R(II) = J1R(II)
      J1R(II) = III
      III = I2R(II)
      I2R(II)= J2R(II)
11    J2R(II)= III
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. I)) GO TO 7
      DO 9 JJ = 1,NO
    9 X(JJ) = X(JJ) + C*P(J,JJ)*RR(JJ)
```

```
    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 = .0000001*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,DELTAE,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),NCRJ(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 = IB, NWF
 1    EK(I) = -.5*(EKIN(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))
      ET(N1,N2) = ET(N1,N2) + CONT
 13   ET(N2,N1) = ET(N2,N1) + CONT
 12   IF (NR .EQ. 0) GO TO 14
      DO 15 I =1,NR
```

```
      N1 = NCRI(I)
      N2 = NCRJ(I)
      CONT =.5*CR(I)                    *RK(I1R(I),I2R(I),J1R(I),J2R(I),KR(I))
      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)
20    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 )
   33 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,I5,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(I3)
       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   NCRI(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 = I,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*QUADR(I,I,-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/R3(20),RM,RMM,RH,SC,RMMM,RMMMM,SC(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)
      RMMMM=QUADR(I,I,4)
      RH = 3*N(I)*N(I) - L(I)*(L(I) + 1)
      SC = Z - .5*RH/RM
      RH = 3*N(I)*N(I) - L(I)*(L(I) + 1)
      SC = Z - .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),RMMMM
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  I3, 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.,-.2.0., .2.0.,-.08571428,0.,.085714286,0.,
     1 0.,-.6,0., -.6,0.,-.17142857, 0.,-.08571428,0.,.257142857,0.,
     2 -0.02857142857,
     3 0.,0.,-.42857143, 0.,-.34285714,0., -.51428571,0.,-.085714285,
     4   0.,-.057142857,0.,
     5 0.,0.,0., 0.,0.,-.23809523, 0.,-.28571428,0., -.476190476,0.,
     6 -0.0649350649,
     7 0.,0.,0., 0.,0.,0., 0.,0.,-.19480519, 0.,-.259740259,0.,
     8 0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,-0.174825175)
      DATA(CN=2.,0.,0., 0.,.8,),., .8,0., .514285714, 0.,.514285714,0.,
     1  0.,1.8,0., -1.0,0.,.85714285, 0.,-.6,0., 1.28571428,0.,
     2 -0.4285714285,
     3 -1.,0.,1.7142857, 0.,-.14285714,0., -1.6857143,0.,-.25714285,
     40.,-.714285714,0.,0.,-1.2,0.,0.,0.,-.04761905,0.,-.17142857,0.,
     5-2.4761905,0.,-0.142857142,
     6 0.,0.,-1.28571428, 0.,-.34285714,0., .51428571,0.,.033766233,
     70.,-.3688311688,0.,0.,0.,0.,0.,0.,-.47619047,0.,0.,0.,.9523809524,
     80.,-0.06493506492,
     9 0.,0.,0., 0.,0.,0., 0.,0.,-.19480519, 0., .2597402597,0.)
      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 = 7*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(20X11HZETACVN-SSD   ,1H(A3,3H,M2,4H) = F10.2,5X2F10.5/)
      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(20X11HZETACVN-SSF   ,1H(A3,3H,M4,4H) = F10.2,5X4F10.5/)
      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(20XI4,6H 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,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)/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,NO,EL(20),D(100),MAX(20),DD(1060),
     1   P(20,200)/SCRAP/IW(20)
      DIMENSION EK(20),EKPNCH(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,I6,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)
      EKPNCH(I) = EK(KK)
      I = I +1
9     CONTINUE
      PUNCH 25, (EKPNCH(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,I,0))
      DO 10 J = 1,NO
   10 P(I,J) = P(I,J)/PNORM
      CALL YKF(I,I,0)
      DO 11 J = 1,NO
   11 Y(I,J) = YK(J)
      MAX(I) = K
      E(I,I) = E(I,I)*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  00.397                          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  12.732                          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  00.397                          1  2
 2S  2  0 1.965                         1  2
 2P  2  12.732                          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 $\overline{P}_i$'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 $\overline{P}_i$'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  045.   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  9.0265515  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	4.4357545	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				

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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

$$R^k(i,j,\ell,m) = \int_0^\infty \int_0^\infty P_i(r_1)P_j(r_2)P_\ell(r_1)P_m(r_2)\frac{r_<^k}{r_>^{k+1}}\,dr_1\,dr_2,$$

