REFERENCES

1. Pullman,A.,Pullman,B., Q. Rev. Biophys, 7, (1975) : 505
2. Tsc,Y.C.,Newton,M.D.,Vishveshwera,S.and Pople,J.A., J. Am. Chem. Soc., 100, (1978) : 4329
3. Soenram,R.D.,Lovas,F.J., J. Am Chem. Soc., 102,(1980) : 7180
4. Palla,P.,Petrongolo,C.and Tomasi,J., J. Phys. Chem. 84, (1980) : 435
5. Ramachandran,G.N.and Scheraga,H.A., J. Biol. chem. 241, (1966) : 1004
6. Carozzo,L.,Corongiv,G.,Petrongolo,C.C., Kmenti,E., J.Chem. Phys. 63(3), (1978) : 787
7. Bonaccorsi,R.,Palla,P.and Tomasi,J., J. Am. Chem. Soc. 106, (1984) : 1945
8. Rode, B.M.,Monatsh. Chem. 106,(1975) : 339.
9. Rode B.M., and Sagarik K.P., Chem. Phys. Lett, 88,(1982) : 337.
10. Pople J.A., Santry D.P., and Segal G.A., J. Chem. Phys. 43,(19659 : s129.
11. Mulliken,R,S. J. Chem. Phys.,61 (1957) : 6-13
12. Wolfsberg, M.,and Helmholtz, L., J. Chem. Phys., 20, (1952) : 837-850
13. Pople J.A., Segal G.A., J. Chem. Phys. 43 (1965) : s 136
14. Mulliken, R. S., C. A. Rieke, D. Orloff, and M. Orloff, J.Chem. Phys., 17(19499 :1248
15. Klopman, G., Chem. Phys. Lett.,1 (1967) : 200

Referenced continued

16. Hobza P., and Zabradnik R., Weak IntermolecularInteractions in Chemistry and Biology, 200 ff.,Elsevier Scientific Publishing Company,(1980)

17. Metropolis, N., Rosenbluth, A, W., Teller, A. H., Teller,E. J.Chem. Phys.,21(1953) : 1078

18. Clementi E., Lecture Notes in Chemistry, Vol 19, 94 ff. Springer-Verlag Berlin, 94 ff.(1980)

19. Boys S.F., and Bernardi F., Molecular Physics., 19,(1970) : 553.

20. Segal, G, A., Semiempirical Method of Electronic Structure Calculation, Part B, pp. 95-96., Plenum Press, New York and London, 1977

21. Imamura A., Fujita H., and Nagata C., Bull. Chem. Soc Jap., 42 (1969) : 3118.

22. Scheraga, H, A., Adv. Phys. Org. Chem.,6(1968) : 103

23. Benedict, W. S., Gailar, N., Plyler, E. k., J. Chem. Phys. 24(1956) : 1139

24. Schuster, P., Jakubetz, W., Beier, G., Mayer, W., Rode, B. M.,Chemical and Biochemical Reactivity, vol VI., pp. 257-282 Bergmann and Pullman Ed.(Jerusalem), 1974

25. Popkie H., Kistenmacher H., and Clementi E., J.Chem. Phys., 59, (1973) : 1325

26. Leland, Hollenberg, L. and Ifft, James, B., J. phys. Chem, 86(1982) : 1938

27. Isemura, G, S., J. Bull. Chem. Soc. Jpn., 37(1964) : 1678

References continued

28. Gaffney, J, S., Pierce, R. C., Friedman, L., J. Am. Chem. soc.,99(1977) : 4293

29. Vishveshwara,S.,Pople,J.A., J. Am. Chem. Soc., 99,(1977) : 2422

APPENDIX A

Ab Initio Program

This appendix gives the FORTRAN listing and a sample input for water molecules(H_2O) which illustrates ab initio calculation (Chapter I)

The program will calculate GLO wave functions for any molecule which contains not more than 50 atoms, not more than 60 group functions, and not more than 100 gaussian functions, and for which the type of function cannot be higher than a p-type function. This program was supported by the Quantum Chemistry Group of Innsbruck University, which used a CDC computer and a FORTRAN V compiler. However, the program has been corrected for use with an IBM 3010/8M, which is a 32-bit computer, and a VS FORTRAN compiler.

The program consists mainly of five parts: the main program, subroutine over 1, subroutine over 2, subroutine over 3, and subroutine over 4.

The main program calls the four required subroutines, namely subroutines over 1 through 4, and there is one block data in the program.

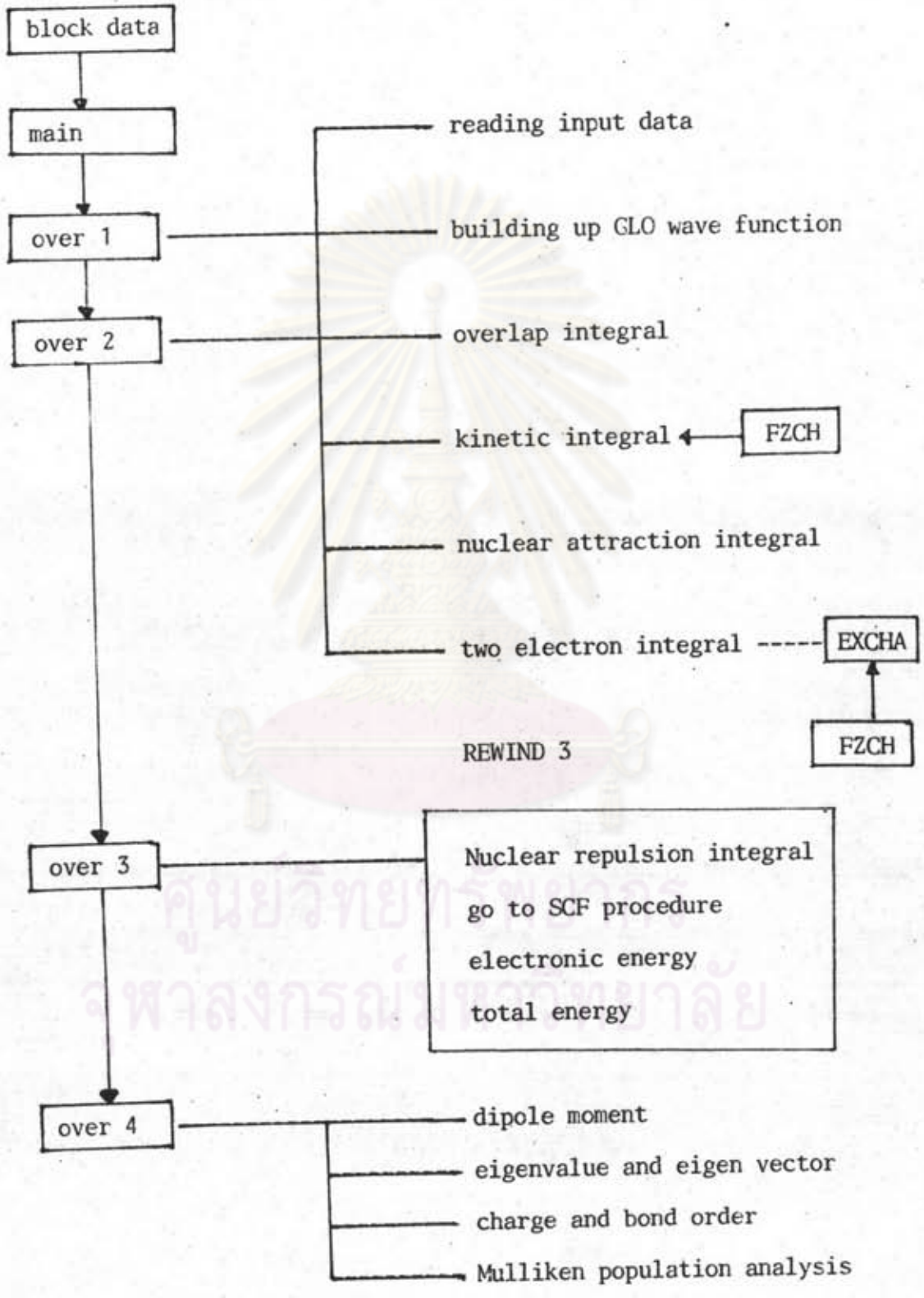
Subroutine over 1 is required for calling input data and building up the GLO wave function. All of the integrals are calculated in subroutine over 2, helped by two function subroutines. The EXCNA calculates four center integrals in two electron integral parts, and function FZCH is an auxiliary function for calculation of nuclear attraction integrals and calculation of function EXCNA. All of the two electron integrals which are required for the SCF procedure are stored in a temporary disk by statement REWIND 3. Subroutine over 3 is the SCF part of the program. The SCF iteration procedure uses the Core-Hamiltonian for an initial guess at the Fock matrix, and

convergence is assumed when the difference of the energy is less than 10^{-5} a.u. Subroutine over 4 is required for calculation of various interpretations such as dipole moment, eigenvalue and eigen vector, charge and bond order, and Mulliken population analysis.

Input for the ab Initio Program

The first card is the name card, the second card is the number of atoms (Format I2), and the next cards are charge and coordinate of each atom. The number of charge and coordinate cards is equal to the number of atoms. After one blank card, the function exponents are assigned to each atom. The reading of the function exponent will be stopped by character E, and the next card is required for convergent factors and the iteration limit.

Flow Chart of ab Initio Program



```
FILE: A        F        F1                VM/SP CONVERSATIONAL MONITOR SYSTEM

//FXDHDD1G     JOB CLASS=1,MSGCLASS=R,MSGLEVEL=(0,0),TYPRUN=HOLD          GLY00010
//      EXEC OFRTVCLG,FVSOURCE=NOSOURCE,FVSRCFL=NOSRCFLG,TIME=160        GLY00020
//FORT.SYSIN DD *                                                        GLY00030
C     THIS PROGRAM COPY FROM ABIN ORIGIN3
      BLOCK DATA                                                       ABI00060
      IMPLICIT REAL*8(A-H,O-Z)                                         ABI00070
      COMMON/CONST/QWERT,NADIM,NFDIM,NGDIM                             ABI00080
      DATA NADIM,NGDIM,NFDIM,QWERT/50,60,100,1.128379167D00/           ABI00090
      END                                                              ABI00100
C
C     PROGRAM MINIG                                                    ABI00110
      IMPLICIT REAL*8(A-H,O-Z)                                         ABI00160
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)        ABI00170
      COMMON/B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)       ABI00180
      COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)               ABI00190
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                  ABI00200
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                       ABI00210
      COMMON/CONST/ QWERT,NADIM,NFDIM,NGDIM                            ABI00230
      DO 1248 I=1,60                                                   ABI00250
      DO 1248 J=1,60                                                   ABI00260
 1248 F(I,J)=0.0D0                                                     ABI00270
      WRITE(6,1000)                                                    ABI00300
      CALL OVER1                                                       ABI00330
      CALL OVER2                                                       ABI00370
      CALL OVER3                                                       ABI00400
      CALL OVER4                                                       ABI00440
      CALL OVER5                                                       ABI00480
 1000 FORMAT(//4X,'OSCF-MO-LC(LCGC)-METHODE'//)                        ABI00490
      STOP
      END                                                              ABI00500
C
      SUBROUTINE SDIAG2 (A)                                            ABI00510
      IMPLICIT REAL*8(A-H,O-Z)                                         ABI00530
      DIMENSION A(60,60),EE(60)                                        ABI00540
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)        ABI00170
      COMMON/B2/RA(50,3),LABGL(60,2),SS(60,60),SC(60,60),HH(60,60)     ABI00180
      COMMON/B3/P(60,60),FF(60,60),RF(100,3),SGF(100,100)              ABI00190
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                  ABI00200
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                       ABI00210
      EQUIVALENCE (EE,FF)                                              ABI00620
      DATA EPS,TOL/1.5D-08,2.5D-31/                                    ABI00630
      IF (NG.EQ.1) GO TO 400                                           ABI00640
      DO 10 I=1,NG                                                     ABI00650
C     PROGRAM ENGINT                                                   ABI00660
      DO 10 J=1,I                                                      ABI00670
   10 P(I,J)=A(I,J)                                                    ABI00680
C     HOUSEHOLDER-S REDUCTION                                          ABI00690
C     SIMULATION OF LOOP DO 150 I=N,2,(-1)                             ABI00700
      DO 150 NI=2,NG                                                   ABI00710
      L=NG-NI                                                          ABI00720
      I=L+2                                                            ABI00730
      H=0.0D0                                                          ABI00740
      G=P(I,I-1)                                                       ABI00750
      IF (L.EQ.0) GO TO 140                                            ABI00760
   20 DO 30 K=1,L                                                      ABI00770
   30 H=H+P(I,K)**2                                                    ABI00780
      S=H+G*G                                                          ABI00790
      IF(S.GE.TOL) GO TO 50                                            ABI00800
      H=0.0D0                                                          ABI00810
   50 IF (H.EQ.0.0D0) GO TO 140                                        ABI00820
      L=L+1                                                            ABI00830
      F=G                                                              ABI00840
      G=DSQRT(S)                                                       ABI00850
      IF(F) 75,75,70                                                   ABI00860
   70 G=-G                                                             ABI00870
   75 H=S-F*G                                                          ABI00880
      P(I,I-1)=F-G                                                     ABI00890
      F=0.0D0                                                          ABI00900
      DO 110 J=1,L                                                     ABI00910
      P(J,I)=P(I,J)/H                                                  ABI00920
      S=0.0D0                                                          ABI00930
      DO 80 K=1,J                                                      ABI00940
   80 S=S+P(J,K)*P(I,K)                                                ABI00950
      J1=J+1                                                           ABI00960
      DO 90 K=J1,L                                                     ABI00970
   90 S=S+P(K,J)*P(I,K)                                                ABI00980
  100 EE(J)=S/H                                                        ABI00990
  110 F=F+S*P(J,I)                                                     ABI01000
      F=0.5D0*F/H                                                      ABI01010
      DO 120 J=1,L                                                     ABI01020
  120 EE(J)=EE(J)-F*P(I,J)                                             ABI01030
      DO 130 J=1,L                                                     ABI01040
      F=P(I,J)                                                         ABI01050
```

```
      S=EE(J)                                                          AB101060
      DO 130 K=1,J                                                     AB101070
  130 P(J,K)=P(J,K)-F*EE(K)-P(I,K)*S                                   AB101080
  140 E(I)=H                                                           AB101090
  150 EE(I-1)=G                                                        AB101100
C     ACCUMULATION OF TRANSFORMATION MATRICES                          AB101110
  160 E(1)=P(1,1)                                                      AB101120
      P(1,1)=1.000                                                     AB101130
      DO 220 I=2,NG                                                    AB101140
      L=I-1                                                            AB101150
      IF(E(I)) 200,200,170                                             AB101160
  170 DO 190 J=1,L                                                     AB101170
      S=0.000                                                          AB101180
      DO 180 K=1,L                                                     AB101190
  180 S=S+P(I,K)*P(K,J)                                                AB101200
      DO 190 K=1,L                                                     AB101210
  190 P(K,J)=P(K,J)-S*P(K,I)                                           AB101220
  200 E(I)=P(I,I)                                                      AB101230
      P(I,I)=1.000                                                     AB101240
  210 DO 220 J=1,L                                                     AB101250
      P(I,J)=0.000                                                     AB101260
  220 P(J,I)=0.000                                                     AB101270
C     DIAGONALIZATION OF THE TRIDIAGONAL MATRIX                        AB101280
      B=0.000                                                          AB101290
      F=0.000                                                          AB101300
      EE(NG)=0.000                                                     AB101310
      DO 340 L=1,NG                                                    AB101320
      H=EPS*(DABS(E(L))+DABS(EE(L)))                                   AB101330
      IF (H.GT.B) B=H                                                  AB101340
C     TEST FOR SPLITTING                                               AB101350
      DO 240 J=L,NG                                                    AB101360
      IF (DABS(EE(J)).LE.B) GOTO 250                                   AB101370
  240 CONTINUE                                                         AB101380
C     TEST FOR CONVERGENCE                                             AB101390
  250 IF (J.EQ.L) GOTO 340                                             AB101400
C     SHIFT FROM UPPER 2*2 MINOR                                       AB101410
  260 PP=(E(L+1)-E(L))*0.500/EE(L)                                     AB101420
      R=DSQRT(PP*PP+1.000)                                             AB101430
      IF(PP) 270,280,280                                               AB101440
  270 PP=PP-R                                                          AB101450
      GO TO 290                                                        AB101460
  280 PP=PP+R                                                          AB101470
  290 H=E(L)-EE(L)/PP                                                  AB101480
      DO 300 I=L,NG                                                    AB101490
  300 E(I)=E(I)-H                                                      AB101500
      F=F+H                                                            AB101510
C     QR TRANSFORMATION                                                AB101520
      PP=E(J)                                                          AB101530
      C=1.000                                                          AB101540
      S=0.000                                                          AB101550
C     SIMULATION OF LOOP DO 330 I=J-1,L,(-1)                           AB101560
      JL=J-1                                                           AB101570
      DO 330 NI=L,JL                                                   AB101580
C     FAKE LOOP FOR RECURSIVE ADDRESS CALCULATION                      AB101590
      I=L+JL-NI                                                        AB101600
      G=C*EE(I)                                                        AB101610
      H=C*PP                                                           AB101620
C     PROTECTION AGAINST UNDERFLOW OF EXPONENTS                        AB101630
      IF (DABS(PP).LT.DABS(EE(I))) GOTO 310                            AB101640
      C=EE(I)/PP                                                       AB101650
      R=DSQRT(C*C+1.000)                                               AB101660
      EE(I+1)=S*PP*R                                                   AB101670
      S=C/R                                                            AB101680
      C=1.000/R                                                        AB101690
      GO TO 320                                                        AB101700
  310 C=PP/EE(I)                                                       AB101710
      R=DSQRT(C*C+1.000)                                               AB101720
      EE(I+1)=S*EE(I)*R                                                AB101730
      S=1.000/R                                                        AB101740
      C=C/R                                                            AB101750
  320 PP=C*E(I)-S*G                                                    AB101760
      E(I+1)=H+S*(C*G+S*E(I))                                          AB101770
      DO 330 K=1,NG                                                    AB101780
      H=P(K,I+1)                                                       AB101790
      P(K,I+1)=P(K,I)*S+H*C                                            AB101800
  330 P(K,I)=P(K,I)*C-H*S                                              AB101810
      EE(L)=S*PP                                                       AB101820
      E(L)=C*PP                                                        AB101830
      IF (DABS(EE(L)).GT.B) GO TO 260                                  AB101840
C     CONVERGENCE                                                      AB101850
  340 E(L)=E(L)+F                                                      AB101860
C     ORDERING OF EIGENVALUES                                          AB101870
```

```
      NI=NG-1                                                          ABI01380
  350 DO 380 I=1,NI                                                    ABI01390
      K=I                                                              ABI01900
      J1=K+1                                                           ABI01910
      PP=E(I)                                                          ABI01920
      DO 360 J=J1,NG                                                   ABI01930
      IF(E(J).GE.PP) GOTO 360                                          ABI01940
      K=J                                                              ABI01950
      PP=E(J)                                                          ABI01960
  360 CONTINUE                                                         ABI01970
      IF (K.EQ.I) GOTO 380                                             ABI01980
      E(K)=E(I)                                                        ABI01990
      E(I)=PP                                                          ABI02000
      DO 370 J=1,NG                                                    ABI02010
      PP=P(J,I)                                                        ABI02020
      P(J,I)=P(J,K)                                                    ABI02030
  370 P(J,K)=PP                                                        ABI02040
  380 CONTINUE                                                         ABI02050
  390 GO TO 410                                                        ABI02060
C     SPECIAL TREATMENT OF CASE N = 1                                  ABI02070
  400 E(1)=A(1,1)                                                      ABI02080
      P(1,1)=1.000                                                     ABI02090
  410 RETURN                                                           ABI02100
      END                                                              ABI02110
C                                                                      ABI02130
C     PROGRAM EINS                                                     ABI02140
      SUBROUTINE OVER1                                                 ABI02120
      IMPLICIT REAL*8(A-H,O-Z)                                         ABI02160
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)        ABI00170
      COMMON/B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)       ABI00180
      COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)               ABI00190
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                  ABI00200
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                       ABI00210
      COMMON/CONST/ QWERT,NADIM,NFDIM,NGDIM                            ABI02240
      DIMENSION BUFFER(10),IBUFF(20),NGL(60),RKNR(50),RAPR(50,3)       ABI02250
C CHARACTER 'E' USE FOR STOP READING THE GUSS FUNCTION.                ABI02270
      REAL SPALTE(80)                                                  ABI02280
      CHARACTER*1 KRIS,KRIS1,ISYM                                      ABI02290
      CHARACTER*10 BUFFER                                              ABI02300
      DATA KRIS/'S'/                                                   ABI02310
      DATA KRIS1/'E'/                                                  ABI02320
      EQUIVALENCE (BUFFER,IBUFF,SPALTE,S),(NGL,E),(RKNR,SC)           ABI02330
      READ(5,1000) BUFFER                                              ABI02340
      WRITE(6,1005) BUFFER                                             ABI02350
      ELEK=0.000                                                       ABI02360
      NA=0                                                             ABI02370
      NG=0                                                             ABI02380
      NF=0                                                             ABI02390
      READ(5,100) NATOM                                                ABI02400
  100 FORMAT(I2)                                                       ABI02430
      DO 1 I=1,NATOM                                                   ABI02440
      NA=NA+1                                                          ABI02520
      IF (NA.GT.NADIM) GO TO 500                                       ABI02530
   28 READ(5,1002)RKNR(NA),INAM(NA),Q(NA)                              ABI02540
     *                        ,RA(NA,1),RA(NA,2),RA(NA,3)             ABI02560
C     CONVERT COORDINATES TO ATOMIC UNIT FOR CALCULATIONS              ABI02550
      RA(NA,1)=RA(NA,1)/0.529167                                       ABI02450
      RA(NA,2)=RA(NA,2)/0.529167                                       ABI02470
      RA(NA,3)=RA(NA,3)/0.529167                                       ABI02480
      ELEK=ELEK+Q(NA)                                                  ABI02490
    1 CONTINUE                                                         ABI02570
      GO TO 2                                                          ABI02590
  500 WRITE(6,5000) NADIM,NGDIM,NFDIM,BUFFER                           ABI02600
 5000 FORMAT('0*** LIMITUEBERSCHREITUNG  */'0MAX.NO.OF ATOMS.:',I3/1CX,ABI02650
     ,'GROUPS. :',I3/7X,'FUNCTIONS. :',I3/'0 FEHLER TRAT BEI FOLGENDER KABI02660
     KARTE AUF : ',10A8)                                               ABI02670
      STOP                                                             ABI02680
    2 READ(5,100) NFUNC                                                ABI02700
   29 READ(5,1003) RKNRG,ISYM,ETAG                                     ABI02710
      IF(ISYM.EQ.KRIS1) GOTO60                                         ABI02720
      DO 32 I=1,NA                                                     ABI02730
      IF (RKNRG.EQ.RKNR(I)) GO TO 33                                   ABI02740
   32 CONTINUE                                                         ABI02750
      WRITE(6,1001) BUFFER                                             ABI02760
   33 EINS=1.000                                                       ABI02780
      J=2                                                              ABI02790
      NG=NG+1                                                          ABI02800
      NGL(NG)=1                                                        ABI02810
      LABGL(NG,1)=NF+1                                                 ABI02820
      LABGL(NG,2)=LABGL(NG,1)                                          ABI02830
      IKNR(NG)=I                                                       ABI02840
      IF(ISYM.EQ.KRIS) GOTO 34                                         ABI02850
      NGL(NG)=2                                                        ABI02860
```

```
      NGL(NG+1)=2                                                        ABI02800
      NGL(NG+2)=2                                                        ABI02810
      IKNR(NG+1)=1                                                       ABI02320
      IKNR(NG+2)=I                                                       ABI02830
      LABGL(NG,2)=NF+2                                                   ABI02840
      LABGL(NG+1,1)=LABGL(NG,2)+1                                        ABI02850
      LABGL(NG+1,2)=LABGL(NG+1,1)+1                                      ABI02860
      LABGL(NG+2,1)=LABGL(NG+1,2)+1                                      ABI02870
      LABGL(NG+2,2)=LABGL(NG+2,1)+1                                      ABI02880
      NG=NG+2                                                            ABI02890
      XPW=0.100/DSQRT(ETAG)                                              ABI02900
      J=8                                                                ABI02910
   34 IF (NG.GT.NGDIM) GO TO 500                                         ABI02920
   35 NF=NF+1                                                            ABI02930
      IF (NF.GT.NFDIM) GO TO 500                                         ABI02940
      ETA(NF)=ETAG                                                       ABI02950
      CFL(NF)=EINS                                                       ABI02960
      RF(NF,1)=RA(I,1)                                                   ABI02970
      RF(NF,2)=RA(I,2)                                                   ABI02980
      RF(NF,3)=RA(I,3)                                                   ABI02990
      EINS=-EINS                                                         ABI03000
      J=J-1                                                              ABI03010
      GOTO(29,38,33,37,37,36,36),J                                       ABI03020
   36 RF(NF,1)=RA(I,1)-EINS*XPW                                          ABI03030
      GO TO 35                                                           ABI03040
   37 RF(NF,2)=RA(I,2)-EINS*XPW                                          ABI03050
      GO TO 35                                                           ABI03060
   38 RF(NF,3)=RA(I,3)-EINS*XPW                                          ABI03070
      IF (J.NE.2) GO TO 35                                               ABI03080
      GO TO 29                                                           ABI03090
   50 READ(5,1004) GESLAD,EKRIT,FAKTOR,ITLIM                             ABI03120
      NE=ELEK-GESLAD+0.500                                               ABI03130
      NEH=NE/2                                                           ABI03140
      WRITE(6,1006)  NF,NG,NA,NE                                         ABI03150
      WRITE(6,1007)                                                      ABI03160
      LINE=29                                                            ABI03170
      DO  4  I=1,NA                                                      ABI03180
      LINE=LINE+1                                                        ABI03190
      IF(LINE-50) 3,3,14                                                 ABI03200
   14 WRITE(6,1027)                                                      ABI03210
      LINE=0                                                             ABI03220
C     CONVERT COORDINATES TO AUNGSTRUM FOR PRINTING
    3 RAPR(I,1)=RA(I,1)*0.529167
      RAPR(I,2)=RA(I,2)*0.529167
      RAPR(I,3)=RA(I,3)*0.529167
    4 WRITE(6,1008)  I,INAM(I),RAPR(I,1),RAPR(I,2),RAPR(I,3),C(I)        ABI03230
      WRITE(6,1009)                                                      ABI03240
      DO  10  IG=1,NG                                                    ABI03250
      IGSS=LABGL(IG,1)                                                   ABI03260
      IGSE=LABGL(IG,2)                                                   ABI03270
      IF(IGSE-IGSS)  7,10,7                                              ABI03280
    7 SN=0.000                                                           ABI03290
      DO  8  IGS1=IGSS,IGSE                                              ABI03300
      DO  8  IGS2=IGSS,IGSE                                              ABI03310
      AIJ=2.000*ETA(IGS1)*ETA(IGS2)/(ETA(IGS1)+ETA(IGS2))                ABI03320
      EXPARG=AIJ*((RF(IGS1,1)-RF(IGS2,1))*(RF(IGS1,1)-RF(IGS2,1))        ABI03330
     1       +(RF(IGS1,2)-RF(IGS2,2))*(RF(IGS1,2)-RF(IGS2,2))            ABI03340
     2       +(RF(IGS1,3)-RF(IGS2,3))*(RF(IGS1,3)-RF(IGS2,3)))*0.500     ABI03350
      IF(65.00-EXPARG)21,20,20                                           ABI03360