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 $\overline{P}_i$ 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 $\overline{P}_i$. 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 $\overline{P}_i$'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,I6/(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,I1,1H( 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),
     1DD(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),
     1R(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
```

C. Sample Data for R^k

The example given here will read in five sets of $\overline{P}_i$'s. The first three are 3d, 4s, and 4p obtained from a solution for the configuration 3d4s4p of ScI. The last two are 3d and 4p obtained from a solution for $3d^24p$ of ScI.

The specified R^k integrals output will be

$R^2(3d4p,3d4p) \equiv F^2(3d4p)$ of 3d4s4p,

$R^2(3d4p,3d4p) \equiv F^2(3d4p)$ of $3d^24p$,

and the configuration interaction integrals,

$R^1(4s4p,4p3d)$,

$R^2(4s4p,3d4p)$,

and

$R^2(3d4s,3d3d)$.

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

```
 5SC I          21.  5
 3  2  4  0  4  1  3  2  4  1
ATOM SC I    TERM    AV. ELECTRON 3D    147     21
 0.0000121  0.0000142  0.0000165  0.0000193  0.0000225  0.0000263  0.0000307
 0.0000359  0.0000419  0.0000489  0.0000570  0.0000665  0.0000776  0.0000905
 0.0001056  0.0001232  0.0001436  0.0001674  0.0001951  0.0002274  0.0002649
 0.0003086  0.0003594  0.0004184  0.0004870  0.0005667  0.0006592  0.0007666
 0.0008913  0.0010358  0.0012033  0.0013973  0.0016219  0.0018818  0.0021823
 0.0025296  0.0029305  0.0033931  0.0039264  0.0045406  0.0052475  0.0060602
 0.0069935  0.0080643  0.0092913  0.0106957  0.0123011  0.0141337  0.0162228
 0.0186006  0.0213026  0.0243681  0.0278396  0.0317636  0.0361903  0.0411735
 0.0467710  0.0530438  0.0600560  0.0678746  0.0765683  0.0862075  0.0968624
 0.1086026  0.1214953  0.1356040  0.1509863  0.1676926  0.1857633  0.2052274
 0.2260995  0.2483780  0.2720429  0.2970531  0.3233447  0.3508288  0.3793896
 0.4088825  0.4391327  0.4699335  0.5010459  0.5321973  0.5630823  0.5933636
 0.6226744  0.6506230  0.6767982  0.7007781  0.7221404  0.7404745  0.7553965
 0.7665629  0.7736861  0.7765473  0.7750075  0.7690148  0.7586075  0.7439132
 0.7251426  0.7025809  0.6765761  0.6475250  0.6158605  0.5820379  0.5465240
 0.5097867  0.4722874  0.4344746  0.3967782  0.3596053  0.3233357  0.2883171
 0.2548609  0.2232374  0.1936711  0.1663370  0.1413560  0.1188034  0.0986896
 0.0809825  0.0656019  0.0524273  0.0413054  0.0320579  0.0244902  0.0183996
 0.0135827  0.0098427  0.0069945  0.0048695  0.0033176  0.0022098  0.0014376
 0.0009125  0.0005648  0.0003405  0.0002000  0.0001143  0.0000636  0.0000345
 0.0000182  0.0000094  0.0000047  0.0000023  0.0000011  0.0000005  0.0000000
ATOM SC I    TERM    AV. ELECTRON 4S    152     21
 0.2269389  0.2333831  0.2399594  0.2466652  0.2534971  0.2604513  0.2675227
 0.2747057  0.2819934  0.2893779  0.2968501  0.3043995  0.3120144  0.3196812
 0.3273849  0.3351084  0.3428329  0.3505374  0.3581985  0.3657905  0.3732851
 0.3806513  0.3878550  0.3948591  0.4016235  0.4081044  0.4142547  0.4200237
 0.4253569  0.4301960  0.4344791  0.4381404  0.4411103  0.4433159  0.4446806
 0.4451250  0.4445669  0.4429219  0.4401039  0.4360262  0.4306021  0.4237461
 0.4153749  0.4054094  0.3937759  0.3804079  0.3652484  0.3482522  0.3293882
```

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	-0.1487302	-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			

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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			

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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			

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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	

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 $\overline{P}_i$ 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 $\overline{P}_i$ 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**(I2,
     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 $\overline{P}_i$'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 -0.2223236
-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  0.0308620
 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     GENERATE R ARRAY
C
      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 II = 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
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  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
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  0.3750792   0.3578658   0.3394928   0.3200607   0.2996670   0.2784061
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```

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621 2 -0.7408393 2 441 2996.8994403 90

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-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 ith orbital.

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

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

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 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. I) 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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