   20 OVERL=DSQRT((AIJ/DSQRT(ETA(IGS1)*ETA(IGS2)))**3)/DEXP(EXPARG)      ABI03370
      IF(OVERL-(1.0-18))21,8,8                                           ABI03380
   21 OVERL=0.00                                                         ABI03390
    8 SN=SN+CFL(IGS1)*CFL(IGS2)*OVERL                                    ABI03400
      SNN=1.00/DSQRT(SN)                                                 ABI03410
      DO  9  IGS=IGSS,IGSE                                               ABI03420
    9 CFL(IGS)=CFL(IGS)*SNN                                              ABI03430
   10 CONTINUE                                                           ABI03440
      LINE=9                                                             ABI03450
      DO  13  IG=1,NG                                                    ABI03460
      IF(LINE-62) 16,16,15                                               ABI03470
   15 WRITE(6,1027)                                                      ABI03480
      LINE=5                                                             ABI03490
   16 LINE=LINE+NGL(IG)+1                                                ABI03500
      IGSS=LABGL(IG,1)                                                   ABI03510
      IGSE=LABGL(IG,2)                                                   ABI03520
      DO  13  IGG=IGSS,IGSE                                              ABI03530
      IF(IGSS-IGG)  12,11,12                                             ABI03540
   11 WRITE(6,1010)  IG,NGL(IG),CFL(IGG),(RF(IGG,J),J=1,3),ETA(IGG)      ABI03550
      GO  TO  13                                                         ABI03560
   12 WRITE(6,1011)  CFL(IGG),(RF(IGG,J),J=1,3),ETA(IGG)                 ABI03570
   13 CONTINUE                                                           ABI03580
 1000 FORMAT (10A8)                                                      ABI03590
```

```
1001 FORMAT('0*** KERNNUMMER NICHT VORHANDEN'/'OFEHLERHAFTE KARTE : ', AB103600
     *10A8)                                                          AB103610
1002 FORMAT(F10.8,A4,6X,4F10.5)                                      AB103620
1003 FORMAT(10X,F10.4,A1,9X,F10.5)                                   AB103640
1004 FORMAT(3F10.8,I5)                                               AB103650
1005 FORMAT(1X,10A8)                                                 AB103660
1006 FORMAT(//14X,'NO.OF GAUSS FUNCTIONS',T50,I3/14X,'NO.OF GROUPED FUNAB103670
     *CTION',T50,I3/14X,'NO.OF ATOMS',T50,I3,/14X,'NO.OF ELECTRONS',T50,AB103680
     *I3)                                                            AB103690
1007 FORMAT(//T33,'BUILD UP THE SYSTEM'//T15,'NO.OF ELEMENTS',T37,'COORAB103700
     *DINATES',T62,6HCHARGE//T29,'** X **',3X,'** Y **',3X,'** Z **')  AB103710
1008 FORMAT(T16,I3,T22,A3,T26,3F10.5,T60,F9.5)                       AB103720
1009 FORMAT(//T28,'BUILD UP THE WAVEFUNCTIONS'//T35,'GAUSS FUNCTION',  AB103730
     *T62,8HEXPONENT/T37,'COORDINATES',/T29,'** X **',3X,'** Y **',   AB103740
     *3X,'** Z **')                                                  AB103750
1010 FORMAT(T3,I3,T9,I3,T13,F10.5,3X,3F10.5,3X,F10.5)                AB103760
1011 FORMAT(T13,F10.5,3X,3F10.5,3X,F10.5)                            AB103770
1027 FORMAT (//)                                                     AB103780
     RETURN                                                          AB103790
     END                                                             AB103800
C
     SUBROUTINE OVER2                                                AB103810
     IMPLICIT REAL*8(A-H,O-Z)                                        AB103840
     COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)       AB100170
     COMMON/B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)      AB100180
     COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)              AB100190
     COMMON/B4/NF,NA,NG,NEH,TGR(128)                                 AB100200
     COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                      AB100210
     COMMON/CONST/ QWERT,NADIM,NFDIM,NGDIM                           AB103920
     REAL KINET                                                      AB103930
     DO  1  KQ=1,NF                                                  AB103960
     DO  1  KP=1,KQ                                                  AB103970
     AIJ=2.0D0*ETA(KP)*ETA(KQ)/(ETA(KP)+ETA(KQ))                     AB103980
     EXPARG=AIJ*((RF(KP,1)-RF(KQ,1))*(RF(KP,1)-RF(KQ,1))            AB103990
    1       +(RF(KP,2)-RF(KQ,2))*(RF(KP,2)-RF(KQ,2))                AB104000
    2       +(RF(KP,3)-RF(KQ,3))*(RF(KP,3)-RF(KQ,3)))*0.5D0         AB104010
     IF(85.D0-EXPARG)21,20,20                                        AB104020
   20 OVERL=DSQRT((AIJ/DSQRT(ETA(KP)*ETA(KQ)))**3)/DEXP(EXPARG)      AB104030
     IF(OVERL-(1.D-18))21,22,22                                      AB104040
   21 OVERL=0.D0                                                     AB104050
   22 SGF(KP,KQ)=OVERL                                               AB104060
    1 SGF(KQ,KP)=SGF(KP,KQ)                                          AB104070
     DO  3  KQ=1,NG                                                  AB104090
     KQGFS=LABGL(KQ,1)                                               AB104100
     KQGFE=LABGL(KQ,2)                                               AB104110
     DO  3  KP=1,KQ                                                  AB104120
     KPGFS=LABGL(KP,1)                                               AB104130
     KPGFE=LABGL(KP,2)                                               AB104140
     S(KP,KQ)=0.0D0                                                  AB104150
     DO  2  KPGF=KPGFS,KPGFE                                         AB104160
     DO  2  KQGF=KQGFS,KQGFE                                         AB104170
    2 S(KP,KQ)=S(KP,KQ)+CFL(KPGF)*CFL(KQGF)*SGF(KPGF,KQGF)          AB104180
    3 S(KQ,KP)=S(KP,KQ)                                              AB104190
     CALL SDIAG2(S)                                                  AB104200
     DO  4  I=1,NG                                                   AB104210
     DO  4  J=1,NG                                                   AB104220
    4 SC(I,J)=P(I,J)/DSQRT(E(J))                                     AB104230
     DO  5  KQ=1,NG                                                  AB104240
     KQGFS=LABGL(KQ,1)                                               AB104250
     FNEU=1.0D0                                                      AB104260
     KQGFE=LABGL(KQ,2)                                               AB104270
     DO  5  KP=1,KQ                                                  AB104280
     KPGFS=LABGL(KP,1)                                               AB104290
     KPGFE=LABGL(KP,2)                                               AB104300
     H(KP,KQ)=0.0D0                                                  AB104310
     DO  5  KPGF=KPGFS,KPGFE                                         AB104320
     DO  5  KQGF=KQGFS,KQGFE                                         AB104330
     AIJ=2.D0*ETA(KPGF)*ETA(KQGF)/(ETA(KPGF)+ETA(KQGF))              AB104340
     KINET=(AIJ*((RF(KPGF,1)-RF(KQGF,1))**2                          AB104350
    1           +(RF(KPGF,2)-RF(KQGF,2))**2                          AB104360
    2           +(RF(KPGF,3)-RF(KQGF,3))**2)-3.D0)*SGF(KPGF,KQGF)*AIJ AB104370
     H(KP,KQ)=H(KP,KQ)-0.5D0*CFL(KPGF)*CFL(KQGF)*KINET               AB104380
     A=ETA(KPGF)                                                     AB104390
     B=ETA(KQGF)                                                     AB104400
     APB=A+B                                                         AB104410
     WAPB=DSQRT(APB)                                                 AB104420
     SUM=0.D0                                                        AB104430
     AT=A/APB                                                        AB104440
     BT=B/APB                                                        AB104450
     DO 6 K=1,NA                                                     AB104460
     CPSQ=DSQRT((AT*RF(KPGF,1)+BT*RF(KQGF,1)-RA(K,1))**2+            AB104470
    1           (AT*RF(KPGF,2)+BT*RF(KQGF,2)-RA(K,2))**2+            AB104480
    2           (AT*RF(KPGF,3)+BT*RF(KQGF,3)-RA(K,3))**2)            AB104490
```

```
      W=CPSQ*WAPB                                                       ABI04500
      WQ=W*W                                                            ABI04510
    6 SUM=SUM+FZCH(WQ)*QWERT*Q(K)                                       ABI04520
      POTEN=-WAPB*SGF(KPGF,KQGF)*SUM                                    ABI04530
      H(KP,KQ)=H(KP,KQ)+CFL(KPGF)*CFL(KQGF)*POTEN                       ABI04540
    5 H(KQ,KP)=H(KP,KQ)                                                 ABI04550
      REWIND  3                                                         ABI04560
      NBLKS3=0                                                          ABI04580
      NI=0                                                              ABI04590
      IRET=1                                                            ABI04600
      DO 13 KP=1,NG                                                     ABI04610
      KPGFS=LABGL(KP,1)                                                 ABI04620
      KPGFE=LABGL(KP,2)                                                 ABI04630
      DO 13 KR=KP,NG                                                    ABI04640
      KRGFS=LABGL(KR,1)                                                 ABI04650
      KRGFE=LABGL(KR,2)                                                 ABI04660
      DO  13  KS=KR,NG                                                  ABI04670
      KSGFS=LABGL(KS,1)                                                 ABI04680
      KSGFE=LABGL(KS,2)                                                 ABI04690
      IF (NI.EQ.0) GO TO 12                                             ABI04700
      IF (MOD(NI,64).EQ.0) GO TO 30                                     ABI04710
   12 NI=NI+1                                                           ABI04720
      TGR(NI)=0.000                                                     ABI04730
      DO  13  KPGF=KPGFS,KPGFE                                          ABI04740
      C1=CFL(KPGF)                                                      ABI04750
      DO  13  KQGF=KPGFS,KPGFE                                          ABI04760
      C2=C1*CFL(KQGF)                                                   ABI04770
      DO  13  KRGF=KRGFS,KRGFE                                          ABI04780
      C3=C2*CFL(KRGF)                                                   ABI04790
      DO  13  KSGF=KSGFS,KSGFE                                          ABI04800
      C4=C3*CFL(KSGF)                                                   ABI04810
   13 TGR(NI)=TGR(NI)+C4*EXCHA(KPGF,KQGF,KRGF,KSGF)                     ABI04820
      NNG=NG-1                                                          ABI04830
      DO 28 KP=1,NNG                                                    ABI04840
      KPGFS=LABGL(KP,1)                                                 ABI04850
      KPGFE=LABGL(KP,2)                                                 ABI04860
      KQS=KP+1                                                          ABI04870
      DO 28 KQ=KQS,NG                                                   ABI04880
      KQGFS=LABGL(KQ,1)                                                 ABI04940
      KQGFE=LABGL(KQ,2)                                                 ABI04950
      DO 28 KR=KP,NG                                                    ABI04960
      KRGFS=LABGL(KR,1)                                                 ABI04970
      KRGFE=LABGL(KR,2)                                                 ABI04980
      IF(KP-KR) 26,25,25                                                ABI04990
   25 KSS=KQ                                                            ABI05000
      GO TO 27                                                          ABI05010
   26 KSS=KR                                                            ABI05020
   27 IRET=2                                                            ABI05030
      DO 28 KS=KSS,NG                                                   ABI05040
      KSGFS=LABGL(KS,1)                                                 ABI05050
      KSGFE=LABGL(KS,2)                                                 ABI05060
      IF (MOD(NI,64).EQ.0)GO TO 30                                      ABI05070
   24 NI=NI+1                                                           ABI05080
      TGR(NI)=0.00                                                      ABI05090
      DO 28 KPGF=KPGFS,KPGFE                                            ABI05100
      C1=CFL(KPGF)                                                      ABI05110
      DO 28 KQGF=KQGFS,KQGFE                                            ABI05120
      C2=C1*CFL(KQGF)                                                   ABI05130
      DO 28 KRGF=KRGFS,KRGFE                                            ABI05140
      C3=C2*CFL(KRGF)                                                   ABI05150
      DO 28 KSGF=KSGFS,KSGFE                                            ABI05160
      C4=C3*CFL(KSGF)                                                   ABI05170
      TGR(NI)=TGR(NI)+C4*EXCHA(KPGF,KQGF,KRGF,KSGF)                     ABI05180
   28 CONTINUE                                                          ABI05190
      IRET=3                                                            ABI05210
C  30 CONTINUE                                                          ABI05220
C  32 CONTINUE                                                          ABI05310
   30 IF (NI.GT.64) GO TO 33                                            ABI05320
      WRITE(3)(TGR(I),I=1,64)                                           ABI05340
      GO TO 34                                                          ABI05350
   33 WRITE(3)(TGR(I),I=65,128)                                         ABI05370
      NI=0                                                              ABI05390
   34 NBLKS3=NBLKS3+1                                                   ABI05400
      GO TO (12,24,999),IRET                                            ABI05410
      WRITE(6,171) IRET
  171 FORMAT(T5,'***IRET***',I5)                                        ABI05420
  999 CONTINUE                                                          ABI05430
      RETURN                                                            ABI05440
      END
C
      FUNCTION EXCHA(II,JJ,KK,LL)                                       ABI05450
      IMPLICIT REAL*8(A-H,O-Z)                                          ABI05460
```

```
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)          AB100170
      COMMON/B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)         AB100180
      COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)                 AB100190
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                    AB100200
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                         AB100210
      COMMON/CONST/ QWERT,NADIM,NFDIM,NGDIM                              AB105540
      DATA CRIT/1D-08/                                                   AB105550
      I=II                                                               AB105560
      J=JJ                                                               AB105570
      K=KK                                                               AB105580
      L=LL                                                               AB105590
      SS=SGF(I,J)*SGF(K,L)                                               AB105600
      IF(SS-CRIT)   1,2,2                                                AB105610
    1 EXCHA=0.0D0                                                        AB105620
      RETURN                                                             AB105630
    2 A=ETA(I)                                                           AB105640
      B=ETA(J)                                                           AB105650
      APB=A+B                                                            AB105660
      C=ETA(K)                                                           AB105670
      D=ETA(L)                                                           AB105680
      CPD=C+D                                                            AB105690
      ABCD=APB+CPD                                                       AB105700
      TAB=APB*CPD/ABCD                                                   AB105710
      DTAB=DSQRT(TAB)                                                    AB105720
      PQS4=DSQRT(((A*RF(I,1)+B*RF(J,1))/APB-(C*RF(K,1)+                  AB105730
     1            D*RF(L,1))/CPD)**2+((A*RF(I,2)+B*                      AB105740
     2            RF(J,2))/APB-(C*RF(K,2)+D*RF(L,2))/CPD)**2+            AB105750
     3      ((A*RF(I,3)+B*RF(J,3))/APB-(C*RF(K,3)+                       AB105760
     4      D*RF(L,3))/CPD)**2)                                          AB105770
      W=DTAB*PQS4                                                        AB105780
      WQ=W*W                                                             AB105790
      EXCHA=DTAB*SS*FZCH(WQ)*QWERT                                       AB105800
      RETURN                                                             AB105810
      END                                                                AB105820
      FUNCTION FZCH(XX)                                                  AB105830
      IMPLICIT REAL*8(A-H,O-Z)                                           AB105840
      X=XX                                                               AB105850
      IF(X-9.0D0) 10,10,20                                               AB105860
   10 A=0.5D0                                                            AB105870
      TERM=1.0D0/A                                                       AB105880
      PTLSUM=TERM                                                        AB105890
      DO 11 I=2,50                                                       AB105900
      A=A+1.0D0                                                          AB105910
      TERM=TERM*X/A                                                      AB105920
      PTLSUM=PTLSUM+TERM                                                 AB105930
      IF(TERM/PTLSUM-0.00000001D0) 12,11,11                              AB105940
   11 CONTINUE                                                           AB105950
      WRITE(6,999) X                                                     AB105960
   12 FZCH=0.5D0*PTLSUM*DEXP(-X)                                         AB105970
      RETURN                                                             AB105980
   20 A=-0.5D0                                                           AB105990
      APPROX=0.88622692D0/DSQRT(X)                                       AB106000
C     PROTECTION AGAINST UNDERFLOW OF EXPONENTS                          AB106010
      IF(X.GT.174.3D0)GOTO88                                             AB106020
      FIMULT=0.5D0*DEXP(-X)/X                                            AB106030
      FIPROP=FIMULT/APPROX                                               AB106040
      TERM=1.0D0                                                         AB106050
      PTLSUM=TERM                                                        AB106060
      NOTRMS=X                                                           AB106070
      DO 24 I=2,NOTRMS                                                   AB106080
      TERM=TERM*A/X                                                      AB106090
      PTLSUM=PTLSUM+TERM                                                 AB106100
C     PROTECTION AGAINST UNDERFLOW                                       AB106110
      FIPROI=FIPROP                                                      AB106120
      IF(FIPROP.LT.10.0D-60) FIPROI=FIPROP*10.0D10                       AB106130
      IF(DABS(TERM*FIPROI/PTLSUM)-0.00000001D0) 25,25,24                 AB106140
   24 A=A-1.0D0                                                          AB106150
      WRITE(6,999) X                                                     AB106160
   88 FIMULT=0.0D0                                                       AB106170
      PTLSUM=0.0D0                                                       AB106180
   25 FZCH=APPROX-FIMULT*PTLSUM                                          AB106190
      RETURN                                                             AB106200
  999 FORMAT (24H NO CONVERGENCE FOR FZCH,E16.9)                         AB106210
      END                                                                AB106220
C                                                                        AB106230
      SUBROUTINE OVER3                                                   AB106240
      IMPLICIT REAL*8(A-H,O-Z)                                           AB106250
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)          AB100170
      COMMON/B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)         AB100180
      COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)                 AB100190
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                    AB100200
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                         AB100210
      COMMON/CONST/ QWERT,NADIM,NFDIM,NGDIM                              AB105310
```

```
      REAL NUCLE,CEND(60,60),FDIAG(60)                                  ABI06320
      EQUIVALENCE (F,CEND)                                              ABI06330
      DATA FDIAG/60*0.D0/                                               ABI06340
      DATA ENERG2,ENERG1/1D20,1D10/                                     ABI06350
      DATA DIFFAL,DIFFNE,DIFF1,DIFF2,ES,EX,TGRN,TGR2,FALT,FNEU/10*0.D0/ ABI06360
      DATA IT,J,K,KP,KPE,KQ,KS,KS1,KS2,N,IBLK3/11*0/                    ABI06370
      DATA ENERGY/0.D0/                                                 ABI06390
      DATA KR/0/                                                        ABI06400
      DATA KQS/0/                                                       ABI06410
      DATA TGR1/0.D0/                                                   ABI06420
      IRET=1                                                            ABI06430
  300 IF (IBLK3.NE.0) GO TO 303                                         ABI06540
      REWIND 3                                                          ABI06550
      IBLK3=NBLKS3                                                      ABI06560
  303 IF (N.EQ.128) GO TO 304                                           ABI06570
      READ(3)(TGR(I),I=1,64)                                            ABI06590
      GO TO 305                                                         ABI06600
  304 READ(3)(TGR(I),I=65,128)                                          ABI06620
      N=0                                                               ABI06640
  305 IBLK3=IBLK3-1                                                     ABI06650
      GOTO (306,10,25,43),IRET                                          ABI06660
  306 N=128                                                             ABI06670
      NUCLE=0.D0                                                        ABI06680
      NNA=NA-1                                                          ABI06690
      IF (NNA.EQ.0) GO TO 201                                           ABI06700
      DO  200   L=1,NNA                                                 ABI06710
      LL=L+1                                                            ABI06720
      DO  200   M=LL,NA                                                 ABI06730
      SHT=DSQRT((RA(L,1)-RA(M,1))*(RA(L,1)-RA(M,1))                     ABI06740
     1         +(RA(L,2)-RA(M,2))*(RA(L,2)-RA(M,2))                     ABI06750
     2         +(RA(L,3)-RA(M,3))*(RA(L,3)-RA(M,3)))                    ABI06760
  200 NUCLE=NUCLE+Q(L)*Q(M)/SHT                                         ABI06770
  201 CONTINUE                                                          ABI06780
      FAKTO1=FAKTOR+0.D0                                                ABI06790
      WRITE(6,1012) FAKTO1                                              ABI06800
 1012 FORMAT(///17X,'CONVERGENCE FACTOR =',F6.3,                        ABI06820
     *       //17X,'ITERATION STEPS    ',10X,'TOTAL ENERGY ',10X)       ABI06810
      IF (EKRIT.EQ.0.0D0) EKRIT=3D-06                                   ABI06830
      IF (ITLIM.EQ.0) ITLIM=50                                          ABI06840
   66 IT=IT+1                                                           ABI06850
      DO 67 I=1,NG                                                      ABI06860
      FDIAG(I)=FALT*FDIAG(I)+FNEU*F(I,I)                                ABI06870
      F(I,1)=FDIAG(I)+H(I,1)                                            ABI06880
      DO 67 J=2,I                                                       ABI06890
      H(I,J-1)=FALT*H(I,J-1)+FNEU*F(J-1,I)                              ABI06900
      F(I,J-1)=H(I,J-1)+H(J-1,I)                                        ABI06910
   67 F(J-1,I)=F(I,J-1)                                                 ABI06920
C     CALL MATMULT(SC,F,P,NGDIM,NG)                                     ABI06930
      DO  1  I=1,NG                                                     ABI06950
      DO  1  K=1,NG                                                     ABI06960
      P(I,K)=0.D0                                                       ABI06970
      DO  1  J=1,NG                                                     ABI06980
    1 P(I,K)=P(I,K)+SC(J,I)*F(J,K)                                      ABI06990
      DO  2  I=1,NG                                                     ABI07000
      DO  2  K=1,NG                                                     ABI07010
      F(I,K)=0.D0                                                       ABI07020
      DO  2  J=1,NG                                                     ABI07030
    2 F(I,K)=F(I,K)+P(I,J)*SC(J,K)                                      ABI07040
      CALL SDIAG2(F)                                                    ABI07050
C     CALL MATMULT(SC,P,CEND,NGDIM,NG)                                  ABI07060
      DO  3  I=1,NG                                                     ABI07070
      DO  3  K=1,NG                                                     ABI07080
      CEND(I,K)=0.D0                                                    ABI07090
      DO  3  J=1,NG                                                     ABI07100
    3 CEND(I,K)=CEND(I,K)+SC(I,J)*P(J,K)                                ABI07110
      DO  4  K=1,NG                                                     ABI07120
      DO  4  L=K,NG                                                     ABI07130
      P(K,L)=0.D0                                                       ABI07140
      DO  7  I=1,NEH                                                    ABI07150
    7 P(K,L)=P(K,L)+CEND(K,I)*CEND(L,I)*2.D0                            ABI07160
    4 P(L,K)=P(K,L)                                                     ABI07170
      ES=0.D0                                                           ABI07180
      DO  68  K=1,NG                                                    ABI07190
      ES=0.5D0*H(K,K)*P(K,K)+ES                                         ABI07200
      DO  68  L=2,K                                                     ABI07210
   68 ES=ES+H(L-1,K)*P(L-1,K)                                           ABI07220
      EX=0.D0                                                           ABI07230
      DO 70 I=1,NEH                                                     ABI07240
   70 EX=EX+E(I)                                                        ABI07250
      ENERGY=EX+ES+NUCLE                                                ABI07260
      IF (IT.NE.1) GO TO 71                                             ABI07270
      FALT=0.4D0                                                        ABI07280
```

```
      GO TO 72                                                          AB107290
   71 FALT=FALT*FAKTOR                                                  AB107300
      IF (FALT.LT.1D-10) FALT=0.000                                     AB107310
      FAKTOR=FAKTOR*FAKTOR                                              AB107320
   72 DIFF2=DABS(ENERGY-ENERG2)                                         AB107330
      DIFF1=DABS(ENERGY-ENERG1)                                         AB107340
      DIFFNE=0.2500*DIFF1-DIFF2                                         AB107350
      IF (DIFF1.GE.EKRIT) GO TO 73                                      AB107360
      IF (DIFF2.LT.EKRIT) GO TO 76                                      AB107370
   73 IF (IT.GT.ITLIM) GO TO 76                                         AB107380
      WRITE(6,1013)IT,ENERGY                                            AB107390
      IF (DIFFAL.LE.0.000) GO TO 74                                     AB107400
      IF (DIFFNE.LE.0.000) GO TO 74                                     AB107410
      FALT=0.500                                                        AB107420
      FAKTOR=0.900                                                      AB107430
      FAKTOR=FAKTOR                                                     AB107440
      WRITE(6,1073)                                                     AB107450
   74 DIFFAL=DIFFNE                                                     AB107460
      ENERG2=ENERG1                                                     AB107470
      ENERG1=ENERGY                                                     AB107480
      FNEW=1.000-FALT                                                   AB107490
      DO 8 I=1,NG                                                       AB107500
      DO 8 J=1,NG                                                       AB107510
    8 F(I,J)=0.000                                                      AB107520
      LASTIN=I                                                          AB107550
      N=((N+63)/64)*64                                                  AB107560
      IRET=2                                                            AB107570
      DO 17 KP=1,NG                                                     AB107580
      DO 17 KR=KP,NG                                                    AB107590
      DO 17 KS=KR,NG                                                    AB107600
      IF (MOD(N,64).EQ.0) GO TO 300                                     AB107610
   10 N=N+1                                                             AB107620
      TGRN=TGR(N)                                                       AB107630
      TGR1=-.500*TGRN                                                   AB107640
      IF(TGR1) 11,17,11                                                 AB107650
   11 F(KP,KP)=F(KP,KP)+P(KR,KS)*TGRN                                   AB107660
      F(KP,KS)=F(KP,KS)+P(KP,KR)*TGR1                                   AB107670
      IF(KP-KR) 14,12,12                                                AB107680
   12 IF(KR-KS) 13,17,17                                                AB107690
   13 F(KP,KP)=F(KP,KP)+P(KS,KR)*TGRN                                   AB107700
      F(KP,KR)=F(KP,KR)+P(KP,KS)*TGR1                                   AB107710
      F(KR,KS)=F(KR,KS)+P(KP,KP)*TGRN                                   AB107720
      F(KR,KP)=F(KR,KP)+P(KS,KP)*TGR1                                   AB107730
      GO TO 17                                                          AB107740
   14 IF(KR-KS) 15,16,16                                                AB107750
   15 F(KP,KP)=F(KP,KP)+P(KS,KR)*TGRN                                   AB107760
      F(KP,KR)=F(KP,KR)+P(KP,KS)*TGR1                                   AB107770
   16 F(KR,KS)=F(KR,KS)+P(KP,KP)*TGRN                                   AB107780
   17 CONTINUE                                                          AB107790
      KPE=NG-1                                                          AB107800
      DO 42 KP=1,KPE                                                    AB107810
      KQS=KP+1                                                          AB107820
      DO 42 KQ=KQS,NG                                                   AB107830
      DO 42 KR=KP,NG                                                    AB107840
      IF(KP-KR) 30,26,26                                                AB107850
   26 IRET=3                                                            AB107860
      DO 29 KS1=KQ,NG                                                   AB107870
      IF (MOD(N,64).EQ.0) GO TO 300                                     AB107880
   25 N=N+1                                                             AB107890
      TGRN=TGR(N)                                                       AB107900
      TGR1=-.500*TGRN                                                   AB107910
      IF(TGR1) 27,29,27                                                 AB107920
   27 F(KP,KQ)=F(KP,KQ)+P(KR,KS1)*TGRN                                  AB107930
      F(KP,KS1)=F(KP,KS1)+P(KQ,KR)*TGR1                                 AB107940
      F(KP,KQ)=F(KP,KQ)+P(KS1,KR)*TGRN                                  AB107950
      F(KP,KR)=F(KP,KR)+P(KQ,KS1)*TGR1                                  AB107960
      F(KQ,KS1)=F(KQ,KS1)+P(KP,KR)*TGR1                                 AB107970
      IF(KQ-KS1) 28,29,29                                               AB107980
   28 F(KR,KS1)=F(KR,KS1)+P(KP,KQ)*TGRN                                 AB107990
      F(KR,KQ)=F(KR,KQ)+P(KS1,KP)*TGR1                                  AB108000
      F(KR,KS1)=F(KR,KS1)+P(KQ,KP)*TGRN                                 AB108010
      F(KR,KP)=F(KR,KP)+P(KS1,KQ)*TGR1                                  AB108020
   29 CONTINUE                                                          AB108030
      GO TO 42                                                          AB108040
   30 IRET=4                                                            AB108050
      DO 41 KS2=KR,NG                                                   AB108060
      IF (MOD(N,64).EQ.0) GO TO 300                                     AB108070
   43 N=N+1                                                             AB108080
      TGRN=TGR(N)                                                       AB108090
      TGR1=-.500*TGRN                                                   AB108100
      IF(TGR1) 31,41,31                                                 AB108110
   31 F(KP,KQ)=F(KP,KQ)+P(KR,KS2)*TGRN                                  AB108120
      F(KP,KS2)=F(KP,KS2)+P(KQ,KR)*TGR1                                 AB108130
```

```
      F(KR,KS2)=F(KR,KS2)+P(KP,KQ)*TGRN                                 ABI08140
      F(KR,KS2)=F(KR,KS2)+P(KQ,KP)*TGRN                                 ABI08150
      IF(KR-KS2) 32,37,37                                               ABI08160
   32 F(KP,KQ)=F(KP,KQ)+P(KS2,KR)*TGRN                                  ABI08170
      F(KP,KR)=F(KP,KR)+P(KQ,KS2)*TGRN                                  ABI08180
      IF(KQ-KR) 33,33,34                                                ABI08190
   33 F(KQ,KR)=F(KQ,KR)+P(KP,KS2)*TGRN                                  ABI08200
   34 IF((KP+1)-KQ) 35,37,37                                            ABI08210
   35 IF(KQ-KS2) 37,36,36                                               ABI08220
   36 F(KS2,KQ)=F(KS2,KQ)+P(KR,KP)*TGRN                                 ABI08230
   37 IF(KQ-KR) 39,38,38                                                ABI08240
   38 F(KR,KQ)=F(KR,KQ)+P(KS2,KP)*TGRN                                  ABI08250
   39 IF(KQ-KS2) 40,40,41                                               ABI08260
   40 F(KQ,KS2)=F(KQ,KS2)+P(KP,KR)*TGRN                                 ABI08270
   41 CONTINUE                                                          ABI08280
   42 CONTINUE                                                          ABI08290
      GO TO 66                                                          ABI08300
 1013 FORMAT(I24,F32.5)                                                 ABI08310
 1073 FORMAT(1H+,74X,5H**OSZ)                                           ABI08320
   76 CONTINUE                                                          ABI08330
      WRITE(6,1014) NUCLE                                               ABI08340
 1014 FORMAT(/20X,'NUCLEAR REPULSION ENERGY',F12.5/)                    ABI08350
      WRITE(6,1013) IT,ENERGY                                           ABI08360
      RETURN                                                            ABI08370
      END                                                               ABI08380
C                                                                       ABI08390
      SUBROUTINE OVER4                                                  ABI08400
      IMPLICIT REAL*8(A-H,O-Z)                                          ABI00170
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)         ABI00180
      COMMON/ B2/RA(50,3),LABGL(60,2),S(60,60),SC(60,60),H(60,60)       ABI00190
      COMMON/B3/P(60,60),CEND(60,60),RF(100,3),SGF(100,100)             ABI00200
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                   ABI00210
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                        ABI08500
      REAL QETA(100),ETXYZ2(100),ALAD(50),AL(60),RO(50)                 ABI08510
      INTEGER KERN(60),NAME(60)                                         ABI08520
      EQUIVALENCE (AL,S),(ALAD,SC,RO)                                   ABI08530
      EQUIVALENCE (H,QETA),(SC,NAME),(SC(1,4),ETXYZ2)                   ABI08540
      EQUIVALENCE (SC(1,2),KERN)                                        ABI08550
      DATA DXGES,DYGES,DZGES,DXNUC,DYNUC,DZNUC/6*0.000/                 ABI08790
      DO 60 JR=1,NG                                                     ABI08800
      NGRS=LABGL(JR,1)                                                  ABI08810
      NGRE=LABGL(JR,2)                                                  ABI08820
      DO 60 JS=1,NG                                                     ABI08830
      NGSS=LABGL(JS,1)                                                  ABI08840
      NGSE=LABGL(JS,2)                                                  ABI08850
      DXGS=0.00                                                         ABI08860
      DYGS=0.00                                                         ABI08870
      DZGS=0.00                                                         ABI08880
      DO 70 NGR=NGRS,NGRE                                               ABI08890
      DO 70 NGS=NGSS,NGSE                                               ABI08900
      GF=SGF(NGR,NGS)/(ETA(NGR)+ETA(NGS))                               ABI08910
      DXG=(ETA(NGR)*RF(NGR,1)+ETA(NGS)*RF(NGS,1))*GF                    ABI08920
      DYG=(ETA(NGR)*RF(NGR,2)+ETA(NGS)*RF(NGS,2))*GF                    ABI08930
      DZG=(ETA(NGR)*RF(NGR,3)+ETA(NGS)*RF(NGS,3))*GF                    ABI08940
      DXGS=DXGS+CFL(NGR)*CFL(NGS)*DXG                                   ABI08950
      DYGS=DYGS+CFL(NGR)*CFL(NGS)*DYG                                   ABI08960
      DZGS=DZGS+CFL(NGR)*CFL(NGS)*DZG                                   ABI08970
   70 CONTINUE                                                          ABI08980
      DXGES=DXGES+P(JR,JS)*DXGS                                         ABI08990
      DYGES=DYGES+P(JR,JS)*DYGS                                         ABI09000
      DZGES=DZGES+P(JR,JS)*DZGS                                         ABI09010
   60 CONTINUE                                                          ABI09020
      DO 50 IA=1,NA                                                     ABI09030
      DXNUC=DXNUC+Q(IA)*RA(IA,1)                                        ABI09040
      DYNUC=DYNUC+Q(IA)*RA(IA,2)                                        ABI09050
   50 DZNUC=DZNUC+Q(IA)*RA(IA,3)                                        ABI09060
      DXGES=DXNUC-DXGES                                                 ABI09070
      DYGES=DYNUC-DYGES                                                 ABI09080
      DZGES=DZNUC-DZGES                                                 ABI09090
      DIP=DSQRT(DXGES*DXGES+DYGES*DYGES+DZGES*DZGES)                    ABI09100
      DIPDEB=2.541603500*DIP                                            ABI09110
      WRITE(6,1015) DIPDEB                                              ABI09120
      WRITE(6,1017)  DXGES                                              ABI09130
      WRITE(6,1018)  DYGES                                              ABI09140
      WRITE(6,1019)  DZGES                                              ABI09150
      WRITE(6,1020)                                                     ABI09160
      DO  1  I=1,NEH                                                    ABI09170
    1 WRITE(6,1022) I,E(I),(CEND(J,I),J=1,NG)                           ABI09180
      WRITE(6,1023)                                                     ABI09190
      K=NEH+1                                                           ABI09200
      DO 11 I=K,NG                                                      ABI09210
   11 WRITE(6,1022) I,E(I),(CEND(J,I),J=1,NG)
```

```
      I=0                                                                AB109300
      DO 93 I=1,NA                                                       AB109310
      K=0                                                                AB109320
      DO 93 J=1,NG                                                       AB109330
      IF (IKNR(J).NE.I) GO TO 93                                         AB109340
      IF (K.NE.0) GO TO 91                                               AB109350
      N=N+1                                                              AB109360
      KERN(N)=I                                                          AB109370
      NAME(N)=INAM(I)                                                    AB109380
      DO 90 K=1,NEH                                                      AB109390
      E(K)=0.D0                                                          AB109400
   90 SGF(N,K)=0.D0                                                      AB109410
   91 DO 92 K=1,NEH                                                      AB109420
   92 SGF(N,K)=SGF(N,K)+CEND(J,K)**2                                     AB109430
   93 CONTINUE                                                           AB109440
      DO 94 I=1,NEH                                                      AB109450
      DO 94 J=1,N                                                        AB109460
   94 E(I)=E(I)+SGF(J,I)                                                 AB109470
      LINE=100                                                           AB109480
      DO 97 I=1,NEH                                                      AB109490
      DO 95 J=1,N                                                        AB109500
   95 SGF(J,I)=SGF(J,I)/E(I)                                             AB109510
      IF (LINE.LT.62) GO TO 96                                           AB109520
      WRITE(6,1031) (KERN(K),NAME(K),K=1,N)                              AB109530
      WRITE(6,1032)                                                      AB109540
      LINE=5                                                             AB109550
   96 WRITE(6,1033) I,(SGF(J,I),J=1,N)                                   AB109560
   97 LINE=LINE+N/10+2                                                   AB109570
      WRITE(6,1023)                                                      AB109580
      DO  2  I=1,NG                                                      AB109590
      DO  2  J=1,NG                                                      AB109600
      CEND(I,J)=P(I,J)*S(I,J)                                            AB109610
    2 CEND(J,I)=CEND(I,J)                                                AB109620
      DO  3  K=1,NG                                                      AB109630
    3 WRITE(6,1024) K,(CEND(K,L),L=K,NG)                                 AB109640
      WRITE(6,1025)                                                      AB109650
      DO 7 K=1,NA                                                        AB109660
    7 ALAD(K)=0.D0                                                       AB109670
      DO  9  I=1,NG                                                      AB109680
      K=IKNR(I)                                                          AB109690
      AL(I)=0.000                                                        AB109700
      DO  4  J=1,NG                                                      AB109710
    4 AL(I)=AL(I)+CEND(I,J)                                              AB109720
    9 ALAD(K)=ALAD(K)+AL(I)                                              AB109730
      WRITE(6,1026)  (AL(I),I=1,NG)                                      AB109740
      WRITE(6,1030) (K,INAM(K),ALAD(K),K=1,NA)                           AB109750
 1016 FORMAT (//12X,11HDIPOLMOMENT,F18.5,5X,3HDE8)                       AB109790
 1017 FORMAT (/17X,1HX,F23.5,5X,5HAT.E.)                                 AB109800
 1018 FORMAT (17X,1HY,F23.5)                                             AB109810
 1019 FORMAT (17X,1HZ,F23.5)                                             AB109820
 1020 FORMAT (//11X,28HEIGENVALUES AND EIGENVECTORS)                     AB109830
 1022 FORMAT (/15,F11.5,5X,5F10.5,2X,5F10.5/(21X,5F10.5,2X,5F10.5))     AB109840
 1023 FORMAT (//10X,29HCHARGES AND BONDORDER          )                  AB109850
 1024 FORMAT(15,(T12,10F11.5))                                           AB109860
 1025 FORMAT(//10X,'MULLIKEN-POPULATIONS OF GAUSSIAN GROUPS')            AB109870
 1026 FORMAT(10F13.5)                                                    AB109880
 1028 FORMAT (1H1///)                                                    AB109890
 1030 FORMAT(//10X,'CHARGE OF THE ATOMS'//T12,'NO.',T17,'ELEMENT'        AB109760
     *,T28,'CHARGE',/(I14,5X,A4,F11.5))                                  AB109770
 1031 FORMAT(//11X,'PERC.CONTRIBUTIONS OF AOIS TO MOIS'//(15X,10(I3,     AB109900
     ,A4)))                                                              AB109910
 1032 FORMAT(/)                                                          AB109920
 1033 FORMAT(I10,(T15,10(2PF7.2)))                                       AB109930
      RETURN                                                             AB109940
      END                                                                AB109950
C                                                                        AB109960
      SUBROUTINE OVERS                                                   AB109970
      IMPLICIT REAL*8(A-H,O-Z)                                           AB100170
      COMMON/B1/Q(50),INAM(50),IKNR(60),E(60),ETA(100),CFL(100)          AB100180
      COMMON/B2/RA(50,3),LABEL(60,2),S(60,60),SC(60,60),H(60,60)         AB100190
      COMMON/B3/P(60,60),F(60,60),RF(100,3),SGF(100,100)                 AB100200
      COMMON/B4/NF,NA,NG,NEH,TGR(128)                                    AB100210
      COMMON/B5/LASTIM,ITLIM,EKRIT,FAKTOR,NBLKS3                         AB110370
      DIMENSION QETA(100)                                                AB110380
      EQUIVALENCE (QETA,H)                                               AB110120
      RETURN                                                             AB110130
      END
/*
//GO.FT03F001 DD UNIT=SYSDA,SPACE=(CYL,(100))
//GO.SYSIN DD *
WATERMOLECULE GLO MINIMUM BASIS SET OH=0.9572,HOH=104.5                  V  10150
                                                                         V  10160
 3
 1.0000   H            1.0000    0.7568    0.5860    0.0000
 2.0000   O            8.0000    0.0000    0.0000    0.0000
 3.0000   H            1.0000   -0.7568    0.5860    0.0000
10                                                                       V  10310
G          1.0000   S              0.39500
G          2.0000   S             17.360
G          2.0000   S              0.636
G          2.0000   P              0.505
G          3.0000   S              0.39500                              V  10320
                    E                                                   V  10560
   0.0000   .000010  0.100000    50                                      V  10570
/*                                                                       V  10580
//                                                                       V  10590
```

APPENDIX B

CNDO Program

This program was originally written in FORTRAN IV, using an IBM 360/65 digital computer. The CNDO program which we have used here was supported by the Quantum Chemistry Group of Innsbruck University. More parts from the original which were helpful in optimization of the molecular structure were added, and the program was run on a CDC computer system with a FORTRAN V compiler.

When it was applied to the IBM 3010/8M digital computer at Chulalongkorn University, the optimization and INDO parts of the program were cut. Thus only the CNDO closed shell part of the program was run. (However, the program can now be run in full.)

Thus only the CNDO closed shell part of the program will be discussed. The program is capable of computing CNDO wavefunctions for closed-shell molecules containing the elements H to Cl.

The matrices in the program are large enough to allow molecules containing up to 35 atoms or 80 basis functions (whichever is smaller). One atomic orbital basis function is allowed for hydrogen (1s), four each to the elements Li through F (2s, 2px, 2py, 2pz) and nine each to the elements Na through Cl (3s, 2px, 3py, 3pz, $3dx^2$, $3dy^2$, 3dxy, 3dyz, $3d(x^2-y^2)$.

The following is a qualitative description of the operation of each subroutine:

OVER 1 is required for calling input data and assigns the coefficients used in the calculation of overlap and coulomb integrals. In subroutine OVER 2 the overlap matrix (stored in the first array of

COMMON /C1/) and the coulomb integral matrix (stored in COMMON/C6/) are computed. Integrals are calculated for pairs of atoms using a local diatomic coordinate system. Then the rotation matrix formed in subroutine HARMTR is used to transform the overlap integrals to the molecular coordinate system.

The SCF procedure begin in subroutine OVER 4 which consists of two main original subroutine. They are HUCKCL and SCFCLO. The first one prepares the initial guess density matrixes. The second takes as input initial density matrixes and CNDO core Halmitonian. Then, the Fock matrix is formed by first adding the integrals. The Fock matrix is diagonalized and a new density matrix is formed which is used to construct a new Fock matrix. The procedure is repeated until the electronic energy converges to 10^{-6} . At this point, the Fock matrix is printed, then diagonalized once more, and the resulting eigen vectors are printed. The electronic energy is computed after each new Fock matrix is formed and before it is diagonalized. A limit of 25 iterations is allowed (IT = 25).

Subroutine CPRINT computes dipole moments, atom densities, and nuclear repulsion energy.

The subroutines SS, HARMER, RELVEC, FACT, BINTGS, AINTGS, and MATOVE are called only by OVER 1. EIGN, SCFOUT, and EIGOUT are needed in the subroutines OVER 4 for HUCKCL.

Input for the CNDO Program

The first card is the name card, the second card is the CNDO closed shell option, the third card is number of atoms, charge, multiplicity, iteration limit, the fourth card is the atomic number of the atoms and the next cards are the coordinates of the atoms. The number of coordinate cards is equal to the number of atoms.

```
FILE: C        F        F1                    VM/SP CONVERSATIONAL MONITOR SYSTEM

//FXDBJDIW     JOB CLASS=1,MSGCLASS=R,MSGLEVEL=(0,0),TYPRUN=HOLD          GLY00010
//      EXEC OFRTVCLG,FVSOURC=NOSOURCE,FVSRCFL=NOSRCFLG,TIME=100          GLY00020
//FORT.SYSIN DD *                                                         GLY00030
      BLOCK DATA                                                        CND00040
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C0/EPS
      COMMON/C2/C(35,3),AN(35)                                          CND00080
      COMMON/C4/EL(18)                                                  CND00090
      COMMON/C5/ORB(9)                                                  CND00100
      COMMON/C8/AA(3,4),ES,XX(3)                                        CND00110
      COMMON/C9/OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN                 CND00120
      CHARACTER*4 EL,ORB,OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN*80     CND00130
      DATA OPTION,CNDO,INDO/'CNDO','CNDO','INDO'/                       CND00200
      DATA OPNCLO,CLOSED,OPEN/'CLSD','CLSD','OPEN'/                     CND00210
      DATA ORB(1),ORB(2)/'   S',' PX'/                                  CND00220
      DATA ORB(3),ORB(4)/' PY',' PZ'/                                   CND00230
      DATA ORB(5),ORB(6)/' DZ2',' DXZ'/                                 CND00240
      DATA ORB(7),ORB(8)/' DYZ',' DX-Y'/                                CND00250
      DATA ORB(9)/' DXY'/                                               CND00260
      DATA EL(1),EL(2),EL(3)/'   H','  HE','  LI'/                      CND00270
      DATA EL(4),EL(5),EL(6)/'  BE','   B','   C'/                     CND00280
      DATA EL(7),EL(8),EL(9)/'   N','   O','   F'/                     CND00290
      DATA EL(10),EL(11),EL(12)/'  NE','  NA','  MG'/                  CND00300
      DATA EL(13),EL(14),EL(15)/'  AL',' SI','   P'/                   CND00310
      DATA EL(16),EL(17),EL(18)/'   S','  CL','  AR'/                  CND00320
      END                                                               CND00330
C                                                                       CND00340
      SUBROUTINE KOORD                                                  CND00360
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C0/EPS
      COMMON/C2/C(35,3),AN(35)                                          CND00400
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,ITER,LIMEX                       CND00410
      INTEGER CHARGE                                                    CND00420
      DATA FAKT/0.01745329252/                                          CND00450
      DO 1 I=1,NATOMS                                                   CND00460
    1 READ2,C(I,1),C(I,2),C(I,3)                                        CND00480
    2 FORMAT(3X,3F10.7)                                                 CND00490
      RETURN                                                            CND00500
      END                                                               CND00510
C                                                                       CND00520
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C0/EPS
      COMMON/C1/A(70,70,3)                                              CND00560
      COMMON/C2/C(35,3),AN(35)                                          CND00580
      COMMON/C3/CZ(35),U(70),ULIM(35),LLIM(35),NELECS,OCCA,OCCB         CND00590
      COMMON/C4/EL(18)                                                  CND00600
      COMMON/C5/ORB(9)                                                  CND00610
      COMMON/C6/G(35,35),XXX(70,7),ENERGY,ENERG                         CND00620
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,ITER,LIMEX                       CND00630
      COMMON/C8/AA(3,4),ES,XX(3)                                        CND00680
      COMMON/C9/OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN                 CND00660
      INTEGER AN,CHARGE,CZ,U,ULIM,OCCA,OCCB                             CND00700
      CHARACTER*4 EL,ORB,OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN*80     CND00670
      DO 60 I=1,3                                                       CND00820
      DO 60 J=1,4                                                       CND00830
      AA(I,J)=1.0                                                       CND00840
   60 CONTINUE                                                          CND00850
      DO 65 I=1,35                                                      CND00860
      DO 65 J=1,3                                                       CND00870
      C(I,J)=0.0                                                        CND00880
   65 CONTINUE                                                          CND00890
      DO 70 I=1,70                                                      CND00900
      DO 70 J=1,7                                                       CND00910
      XXX(I,J)=0.0                                                      CND00920
   70 CONTINUE                                                          CND00930
  100 NST=1                                                             CND00940
  200 CALL OVER1                                                        CND00950
      CALL OVER2                                                        CND00960
      CALL OVER4                                                        CND00980
   95 CONTINUE                                                          CND01010
      STOP                                                              CND01020
      END                                                               CND01030
C                                                                       CND01040
      SUBROUTINE SCFOUT(OP,MOP)                                         CND01090
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C0/EPS
      COMMON/C1/A(70,70,3)                                              CND01120
      COMMON/C2/C(35,3),AN(35)                                          CND00080
      COMMON/C3/CZ(35),U(70),ULIM(35),LLIM(35),NELECS,OCCA,OCCB         CND01150
      COMMON/C4/EL(18)                                                  CND01170
      COMMON/C5/ORB(9)                                                  CND01160
      COMMON/C6/G(35,35),XXX(70,3),EPSILN(70)                           CND01130
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,ITER,LIMEX                       CND00630
```

```
      INTEGER OP,AN,ANII,CZ,U,ULIM,CHARGE,OCCA,OCCB                    CND01190
      CHARACTER*4 EL,ORB                                               CND01180
      DO 120 M=1,N,12                                                  CND01200
      K=M+11                                                           CND01210
      IF (K.GT.N) K=N                                                  CND01220
      PRINT100                                                         CND01230
      IF (OP.EQ.0) GO TO 50                                            CND01240
      PRINT40,  (EPSILN(I) ,I=M,K)                                     CND01250
   40 FORMAT(//'0EIGENVALUES---',12F9.4//)                             CND01260
   50 CONTINUE                                                         CND01270
      PRINT60,  (I,I=M,K)                                              CND01280
   60 FORMAT(14X,1219)                                                 CND01290
      DO 120 I=1,N                                                     CND01300
      II=U(I)                                                          CND01310
      ANII=AN(II)                                                      CND01320
      L=I-LLIM(II)+1                                                   CND01330
      PRINT80,  I,II,EL(ANII),ORB(L),(A(I,J,MOP),J=M,K)                CND01340
   80 FORMAT(1X,2I3,A1,1X,A1,12(F9.4))                                 CND01350
      IF (I.EQ.ULIM(II)) PRINT100                                      CND01360
  100 FORMAT(1X)                                                       CND01370
  120 CONTINUE                                                         CND01380
      PRINT200                                                         CND01390
  200 FORMAT(//)                                                       CND01400
      RETURN                                                           CND01410
      END                                                              CND01420
C                                                                      CND01430
      SUBROUTINE OVER2                                                 CND01450
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CO/EPS
      COMMON/C1/S(70,70),Y(9,5,203),Z(17,45)                           CND01490
      COMMON/C2/C(35,3),AN(35)                                         CND01500
      COMMON/C3/CZ(35),U(70),ULIM(35),LLIM(35),NELECS,OCCA,OCCB        CND01510
      COMMON/C6/GAMMA(35,35),T(9,9),PAIRS(9,9),TEMP(9,9)               CND01520
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,ITER,LIMEX                      CND01530
      COMMON/C9/OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN                CND01540
      DIMENSION MU(18),NC(18),LC(9),MC(9),E(3)                         CND01560
      DIMENSION P(70,70)                                               CND01570
      INTEGER AN,ULIM,ULK,ULL,CZ,U,CHARGE,ANL,ANK,OCCA,OCCB,Y,Z        CND01610
      REAL MU,NUM,K1,K2                                                CND01590
      CHARACTER ERRMSG*60                                              CND01600
      CHARACTER*4 EL,ORB,OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN*80    CND01550
      EQUIVALENCE (P(1,1),Y(1,1,1))                                    CND01580
C     ASSIGNMENT OF ANGULAR MOMENTUM QUANTUM NOS. TO ATOMIC ORBITALS   CND01620
      DATA LC/0,1,1,1,2,2,2,2,2/                                       CND01630
      DATA MC/0,1,-1,0,0,1,-1,2,-2/                                    CND01640
C     DETERMINATION OF SIZE OF AO BASIS IN AND CORE CHARGE CZ          CND01650
      N=0                                                              CND01660
      DO 50 I=1,NATOMS                                                 CND01670
      LLIM(I)=N+1                                                      CND01680
      K=1                                                              CND01690
      IF (AN(I).LT.11) GO TO 20                                        CND01700
      N=N+9                                                            CND01710
      CZ(I)=AN(I)-10                                                   CND01720
      GO TO 50                                                         CND01730
   20 IF (AN(I).LT.3) GO TO 40                                         CND01740
      N=N+4                                                            CND01750
      CZ(I) = AN(I)-2                                                  CND01760
      GO TO 50                                                         CND01770
   40 N=N+1                                                            CND01780
      CZ(I)= AN(I)                                                     CND01790
   50 CONTINUE                                                         CND01800
      ULIM(I) = N                                                      CND01810
   60 CONTINUE                                                         CND01820
      IF (N.LE.(70)) GO TO 65                                          CND01830
      WRITE(ERRMSG,666)N,70                                            CND01840
  666 FORMAT('0 **** SIZE OF AO BASIS =',I4,9X,'(LIMIT=',I3,') ****')  CND01850
   65 CONTINUE                                                         CND01870
C     FILL J ARRAY---J(I) IDENTIFIES THE ATOM TO WHICH ORBITAL J IS    CND01880
C     ATTACHED E.G. ORBITAL 32 ATTACHED TO  ATOM 7, ETC.               CND01890
      DO 70 K=1,NATOMS                                                 CND01900
      LLK = LLIM(K)                                                    CND01910
      ULK = ULIM(K)                                                    CND01920
      LIM = ULK+1-LLK                                                  CND01930
      DO 70 I=1,LIM                                                    CND01940
      J = LLK+I-1                                                      CND01950
   70 J(J) = K                                                         CND01960
C     ASSIGNMENT OF ORBITAL EXPONENTS TO ATOMS BY SLATERS RULES        CND01970
      MU(2)=1.700                                                      CND01980
      MU(1)=1.200                                                      CND01990
      NC(1)=1                                                          CND02000
      NC(2)=1                                                          CND02010
      DO 80 I=3,10                                                     CND02020
```

```
      NC(I)=2                                                          CND02030
   80 MJ(I)=.32500*(I-1)                                               CND02040
      DO 90 I=11,18                                                    CND02050
      NC(I)=3                                                          CND02060
   90 MJ(I)=(.6500*(I)-4.9500)/3.00                                    CND02070
C     STEP THRU PAIRS OF ATOMS                                         CND02080
      DO 320 K=1,NATOMS                                                CND02090
      DO 320 L=K,NATOMS                                                CND02100
C     CALCULATE UNIT VECTOR ALONG INTERATOM AXIS,E                     CND02110
      R=0.                                                             CND02120
      DO 101 I=1,3                                                     CND02130
      E(I) = C(L,I)-C(K,I)                                             CND02140
      R = R+E(I)**2                                                    CND02150
  101 CONTINUE                                                         CND02160
      IF (K.EQ.L) GO TO 105                                            CND02170
      R=DSQRT(R)                                                       CND02180
      IF (R.GE.1E-6) GO TO 103                                         CND02190
  103 DO 102 I=1,3                                                     CND02210
  102 E(I)=E(I)/R                                                      CND02220
  105 LLK = LLIM(K)                                                    CND02230
      LLL = LLIM(L)                                                    CND02240
      JLK = ULIM(K)                                                    CND02250
      JLL = ULIM(L)                                                    CND02260
      NORBK=JLK-LLK+1                                                  CND02270
      NORBL=JLL-LLL+1                                                  CND02280
      ANK=AN(K)                                                        CND02290
      ANL=AN(L)                                                        CND02300
C     LOOP THRU PAIRS OF BASIS FUNCTIONS, ONE ON EACH ATOM             CND02310
      DO 200 I=1,NORBK                                                 CND02320
      DO 200 J=1,NORBL                                                 CND02330
      IF(K.EQ.L) GO TO 160                                             CND02340
      IF(NC( I).NE.NC(J)) GO TO 180                                    CND02350
      IF(NC(I).LT.0) GO TO 140                                         CND02360
      PAIRS(I,J)=DSQRT((MJ(ANK)*R)**(2*NC(ANK)+1)*(MJ(ANL)*R)**(2*NC(ANLCND02370
     1)+1)/(FACT(2*NC(ANK))*FACT(2*NC(ANL))))*(-1.00)**(LC(J)+MC(J))   CND02380
     2*SS(NC(ANK),LC(I),MC(I),NC(ANL),LC(J),MJ(ANK)*R,MJ(ANL)*R)        CND02390
      GO TO 190                                                        CND02400
  140 PAIRS(I,J)=PAIRS(I-1,J-1)                                        CND02410
      GO TO 190                                                        CND02420
  160 IF (I.EQ.J) GO TO 170                                            CND02430
  180 PAIRS(I,J)=0.000                                                 CND02440
      GO TO 190                                                        CND02450
  170 PAIRS(I,J)=1.000                                                 CND02460
  190 CONTINUE                                                         CND02470
  200 CONTINUE                                                         CND02480
      LCULK=LC(NORBK)                                                  CND02490
      LCULL=LC(NORBL)                                                  CND02500
      MAXL=MAXO(LCULK,LCULL)                                           CND02510
      IF(R.LE.0.000001D0) GO TO 250                                    CND02520
C     ROTATE INTEGRALS FROM DIATOMIC BASIS TO MOLECULAR BASIS          CND02530
      CALL HARMTR(MAXL,E)                                              CND02540
      DO 230 I=1,NORBK                                                 CND02550
      DO 230 J=1,NORBL                                                 CND02560
      TEMP(I,J) = 0.D0                                                 CND02570
      DO 230 KK=1,NORBL                                                CND02580
      TEMP(I,J) = TEMP(I,J)+T(J,KK)*PAIRS(I,KK)                        CND02590
  230 CONTINUE                                                         CND02600
      DO 240 I=1,NORBK                                                 CND02610
      DO 240 J=1,NORBL                                                 CND02620
      PAIRS(I,J) = 0.D0                                                CND02630
      DO 240 KK=1,NORBK                                                CND02640
      PAIRS(I,J) = PAIRS(I,J)+T(I,KK)*TEMP(KK,J)                       CND02650
  240 CONTINUE                                                         CND02660
C     FILL S MATRIX                                                    CND02670
  250 CONTINUE                                                         CND02680
      DO 260 I=1,NORBK                                                 CND02690
      LLKP=LLK+I-1                                                     CND02700
      DO 260 J=1,NORBL                                                 CND02710
      LLLP=LLL+J-1                                                     CND02720
  260 S(LLKP,LLLP)=PAIRS(I,J)                                          CND02730
C     COMPUTATION OF 1-CENTER COULOMB INTEGRALS OVER SLATER S FUNCTIONS CND02740
      N1=NC(ANK)                                                       CND02750
      N2=NC(ANL)                                                       CND02760
      K1=MJ(ANK)                                                       CND02770
      K2=MJ(ANL)                                                       CND02780
      IF(K.NE.L) GO TO 290                                             CND02790
      TERM1 = FACT(2*N1-1)/((2.D0*K2)**(2*N1))                         CND02800
      TERM2 = 0.D0                                                     CND02810
      LIM = 2*N1                                                       CND02820
      DO 280 J=1,LIM                                                   CND02830
      NUM =(J)*(2.D0*K1)**(2*N1-J)*FACT(4*N1-J-1)                      CND02840
      DEN = FACT(2*N1-J)*2.D0*(N1)*(2.D0*(K1+K2))**(4*N1-J)            CND02850
```

```
      TERM2 = TERM2 + NUM/DEN                                          CND02860
  280 CONTINUE                                                         CND02870
      GO TO 310                                                        CND02880
C     COMPUTATION OF 2-CENTER COULOMB INTEGRALS OVER SLATER S FUNCTIONS CND02890
  290 IF (OPNCLO.EQ.OPEN) GO TO 295                                    CND02900
      IF (R.LT.4.0) GO TO 295                                          CND02910
      GAMMA(K,L)=1.0/R                                                 CND02920
      GO TO 320                                                        CND02930
  295 TERM1=(R/2.D0)**(2*N2)*SS(0,0,0,2*N2-1,0,0.D0,2.D0*K2*R)         CND02940
      TERM2 = 0.D0                                                     CND02950
      LIM = 2*N1                                                       CND02960
      DO 300 J=1,LIM                                                   CND02970
  300 TERM2 = TERM2+((J)*(2.D0*K1)**(2*N1-J)*(R/2.D0)**(2*             CND02980
     1N1-J+2*N2))/ (FACT(2*N1-J)*2.D0*(N1))*SS(2*N1-J,0,0,2*N2-1,0     CND02990
     2,2.D0*K1*R,2.D0*K2*R)                                            CND03000
  310 GAMMA(K,L) = ((2.D0*K2)**(2*N2+1)/FACT(2*N2))*(TERM1-TERM2)      CND03010
  320 CONTINUE                                                         CND03020
C     SYMMETRIZATION OF OVERLAP AND COULOMB INTEGRAL MATRICES          CND03030
      DO 330 I=1,N                                                     CND03040
      DO 330 J=1,N                                                     CND03050
  330 S(J,I) = S(I,J)                                                  CND03060
      DO 340 I=1,NATOMS                                                CND03070
      DO 340 J=1,NATOMS                                                CND03080
  340 GAMMA(J,I) = GAMMA(I,J)                                          CND03090
C     IF(PRTOPT.LE.1)GO TO 380                                         CND03100
      PRINT350                                                         CND03110
  350 FORMAT('0'/4(/'+OVERLAP INTEGRAL MATRIX'))                       CND03120
      CALL MATOUT(N,1)                                                 CND03130
C     TRANSFER GAMMA TO 80X80 MATRIX P FOR PRINTING                    CND03140
      DO 360 I=1,NATOMS                                                CND03150
      DO 360 J=1,NATOMS                                                CND03160
  360 P(I,J)=GAMMA(I,J)                                                CND03170
      PRINT370                                                         CND03180
  370 FORMAT(/4(/'+COULOMB INTEGRAL MATRIX'))                          CND03190
      CALL MATOUT(NATOMS,2)                                            CND03200
  380 CONTINUE                                                         CND03210
      RETURN                                                           CND03220
      END                                                              CND03230
C                                                                      CND03240
      SUBROUTINE HARMTR(MAXL,E)                                        CND03260
      IMPLICIT REAL*8 (A-H,O-Z)                                        CND03290
      DIMENSION T(9,9),E(3)                                            CND03300
      COMMON/C6/YYY(35,35),T                                           CND03310
      DATA SQRT3/1.732050808/                                          CND03320
      COST = E(3)                                                      CND03330
      IF((1.-COST**2).GT.0.00000000001) GO TO 20                       CND03340
      SINT = 0.D0                                                      CND03350
      GO TO 30                                                         CND03360
   20 SINT=DSQRT(1.D0-COST**2)                                         CND03370
   30 CONTINUE                                                         CND03380
      IF(SINT.GT.0.00000100) GO TO 50                                  CND03390
      COSP = 1.D0                                                      CND03400
      SINP = 0.D0                                                      CND03410
      GO TO 70                                                         CND03420
   50 COSP = E(1)/SINT                                                 CND03430
      SINP = E(2)/SINT                                                 CND03440
   70 CONTINUE                                                         CND03450
      DO 80 I=1,9                                                      CND03460
      DO 80 J=1,9                                                      CND03470
   80 T(I,J) = 0.D0                                                    CND03480
      T(1,1) =1.D0                                                     CND03490
      IF(MAXL-1)120,110,100                                            CND03500
  100 COS2T = COST**2-SINT**2                                          CND03510
      SIN2T = 2.D0*SINT*COST                                           CND03520
      COS2P = COSP**2-SINP**2                                          CND03530
      SIN2P = 2.D0*SINP*COSP                                           CND03540
C     TRANSFORMATION MATRIX ELEMENTS FOR D FUNCTIONS                   CND03550
      T(5,5) = (3.D0*COST**2-1.D0)/2.D0                                CND03560
      T(5,6) = -SQRT3    *SIN2T/2.D0                                   CND03570
      T(5,8) = SQRT3     *SINT**2/2.D0                                 CND03580
      T(6,5) = SQRT3     *SIN2T*COSP/2.D0                              CND03590
      T(6,6) = COS2T*COSP                                              CND03600
      T(6,7) = -COST*SINP                                              CND03610
      T(6,8)=-T(6,5)/SQRT3                                             CND03620
      T(6,9)=SINT*SINP                                                 CND03630
      T(7,5)=SQRT3   *SIN2T*SINP/2.D0                                  CND03640
      T(7,6)=COS2T*SINP                                                CND03650
      T(7,7)=COST*COSP                                                 CND03660
      T(7,8)=-T(7,5)/SQRT3                                             CND03670
      T(7,9) = -SINT*COSP                                              CND03680
      T(8,5) = SQRT3     *SINT**2*COS2P/2.D0                           CND03690
      T(8,6) = SIN2T*COS2P/2.D0                                        CND03700
      T(8,7) = -SINT*SIN2P                                             CND03710
```

```
      T(8,8) = (1.D0+COST**2)*COS2P/2.D0                                CND03710
      T(8,9) = -COST*SIN2P                                              CND03720
      T(9,5) = SQRT3    *SINT**2*SIN2P/2.D0                             CND03730
      T(9,6) = SIN2T*SIN2P/2.D0                                         CND03740
      T(9,7) = SINT*COS2P                                               CND03750
      T(9,8) = (1.D0+COST**2)*SIN2P/2.D0                                CND03760
      T(9,9) = COST*COS2P                                               CND03770
  110 CONTINUE                                                          CND03780
C     TRANSFORMATION MATRIX ELEMENTS FOR P FUNCTIONS                    CND03790
      T(2,2) = COST*COSP                                                CND03800
      T(2,3) = -SINP                                                    CND03810
      T(2,4) = SINT*COSP                                                CND03820
      T(3,2) = COST*SINP                                                CND03830
      T(3,3) = COSP                                                     CND03840
      T(3,4) = SINT*SINP                                                CND03850
      T(4,2) = -SINT                                                    CND03860
      T(4,4) = COST                                                     CND03870
  120 CONTINUE                                                          CND03880
      DO 130 I=1,9                                                      CND03890
      DO 130 J=1,9                                                      CND03900
      IF(DABS(T(I,J)).LE.1.D-8) T(I,J)=0.                               CND03910
  130 CONTINUE                                                          CND03920
      RETURN                                                            CND03930
      END                                                               CND03940
C                                                                       CND03950
      FUNCTION FACT(N)                                                  CND03970
      IMPLICIT REAL*8 (A-H,O-Z)                                         CND03980
      PRODT = 1.D0
C  PROTECT THE CASE OF N .LT. 2
      IF(N.LT.2)GOTO 40                                                 CND03990
      DO 30 I=2,N                                                       CND04000
   30 PRODT=PRODT*(I)
      FACT= PRODT
      GOTO 50                                                           CND04010
   40 FACT= PRODT                                                       CND04020
   50 RETURN                                                            CND04030
      END                                                               CND04040
C                                                                       CND04060
      FUNCTION SS(NN1,LL1,MM,NN2,LL2,ALPHA,BETA)
      IMPLICIT REAL*8 (A-H,O-Z)                                         CND04100
      COMMON/C1/S(70,70),Y(9,5,203),Z(17,45)                            CND04110
      COMMON/C6/G(35,35),XXX(9,9,3),A(18),B(18)                         CND04120
      INTEGER ULIM,Y,Z                                                  CND04130
      N1=NN1                                                            CND04140
      L1=LL1                                                            CND04150
      M=MM                                                              CND04160
      N2=NN2                                                            CND04170
      L2=LL2                                                            CND04180
      P =(ALPHA + BETA)/2.D0                                            CND04190
      PT=(ALPHA - BETA)/2.D0                                            CND04200
      X = 0.D0                                                          CND04210
      M=IABS(M)                                                         CND04220
C     REVERSE QUANTUM NUMBERS IF NECESSARY                              CND04230
      IF(L2-L1)20,10,30                                                 CND04240
   10 IF(N2.GE.N1)GO TO 30                                              CND04250
   20 K=N1                                                              CND04260
      N1= N2                                                            CND04270
      N2= K                                                             CND04280
      K= L1                                                             CND04290
      L1= L2                                                            CND04300
      L2= K                                                             CND04310
      PT=-PT                                                            CND04320
   30 CONTINUE                                                          CND04330
      K = MOD((N1+N2-L1-L2),2)                                          CND04340
C     FIND A AND B INTEGRALS                                            CND04350
      CALL AINTGS(P,N1+N2)                                              CND04360
      CALL BINTGS(PT,N1+N2)                                             CND04370
      IF((L1.GT.0).OR.(L2.GT.0)) GO TO 60                               CND04380
C     BEGIN SECTION USED FOR OVERLAP INTEGRALS INVOLVING S FUNCTIONS    CND04390
C     FIND Z TABLE NUMBER L                                             CND04400
      L = (90-17*N1+N1**2-2*N2)/2                                       CND04410
      ULIM = N1+N2                                                      CND04420
      LLIM = 0
C  PROTECT LLIM1 CAN NOT .EQ. 0
      LLIM1= LLIM+1
      ULIM1= ULIM+1                                                     CND04430
      DO 50 MJ1=LLIM1,MLIM1
      I=MJ1-1                                                           CND04440
      NN11=N1+N2-I+1                                                    CND04450
   50 X=X+Z(I+1,L)*A(I+1)*B(NN11)/2.D0                                  CND04460
      SS=X                                                              CND04470
      GO TO 80
```

```
C     BEGIN SECTION USED FOR OVERLAPS INVOLVING NON-S FUNCTIONS          CND04480
C     FIND Y TABLE NUMBER L                                             CND04490
   50 L=(5-M)*(24-10*M+M**2)*(83-30*M+3*M**2)/120+                      CND04500
     1  (30-9*L1+L1**2-2*N1)*(28-9*L1+L1**2-2*N1)/8+                    CND04510
     2  (30-9*L2+L2**2-2*N2)/2                                          CND04520
      LLIM = 0                                                         CND04530
C  PROTECT LLIM1 CAN NOT .EQ. 0
      LLIM1=LLIM+1
      DO 70 MK1=LLIM1,9                                                CND04540
      I=MK1-1
      JLIM=4 - MOD(K+1,2)                                              CND04550
      MLIM1=JLIM+1
      DO 70 ML1=LLIM1,MLIM1                                            CND04560
      J=ML1-1
      IIII=2*J+MOD(K+1,2)+1                                            CND04570
   70 X=X+Y(I+1,J+1,L)*A(I+1)*B(IIII)                                  CND04580
      SS = X*(FACT(M+1)/8.D0)**2*DSQRT((2*L1+1)*FACT(L1-M)*            CND04590
     1 (2*L2+1)*FACT(L2-M)/(4.D0*FACT(L1+M)*FACT(L2+M)))               CND04600
   80 CONTINUE                                                         CND04610
      RETURN                                                           CND04620
      END                                                              CND04630
C                                                                      CND04640
      SUBROUTINE AINTGS(X,K)                                           CND04660
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C6/G(35,35),XXX(9,9,3),A(18),B(18)                        CND04690
      A(1) =DEXP(-X)/X                                                 CND04700
      DO 10  I=1,K                                                     CND04710
   10 A(I+1) =(A(I)*(I)+DEXP(-X))/X                                    CND04720
      RETURN                                                           CND04730
      END                                                              CND04740
C                                                                      CND04750
      SUBROUTINE BINTGS(XX,KK)                                         CND04770
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C6/G(35,35),XXX(9,9,3),A(18),B(18)                        CND04910
      DATA IO/0/                                                       CND04920
      K=XX                                                             CND04930
      K=KK                                                             CND04940
      ABSX=DABS(X)                                                     CND04950
      IF(ABSX.GT.3.D0) GO TO 120                                       CND04960
      IF(ABSX.GT.2.D0) GO TO 20                                        CND04970
      IF(ABSX.GT.1.D0) GO TO 50                                        CND04980
      IF(ABSX.GT..5D0) GO TO 80                                        CND04990
      IF(ABSX.GT..00000100) GO TO 110                                  CND05000
C  PROTEC FOR IO .EQ.0
      IIO=IO+1
      DO 130 J=IIO,K,3                                                 CND05010
      I=J-1
      B(I+2)=0.0                                                       CND05020
  130 B(I+1)=2.0/(I+1)                                                 CND05030
      RETURN                                                           CND05040
  110 LAST=5                                                           CND05050
      GO TO 140                                                        CND05060
   80 IF(K..E.5) GO TO 120                                             CND05070
      LAST=7                                                           CND05080
      GO TO 140                                                        CND05090
   50 IF(K..E.7) GO TO 120                                             CND05100
      LAST=12                                                          CND05110
      GO TO 140                                                        CND05120
   20 IF(K.LE.10) GO TO 120                                            CND05130
      LAST=15                                                          CND05140
      GO TO 140                                                        CND05150
  120 EXPX=DEXP(X)                                                     CND05160
      EXPMX=1.D0/EXPX                                                  CND05170
      B(1)=(EXPX-EXPMX)/X                                              CND05180
      DO 130 I=1,K                                                     CND05190
      EXPX=-EXPX                                                       CND05200
  130 B(I+1)=(I*B(I)+EXPX-EXPMX)/X                                     CND05210
      RETURN                                                           CND05220
  140 DO 160 I=IO,K                                                    CND05230
      Y=0.D0                                                           CND05240
      II=MOD(I,2)                                                      CND05250
      DO 150 M=II,LAST,2                                               CND05260
  150 Y=Y+(-X)**M*2.0/(FACT(M)*(M+I+1))                                CND05270
  160 B(I+1)=Y                                                         CND05280
      RETURN                                                           CND05290
      END                                                              CND05300
C                                                                      CND05310
      SUBROUTINE MATOUT(NN,MATOP)                                      CND05330
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C1/A(70,70,3)                                             CND05360
      N=NN                                                             CND05370
      DO 60 M=1,N,12                                                   CND05380
      K=M+11                                                           CND05390
```

```
      IF (K.GT.N) K=N                                                   CND05400
      PRINT40, (J,J=M,K)                                                CND05410
   40 FORMAT('0      ',12I9)                                            CND05420
      DO 60 I=1,N                                                       CND05430
      PRINT50, I,(A(I,J,MATOP),J=M,K)                                   CND05440
   50 FORMAT(I4,4X,12F9.4)                                              CND05450
   60 CONTINUE                                                          CND05460
      PRINT70                                                           CND05470
   70 FORMAT(//)                                                        CND05480
      RETURN                                                            CND05490
      END                                                               CND05500
C                                                                       CND05510
      SUBROUTINE EIGNOP(NN,RHO)                                         CND05580
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C1/A(70,70),VEC(70,70)                                     CND05610
      COMMON/C6/XXX(35,35),GAMMA(70),BETA(70),BETASQ(70),               CND05620
     ,EIG(70),W(70)                                                     CND05630
C     THE FOLLOWING DIMENSIONED VARIABLES ARE EQUIVALENCED              CND05640
      DIMENSION P(70),Q(70)                                             CND05650
      EQUIVALENCE (P(1),BETA(1)),(Q(1),BETA(1))                         CND05660
      DIMENSION IPOSV(70),IVPOS(70),IORD(70)                            CND05670
      EQUIVALENCE (IPOSV(1),GAMMA(1)),(IVPOS(1),BETA(1)),               CND05680
     1(IORD(1),BETASQ(1))                                               CND05690
      RHOSQ=RHO*RHO                                                     CND05700
      N=NN                                                              CND05710
      IF (N .EQ. 0) GO TO 640                                           CND05720
      N1=N-1                                                            CND05730
      N2=N-2                                                            CND05740
      GAMMA(1)=A(1,1)                                                   CND05750
      IF(N2) 200,190,40                                                 CND05760
   40 DO 180 NR=1,N2                                                    CND05770
      B=A(NR+1,NR)                                                      CND05780
      S=0.D0                                                            CND05790
      DO 50 I=NR,N2                                                     CND05800
   50 S=S+A(I+2,NR)**2                                                  CND05810
C     PREPARE FOR POSSIBLE BYPASS OF TRANSFORMATION                     CND05820
      A(NR+1,NR)=0.D0                                                   CND05830
      IF (S) 170,170,60                                                 CND05840
   60 S=S+B*B                                                           CND05850
      SGN=+1.D0                                                         CND05860
      IF (B) 70,80,80                                                   CND05870
   70 SGN=-1.D0                                                         CND05880
   80 SQRTS=DSQRT(S)                                                    CND05890
      D=SGN/(SQRTS+SQRTS)                                               CND05900
      TEMP=DSQRT(.5D0+B*D)                                              CND05910
      W(NR)=TEMP                                                        CND05920
      A(NR+1,NR)=TEMP                                                   CND05930
      D=D/TEMP                                                          CND05940
      B=-SGN*SQRTS                                                      CND05950
C     D IS FACTOR OF PROPORTIONALITY. NOW COMPUTE AND SAVE W VECTOR.    CND05960
C     EXTRA SINGLY SUBSCRIPTED W VECTOR USED FOR SPEED.                 CND05970
      DO 90 I=NR,N2                                                     CND05980
      TEMP=D*A(I+2,NR)                                                  CND05990
      W(I+1)=TEMP                                                       CND06000
   90 A(I+2,NR)=TEMP                                                    CND06010
C     PREMULTIPLY VECTOR W BY MATRIX A TO OBTAIN P VECTOR.              CND06020
C     SIMULTANEOUSLY ACCUMULATE DOT PRODUCT WP,(THE SCALAR K)           CND06030
      WTAW=0.D0                                                         CND06040
      DO 140 I=NR,N1                                                    CND06050
      SUM=0.D0                                                          CND06060
      DO 130 J=NR,I                                                     CND06070
  130 SUM=SUM+A(I+1,J+1)*W(J)                                           CND06080
      I1=I+1                                                            CND06090
      IF(N1-I1) 130,110,110                                             CND06100
  110 DO 120 J=I1,N1                                                    CND06110
  120 SUM=SUM+A(J+1,I+1)*W(J)                                           CND06120
  130 P(I)=SUM                                                          CND06130
  140 WTAW=WTAW+SUM*W(I)                                                CND06140
C     P VECTOR AND SCALAR K  NOW STORED. NEXT COMPUTE Q VECTOR          CND06150
      DO 150 I=NR,N1                                                    CND06160
  150 Q(I)=P(I)-WTAW*W(I)                                               CND06170
C     NOW FORM PAP MATRIX, REQUIRED PART                                CND06180
      DO 160 J=NR,N1                                                    CND06190
      QJ=Q(J)                                                           CND06200
      WJ=W(J)                                                           CND06210
      DO 160 I=J,N1                                                     CND06220
  160 A(I+1,J+1)=A(I+1,J+1)-2.D0*(W(I)*QJ+WJ*Q(I))                      CND06230
  170 BETA(NR)=B                                                        CND06240
      BETASQ(NR)=B*B                                                    CND06250
  180 GAMMA(NR+1)=A(NR+1,NR+1)                                          CND06260
  190 B=A(N,N-1)                                                        CND06270
      BETA(N-1)=B                                                       CND06280
```

```
      BETASQ(N-1)=B*B                                                   CND06290
      GAMMA(N)=A(N,N)                                                   CND06300
  200 BETASQ(N)=0.D0                                                    CND06310
C     ADJOIN AN IDENTITY MATRIX TO BE POSTMULTIPLIED BY ROTATIONS.      CND06320
      DO 220 I=1,N                                                      CND06330
      DO 210 J=1,N                                                      CND06340
  210 VEC(I,J)=0.D0                                                     CND06350
  220 VEC(I,I)=1.D0                                                     CND06360
      M=N                                                               CND06370
      SUM=0.D0                                                          CND06380
      NPAS=1                                                            CND06390
      GO TO 350                                                         CND06400
  230 SUM=SUM+SHIFT                                                     CND06410
      COSA=1.D0                                                         CND06420
      G=GAMMA(1)-SHIFT                                                  CND06430
      PP=G                                                              CND06440
      PPBS=PP*PP+BETASQ(1)                                              CND06450
      PPBR=DSQRT(PPBS)                                                  CND06460
      DO 320 J=1,M                                                      CND06470
      COSAP=COSA                                                        CND06480
      IF (PPBS.GT.1.E-12) GO TO 250                                     CND06490
      SINA=0.D0                                                         CND06500
      SINA2=0.D0                                                        CND06510
      COSA=1.D0                                                         CND06520
      GO TO 290                                                         CND06530
  250 SINA=BETA(J)/PPBR                                                 CND06540
      SINA2=BETASQ(J)/PPBS                                              CND06550
      COSA=PP/PPBR                                                      CND06560
C     POSTMULTIPLY IDENTITY BY P-TRANSPOSE MATRIX                       CND06570
      NT=J+NPAS                                                         CND06580
      IF(NT .LT. N) GO TO 270                                           CND06590
      NT=N                                                              CND06600
  270 DO 280 I=1,NT                                                     CND06610
      TEMP=COSA*VEC(I,J)+SINA*VEC(I,J+1)                                CND06620
      VEC(I,J+1)=-SINA*VEC(I,J)+COSA*VEC(I,J+1)                         CND06630
  280 VEC(I,J)=TEMP                                                     CND06640
  290 DIA=GAMMA(J+1)-SHIFT                                              CND06650
      U=SINA2*(G+DIA)                                                   CND06660
      GAMMA(J)=G+U                                                      CND06670
      G=DIA-U                                                           CND06680
      PP=DIA*COSA-SINA*COSAP*BETA(J)                                    CND06690
      IF(J .NE. M) GO TO 310                                            CND06700
      BETA(J)=SINA*PP                                                   CND06710
      BETASQ(J)=SINA2*PP*PP                                             CND06720
      GO TO 330                                                         CND06730
  310 PPBS=PP*PP+BETASQ(J+1)                                            CND06740
      PPBR=DSQRT(PPBS)                                                  CND06750
      BETA(J)=SINA*PPBR                                                 CND06760
  320 BETASQ(J)=SINA2*PPBS                                              CND06770
  330 GAMMA(M+1)=G                                                      CND06780
C     TEST FOR CONVERGENCE OF LAST DIAGONAL ELEMENT                     CND06790
      NPAS=NPAS+1                                                       CND06800
      IF(BETASQ(M) .GT. RHOSQ) GO TO 370                                CND06810
  340 EIG(M+1)=GAMMA(M+1)+SUM                                           CND06820
  350 BETA(M)=0.D0                                                      CND06830
      BETASQ(M)=0.D0                                                    CND06840
      M=M-1                                                             CND06850
      IF(M .EQ. 0) GO TO 400                                            CND06860
      IF(BETASQ(M) .LE. RHOSQ) GO TO 340                                CND06870
C     TAKE ROOT OF CORNER 2 BY 2 NEAREST TO LOWER DIAGONAL IN VALUE     CND06880
C     AS ESTIMATE OF EIGENVALUE TO USE FOR SHIFT                        CND06890
  370 A2=GAMMA(M+1)                                                     CND06900
      R2=0.5D0*A2                                                       CND06910
      R1=0.5D0*GAMMA(M)                                                 CND06920
      R12=R1+R2                                                         CND06930
      DIF=R1-R2                                                         CND06940
      TEMP=DSQRT(DIF*DIF+BETASQ(M))                                     CND06950
      R1=R12+TEMP                                                       CND06960
      R2=R12-TEMP                                                       CND06970
      DIF=DABS(A2-R1)-DABS(A2-R2)                                       CND06980
      IF(DIF .LT. 0.D0) GO TO 390                                       CND06990
      SHIFT=R2                                                          CND07000
      GO TO 230                                                         CND07010
  390 SHIFT=R1                                                          CND07020
      GO TO 230                                                         CND07030
  400 EIG(1)=GAMMA(1)+SUM                                               CND07040
C     INITIALIZE AUXILIARY TABLES REQUIRED FOR REARRANGING THE VECTORS  CND07050
      DO 410 J=1,N                                                      CND07060
      IPOSV(J)=J                                                        CND07070
      IVPOS(J)=J                                                        CND07080
  410 IORD(J)=J                                                         CND07090
C     USE A TRANSPOSITION SORT TO ORDER THE EIGENVALUES                 CND07100
      M=N                                                               CND07110
```

```
      GO TO 450                                                          CND07120
  420 DO 440 J=1,M                                                       CND07130
      IF (EIG(J) .LE. EIG(J+1)) GO TO 440                                CND07140
      TEMP=EIG(J)                                                        CND07150
      EIG(J)=EIG(J+1)                                                    CND07160
      EIG(J+1)=TEMP                                                      CND07170
      ITEMP=IORD(J)                                                      CND07180
      IORD(J)=IORD(J+1)                                                  CND07190
      IORD(J+1)=ITEMP                                                    CND07200
  440 CONTINUE                                                           CND07210
  450 M=M-1                                                              CND07220
      IF(M .NE. 0) GO TO 420                                             CND07230
      IF(N1 .EQ. 0) GO TO 510                                            CND07240
      DO 500 L=1,N1                                                      CND07250
      NV=IORD(L)                                                         CND07260
      NP=IPOSV(NV)                                                       CND07270
      IF(NP .EQ. L) GO TO 500                                            CND07280
      LV=IVPOS(L)                                                        CND07290
      IVPOS(NP)=LV                                                       CND07300
      IPOSV(LV)=NP                                                       CND07310
      DO 490 I=1,N                                                       CND07320
      TEMP=VEC(I,L)                                                      CND07330
      VEC(I,L)=VEC(I,NP)                                                 CND07340
  490 VEC(I,NP)=TEMP                                                     CND07350
  500 CONTINUE                                                           CND07360
  510 CONTINUE                                                           CND07370
C     BACK TRANSFORM THE VECTORS OF THE TRIPLE DIAGONAL MATRIX           CND07380
      DO 570 NRR=1,N                                                     CND07390
      K=N1                                                               CND07400
  520 K=K-1                                                              CND07410
      IF(K .LE. 0) GO TO 560                                             CND07420
      SUM=0.D0                                                           CND07430
      DO 540 I=K,N1                                                      CND07440
  540 SUM=SUM+VEC(I+1,NRR)*A(I+1,K)                                      CND07450
      SUM=SUM+SUM                                                        CND07460
      DO 550 I=K,N1                                                      CND07470
  550 VEC(I+1,NRR)=VEC(I+1,NRR)-SUM*A(I+1,K)                             CND07480
      GO TO 520                                                          CND07490
  560 CONTINUE                                                           CND07500
  570 CONTINUE                                                           CND07510
  640 RETURN                                                             CND07520
      END                                                                CND07530
C                                                                        CND07540
      SUBROUTINE OVER4                                                   CND07570
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CO/EPS
      COMMON/C1/A(70,70),B(70,70)                                        CND07610
      COMMON/C2/C(35,3),AN(35)                                           CND00080
      COMMON/C3/CZ(35),U(70),ULIM(35),LLIM(35),NELECS,OCCA,OCCB          CND07620
      COMMON/C6/G(35,35),Q(70),XXX(70),YYY(70,5),ENERGY,ENERG            CND07630
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,IT,LIMEX                          CND07640
      COMMON/C9/OPTION,OPNCLC,CNDO,INDO,CLOSED,OPEN,IAN                  CND07650
      DIMENSION ENEG(18,3),BETAO(16)                                     CND07670
      DIMENSION G1(18),F2(18)                                            CND07680
      INTEGER CHARGE,OCCA,OCCB,UL,AN,CZ,U,ULIM,ANI,Z                     CND07690
      DATA BETAO(3) / -9.    /                                           CND08250
      DATA BETAO(4) / -13.   /                                           CND08260
      DATA BETAO(5) / -17.   /                                           CND08270
      DATA BETAO(6) / -21.   /                                           CND08280
      DATA BETAO(7) / -25.   /                                           CND08290
      DATA BETAO(8) / -31.   /                                           CND08300
      DATA BETAO(9) / -39.   /                                           CND08310
      DATA BETAO(11) /-7.7203 /                                          CND08320
      DATA BETAO(12) /-9.4471 /                                          CND08330
      DATA BETAO(13) /-11.3011/                                          CND08340
      DATA BETAO(14) /-13.065 /                                          CND08350
      DATA BETAO(15) /-15.070 /                                          CND08360
      DATA BETAO(16) /-18.150 /                                          CND08370
      DATA BETAO(17) /-22.330 /                                          CND08380
      DATA OLDENG,ELDENG/2*1E10/                                         CND08390
      DATA RHO /1E-6/                                                    CND08400
C     FIND NELECS AND FILL H CORE(DIAGONAL) WITH (I+A)/2                 CND08410
      NELECS=0                                                           CND08420
      DO 60 I=1,NATOMS                                                   CND08430
      NELECS=NELECS+CZ(I)                                                CND08440
      LL =LLIM(I)                                                        CND08450
      JL =ULIM(I)                                                        CND08460
      ANI=AN(I)                                                          CND08470
      L=0                                                                CND08480
      DO 50 J=LL,JL                                                      CND08490
      L=L+1                                                              CND08500
      IF (L.EQ.1) GO TO 10                                               CND08510
```

```
      IF (L.LT.5) GO TO 40                                              CND08520
      A(J,J)=-ENEG(ANI,3)/27.2100                                       CND08530
      GO TO 50                                                          CND08540
   40 A(J,J)=-ENEG(ANI,2)/27.2100                                       CND08550
      GO TO 50                                                          CND08560
   10 A(J,J)   =-ENEG(ANI,1)/27.2100                                    CND08570
   50 CONTINUE                                                          CND08580
   60 CONTINUE                                                          CND08590
      NELECS=NELECS-CHARGE                                              CND08600
      OCCA=NELECS/2                                                     CND08610
C     FORM HUCKEL HAMILTONIAN IN A (OFF DIAGONAL TWO CENTER TERMS)      CND08620
      DO 90 I=2,N                                                       CND08630
      K=J(I)                                                            CND08640
      L=AN(K)                                                           CND08650
      JL=I-1                                                            CND08660
      DO 90 J=1,JL                                                      CND08670
      KK=U(J)                                                           CND08680
      LL=AN(KK)                                                         CND08690
      IF ((L.GT.9).OR.(LL.GT.9)) GO TO 70                               CND08700
      A(I,J)=A(I,J)*(BETAO(L)+BETAO(LL))/54.4200                        CND08710
      A(J,I)=A(I,J)                                                     CND08720
      GO TO 90                                                          CND08730
   70 A(I,J)=0.7500*A(I,J)*(BETAO(L)+BETAO(LL))/54.4200                 CND08740
     *A(J,I)=A(I,J)                                                     CND08750
   90 CONTINUE                                                          CND08760
      DO 100 I=1,N                                                      CND08770
  100 Q(I)=A(I,I)                                                       CND08780
      NN=N                                                              CND08790
      CALL EIGNCL(NN,RHO)                                               CND08800
C     EIGENVECTORS (IN B) ARE CONVERTED INTO DENSITY MATRIX (IN B)      CND08810
      DO 140 I=1,N                                                      CND08820
      DO 120 J=1,N                                                      CND08830
      XXX(J)=0.000                                                      CND08840
      DO 110 K=1,OCCA                                                   CND08850
  110 XXX(J)= XXX(J)+2.00*B(I,K)*B(J,K)                                 CND08860
  120 CONTINUE                                                          CND08870
      DO 130 J=I,N                                                      CND08880
  130 B(I,J)= XXX(J)                                                    CND08890
  140 CONTINUE                                                          CND08900
      DO 150 I=1,N                                                      CND08910
      DO 150 J=I,N                                                      CND08920
  150 B(J,I)=B(I,J)                                                     CND08930
C     ADD V(AB) TO HCORE--CNDO                                          CND08940
      DO 170 I=1,N                                                      CND08950
      J=U(I)                                                            CND08960
      Q(I)=Q(I)  +0.500*G(J,J)                                          CND08970
      DO 160 K=1,NATOMS                                                 CND08980
  160 Q(I)=Q(I)-(CZ(K)*G(J,K))                                          CND08990
  170 CONTINUE                                                          CND09000
C     EXIT SEGMENT IF ONLY CNDO APPROXIMATIONS ARE DESIRED              CND09010
      IF (OPTION.EQ.CNDO) GO TO 290                                     CND09020
C     INDO MODIFICATION (CORRECTION TO U(I,I) )                         CND09030
      DO 280 I=1,NATOMS                                                 CND09040
      K=AN(I)                                                           CND09050
      J=LLIM(I)                                                         CND09060
      IF ((K.GT.1).AND.(K.LT.10)) GO TO 190                             CND09070
      GO TO 280                                                         CND09080
  190 IF (K.LE.3) GO TO 210                                             CND09090
      Q(J)=Q(J)+(CZ(I)-1.5)*G1(K)/6.                                    CND09100
  210 IF(K.EQ.3) GO TO 220                                              CND09110
      IF(K.EQ.4) GO TO 240                                              CND09120
      TEMP=S1(K)/3.+(CZ(I)-2.5)*2.*F2(K)/25.                            CND09130
      GO TO 260                                                         CND09140
  240 TEMP=S1(K)/4.00                                                   CND09150
      GO TO 260                                                         CND09160
  220 TEMP=S1(K)/12.00                                                  CND09170
  260 CONTINUE                                                          CND09180
      DO 270 L=1,3                                                      CND09190
      JPL=J+L                                                           CND09200
  270 Q(JPL)=Q(JPL)+TEMP                                                CND09210
  280 CONTINUE                                                          CND09220
  290 CONTINUE                                                          CND09230
      DO 310 I=1,N                                                      CND09240
      DO 300 J=I,N                                                      CND09250
  300 A(J,I)=A(I,J)                                                     CND09260
  310 A(I,I)=Q(I)                                                       CND09270
C     IF(PRTOPT.LE.1)GO TO 380                                          CND09280
      PRINT320                                                          CND09290
  320 FORMAT(/4(/'+ CORE HAMILTONIAN')/)                                CND09300
      CALL SCFOUT(0,1)                                                  CND09310
  380 CONTINUE                                                          CND09320
  410 CONTINUE                                                          CND09380
      Z = Z+1                                                           CND09390
```

```
      ENERGY = 0.D0                                                          CND09400
C     TRANSFER CORE HAMILTONIAN TO LOWER TRIANGLE OF A                       CND09410
      DO 420 I=1,N                                                           CND09420
      A(I,I)=Q(I)                                                            CND09430
      DO 420 J=I,N                                                           CND09440
  420 A(J,I)=A(I,J)                                                          CND09450
      DO 430 I=1,N                                                           CND09460
      II=U(I)                                                                CND09470
      A(I,I)=A(I,I)-B(I,I)*G(II,II)*0.5D0                                    CND09480
      DO 430 K=1,N                                                           CND09490
      JJ=J(K)                                                                CND09500
  430 A(I,I)=A(I,I)+B(K,K)*G(II,JJ)                                          CND09510
      NM=N-1                                                                 CND09520
      DO 440 I=1,NM                                                          CND09530
      II=U(I)                                                                CND09540
      LL=I+1                                                                 CND09550
      DO 440 J=LL,N                                                          CND09560
      JJ=U(J)                                                                CND09570
  440 A(J,I)=A(J,I)-B(J,I)*G(II,JJ)*0.5D0                                    CND09580
C     INDO MODIFICATION                                                      CND09590
      IF (OPTION.EQ.CNDO) GO TO 490                                          CND09600
      DO 480 II=1,NATOMS                                                     CND09610
      K=AN(II)                                                               CND09620
      I=LLIM(II)                                                             CND09630
      IF (K.EQ.1) GO TO 480                                                  CND09640
      PAA=B(I,I)+B(I+1,I+1)+B(I+2,I+2)+B(I+3,I+3)                            CND09650
      A(I,I)=A(I,I)-(PAA-B(I,I)) *G1(K)/6.D0                                 CND09660
      DO 470 J=1,3                                                           CND09670
      IPJ=I+J                                                                CND09680
      A(IPJ,IPJ)=A(IPJ,IPJ)-B(I,I)*G1(K)/6.D0-(PAA-B(I,I))*7.D0*             CND09690
     1F2(K)/50.D0+B(IPJ,IPJ)*11.D0*F2(K)/50.D0                               CND09700
  470 A(IPJ,I)=A(IPJ,I)+B(I,IPJ)*G1(K)/2.D0                                  CND09710
      I1=I+1                                                                 CND09720
      I2=I+2                                                                 CND09730
      I3=I+3                                                                 CND09740
      A(I2,I1)=A(I2,I1)+B(I2,I1)*11.D0*F2(K)/50.D0                           CND09750
      A(I3,I1)=A(I3,I1)+B(I3,I1)*11.D0*F2(K)/50.D0                           CND09760
      A(I3,I2)=A(I3,I2)+B(I3,I2)*11.D0*F2(K)/50.D0                           CND09770
  480 CONTINUE                                                               CND09780
  490 CONTINUE                                                               CND09790
      DO 500 I=1,N                                                           CND09800
  500 ENERGY=ENERGY+0.5D0*B(I,I)*(A(I,I)+Q(I))                               CND09810
      DO 505 I=1,NM                                                          CND09820
      LL=I+1                                                                 CND09830
      DO 505 J=LL,N                                                          CND09840
  505 ENERGY=ENERGY+B(I,J)*(A(I,J)+A(J,I))                                   CND09850
      IF(DABS(ENERGY-OLDENG).GE.EPS)GOTO 550                                 CND09860
      IF(DABS(ENERGY-ELDENG).GE.EPS)GOTO 550                                 CND09870
  530 PRINT540, ENERGY,Z                                                     CND09880
  540 FORMAT(//10X,'ELECTRONIC ENERGY =',F17.10,' A.U.',T70,'ENERGY SATICND09890
     1FIED AFTER',I4,' ITERATIONS'/)                                         CND09900
      Z=11111                                                                CND09910
      GO TO 1570                                                             CND09920
  550 IZ=IZ+1                                                                CND09930
      YY(IZ)=ENERGY                                                          CND09940
      SUMYY=ENERGY*0.1+SUMYY                                                 CND09950
      IF (IZ.NE.10) GO TO 1560                                               CND09960
C           KONVERGIEREN MITTELWERTE ?                                       CND09970
      IF (DABS(SUMYY-OLSUMY).GT.EPS) GO TO 1530                              CND09980
      ENERGY=SUMYY                                                           CND09990
      PRINT1520, YY                                                          CND10000
 1520 FORMAT('0 LAST ITERATION VALUES'//2X,10F13.5)                          CND10010
      GO TO 530                                                              CND10020
 1530 OLSUMY=SUMYY                                                           CND10030
      SUMYY=0.0                                                              CND10040
      IZ=0                                                                   CND10050
 1560 ELDENG=OLDENG                                                          CND10060
      OLDENG=ENERGY                                                          CND10070
      IF (Z.LE.IT) GOTO 610                                                  CND10080
      IF (Z.EQ.IT+1) PRINT541, ENERGY                                        CND10090
  541 FORMAT(//10X,'ELECTRONIC ENERGY =',F17.5,' A.U.',4(/'+',T70,'++++ CND10100
     ++ ENERGY NOT SATISFIED +++++'))                                        CND10110
C     SYMMETRIZE F FOR PRINTING (MATRIX A)                                   CND10120
 1570 DO 590 I=1,N                                                           CND10130
      DO 590 J=I,N                                                           CND10140
  590 A(I,J)=A(J,I)                                                          CND10150
  610 CONTINUE                                                               CND10160
      NN=N                                                                   CND10170
      CALL EIGNCL(NN,RHO)                                                    CND10180
      IF (Z.LE.IT) GO TO 640                                                 CND10190
C     IF(PRTOPT.LT.1)GO TO 640                                               CND10200
      PRINT630                                                               CND10210
  630 FORMAT(/4(/'+ EIGENVALUES AND EIGENVECTORS'))                          CND10220
      CALL SCFOUT(1,2)                                                       CND10230
  640 CONTINUE                                                               CND10240
C     EIGENVECTORS (IN J) ARE CONVERTED INTO DENSITY MATRIX (IN B)           CND10250
```

```
      DO 680 I=1,N                                                      CND10260
      DO 660 J=I,N                                                      CND10270
      XXX(J)=0.000                                                      CND10280
      DO 650 K=1,DCCA                                                   CND10290
  650 XXX(J)= XXX(J)+B(I,K)*B(J,K)*2.000                                CND10300
  660 CONTINUE                                                          CND10310
      DO 670 J=I,N                                                      CND10320
  670 B(I,J)= XXX(J)                                                    CND10330
  680 CONTINUE                                                          CND10340
      DO 690 I=1,N                                                      CND10350
      DO 690 J=I,N                                                      CND10360
  690 B(J,I)=B(I,J)                                                     CND10370
      IF (J.LE.ITT) GO TO 410                                           CND10380
      CALL OPRINT                                                       CND10390
      RETURN                                                            CND10400
      END                                                               CND10410
C                                                                       CND10420
      SUBROUTINE EIGNCL(P,THR)                                          CND10440
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C1/B(70,70),X(70,70)                                       CND10490
      COMMON/C6/XXX(35,35),GAMMA(70),BETA(70),BETASQ(70),G(70)          CND10500
      INTEGER P,P1                                                      CND10510
      LOGICAL TRANSF                                                    CND10520
      DO 20 I=1,P                                                       CND10530
   20 G(I)=B(I,I)                                                       CND10540
      SR=.5                                                             CND10550
      DO11=1,P                                                          CND10560
      DO2J=1,P                                                          CND10570
    2 X(I,J)=0.                                                         CND10580
    1 X(I,I)=1.00                                                       CND10590
      DO44=1,9                                                          CND10600
    5 TRANSF=.FALSE.                                                    CND10610
      DO61=2,P                                                          CND10620
      I1=I-1                                                            CND10630
      I2=I+1                                                            CND10640
      DO6J=1,I1                                                         CND10650
      IF(DABS(B(I,J)).LT.SR)GOTO6                                       CND10660
      TRANSF=.TRUE.                                                     CND10670
      Z=2.00*B(I,J)                                                     CND10680
      R=G(J)-G(I)                                                       CND10690
      S2=Z/DSIGN(DSQRT(Z*Z+R*R),R)                                      CND10700
      S1=S2/DSQRT(2.*(1.+DSQRT(DABS(1.-S2*S2))))                        CND10710
      S=S1                                                              CND10720
      C=DSQRT(1.00-S1*S1)                                               CND10730
      W=(Z*C-R*S)*S                                                     CND10740
      G(J)=G(J)+W                                                       CND10750
      G(I)=G(I)-W                                                       CND10760
      B(I,J)=0.                                                         CND10770
      IF(J.EQ.1)GOTO7                                                   CND10780
      J1=J-1                                                            CND10790
      DO8K=1,J1                                                         CND10800
      W=B(J,K)                                                          CND10810
      B(J,K)=W*C+B(I,K)*S                                               CND10820
    8 B(I,K)=-W*S+B(I,K)*C                                              CND10830
    7 IF(J.EQ.I1)GOTO9                                                  CND10840
      J1=J+1                                                            CND10850
      DO10K=J1,I1                                                       CND10860
      W=B(K,J)                                                          CND10870
      B(K,J)=W*C+B(I,K)*S                                               CND10880
   10 B(I,K)=-W*S+B(I,K)*C                                              CND10890
    9 IF(I.EQ.P)GOTO11                                                  CND10900
      DO12K=I2,P                                                        CND10910
      W=B(K,J)                                                          CND10920
      B(K,J)=W*C+B(K,I)*S                                               CND10930
   12 B(K,I)=-W*S+B(K,I)*C                                              CND10940
   11 DO13K=1,P                                                         CND10950
      W=X(K,J)                                                          CND10960
      X(K,J)=W*C+X(K,I)*S                                               CND10970
   13 X(K,I)=-W*S+X(K,I)*C                                              CND10980
    6 CONTINUE                                                          CND10990
      IF(TRANSF)GOTO5                                                   CND11000
    4 SR=SR/10.00                                                       CND11010
      P1=P-1                                                            CND11020
      DO151=1,P1                                                        CND11030
      GMAX= 1E10                                                        CND11040
      DO16J=I,P                                                         CND11050
      IF(G(J).GE.GMAX)GOTO16                                            CND11060
      GMAX=G(J)                                                         CND11070
      L=J
```

```
   16 CONTINUE                                                          CND11080
      S(L)=S(I)                                                         CND11090
      S(I)=SMAX                                                         CND11100
      DO15K=1,P                                                         CND11110
      A=X(K,I)                                                          CND11120
      X(K,I)=X(K,L)                                                     CND11130
   15 X(K,L)=A                                                          CND11140
      RETURN                                                            CND11150
      END                                                               CND11160
C                                                                       CND11170
      SUBROUTINE CPRINT                                                 CND11190
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/C0/EPS
      COMMON/C1/A(70,70),B(70,70)                                       CND11230
      COMMON/C2/C(35,3),AN(35)                                          CND11250
      COMMON/C3/CZ(35),J(70),ULIM(35),LLIM(35),NELECS,OCCA,OCCB         CND11260
      COMMON/C4/EL(18)                                                  CND11270
      COMMON/C6/G(35,35),J(70),XXX(70),YYY(70,5),ENERGY,ENERG           CND11240
      COMMON/C7/NATOMS,CHARGE,MULTIP,N,IT,LIMEX                         CND11280
      COMMON/C9/OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN                 CND11290
      CHARACTER*4 EL,OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN*80         CND11300
      INTEGER CHARGE,AN,O,ULIM,OCCA,OCCB,UL,CZ,ANI                      CND11310
      DIMENSION DPM(3),DM(3),DMSP(3),DMPO(3)                            CND11320
      DIMENSION ATENG(18)                                               CND11330
      DATA ATENG(1)/-0.638730240e2 /                                    CND11340
      DATA ATENG(3)/-.23219724O5  /                                     CND11350
      DATA ATENG(4)/-1.1454120355 /                                     CND11360
      DATA ATENG(5)/-2.3774239048 /                                     CND11370
      DATA ATENG(6)/-6.164993626. /                                     CND11380
      DATA ATENG(7)/-11.073874625 /                                     CND11390
      DATA ATENG(8)/-18.081965865 /                                     CND11400
      DATA ATENG(9)/-27.549130288 /                                     CND11410
      DATA ATENG(11)/-.1977009566 /                                     CND11420
      DATA ATENG(12)/-.8671913833 /                                     CND11430
      DATA ATENG(13)/-2.0364557744/                                     CND11440
      DATA ATENG(14)/-3.8979654o86/                                     CND11450
      DATA ATENG(15)/-6.7766009163/                                     CND11460
      DATA ATENG(16)/-10.758174344/                                     CND11470
      DATA ATENG(17)/-16.046701794/                                     CND11480
      IF (OPTION.EQ.CNDO) GO TO 30                                      CND11490
      ATENG(4)=-1.1219620354                                            CND11500
      ATENG(5)=-2.8725750046                                            CND11510
      ATENG(6)=-5.9349548261                                            CND11520
      ATENG(7)=-10.673174125                                            CND11530
      ATENG(8)=-17.292035065                                            CND11540
      ATENG(9)=-26.257437737                                            CND11550
   30 ENERG=ENERGY                                                      CND11560
      K=NATOMS-1                                                        CND11570
C     IF(PRTOPT.LT.1)GO TO 290                                          CND11580
      PRINT40                                                           CND11590
   40 FORMAT(/4(/'* DENSITY MATRIX'))                                   CND11600
      CALL SCFOUT(0,2)                                                  CND11610
  290 DO 50 I=1,K                                                       CND11620
      L=I+1                                                             CND11630
      DO 50 J=L,NATOMS                                                  CND11640
      RA=DSQRT((C(I,1)-C(J,1))**2+(C(I,2)-C(J,2))**2                    CND11650
     1        +(C(I,3)-C(J,3))**2)                                      CND11660
   50 ENERGY=ENERGY+(CZ(I)*CZ(J))/RAD                                   CND11670
      ENERG=ENERGY-ENERG                                                CND11680
      PRINT60, ENERG,ENERGY                                             CND11690
   60 FORMAT(/'0  NUCLEAR REPULSION ENERGY =',F12.4,' A.U.',            CND11700
     */13X,' TOTTAL ENERGY =',F12.4,' A.U.')                            CND11710
      ENERG=ENERGY                                                      CND11720
      DO 70 I=1,NATOMS                                                  CND11730
      ANI=AN(I)                                                         CND11740
   70 ENERGY=ENERGY-ATENG(ANI)                                          CND11750
      PRINT80,  ENERGY                                                  CND11760
   80 FORMAT(11X,'  BINDING ENERGY =',F12.4,' A.U.')                    CND11770
C     IF(PRTOPT.EQ.0)GOTO300                                            CND11780
      PRINT85                                                           CND11790
   85 FORMAT(//16X,'*VALENCE ELECTRON DENSITY*'/)                       CND11800
      DO 110 I=1,NATOMS                                                 CND11810
      TCHG = 0.00                                                       CND11820
      LL=LLIM(I)                                                        CND11830
      JL=JLIM(I)                                                        CND11840
      DO 90 J=LL,JL                                                     CND11850
   90 TCHG = TCHG+B(J,J)                                                CND11860
      ANI=AN(I)                                                         CND11870
      PRINT100,  I,EL(ANI),TCHG                                         CND11880
  100 FORMAT(12O,A1,F15.4)                                              CND11890
      XXX(I)=TCHG                                                       CND11900
  110 CONTINUE                                                          CND11910
      DO 120 I=1,3                                                      CND11920
```

```
      DM(I)=0.000                                                       CND11930
      DMSP(I)=0.000                                                     CND11940
  120 DMPD(I)=0.000                                                     CND11950
      DO 200 J=1,NATOMS                                                 CND11960
      IF (AN(J).LT.3) GO TO 180                                         CND11970
      IF (AN(J).LT.11) GO TO 140                                        CND11980
      SLTR1=(.65*AN(J)-4.95)/3.                                         CND11990
      FACTOR=2.541600*7.00/(2.2500679775*SLTR1)                         CND12000
      INDEX=LLIM(J)                                                     CND12010
      DO 170 K=1,3                                                      CND12020
      INDEXK=INDEX+K                                                    CND12030
  170 DMSP(K)=DMSP(K)-B(INDEX,INDEXK )*10.27175D0/SLTR1
      DMPD(1)=DMPD(1)-FACTOR*(B(INDEX+2,INDEX+8)+B(INDEX+3,INDEX+5)     CND12050
     1  +B(INDEX+1,INDEX+7)-1.00/1.7320508076*B(INDEX+1,INDEX+4))       CND12060
      DMPD(2)=DMPD(2)-FACTOR*(B(INDEX+1,INDEX+8)+B(INDEX+3,INDEX+6)     CND12070
     1  -B(INDEX+2,INDEX+7)-1.00/1.7320508076*B(INDEX+2,INDEX+4))       CND12080
      DMPD(3)=DMPD(3)-FACTOR*(B(INDEX+1,INDEX+5)+B(INDEX+2,INDEX+6)     CND12090
     1  +2.00/1.7320508076*B(INDEX+3,INDEX+4))                          CND12100
      GO TO 180                                                         CND12110
  140 INDEX=LLIM(J)                                                     CND12120
      DO 150 K=1,3                                                      CND12130
      INDEXK=INDEX+K                                                    CND12140
  150 DMSP(K)=DMSP(K)-B(INDEX,INDEXK )*7.3369700/                       CND12150
     1(1.329*(AN(J)-1))                                                 CND12160
  180 DO 190 I=1,3                                                      CND12170
  190 DM(I)=DM(I)+(CZ(J)-XXX(J))*C(J,I)*2.5416                          CND12180
  200 CONTINUE                                                          CND12190
      DP=0.                                                             CND12200
      DO 210 I=1,3                                                      CND12210
      DPM(I)=DM(I)+DMSP(I)+DMPD(I)                                      CND12220
  210 DP=DP+DPM(I)**2                                                   CND12230
      DP=DSQRT(DP)                                                      CND12240
      PRINT220, DM,DMSP,DMPD,DPM,DP                                     CND12250
  220 FORMAT(//22X,'DIPOLE MOMENTS'//6X,'COMPONENTS',5X,'X',9X,'Y',9X,'ZCND12260
     Z'/6X,'DENSITIES',3F10.5/6X,'S-P',6X,3F10.5/6X,'P-D',6X,3F10.5/6X,'CND12270
     'TOTAL',4X,3F10.5/'0  DIPOLE MOMENT=',F10.5,' DEBYES'//)           CND12280
  300 PRINT9999                                                         CND12290
 9999 FORMAT('0END OF SCF-PROCEDURE'/1X,20('*')/)                       CND12300
      RETURN                                                            CND12310
      END                                                               CND12320
C                                                                       CND12330
      SUBROUTINE OVER1                                                  CND12350
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/CO/EPS
      COMMON/C1/S(70,70),Y(9135),Z(765)                                 CND12390
      COMMON/C2/C(35,3),AN(35)                                          CND12470
      COMMON/C3/CZ(35),J(70),JLIM(35),LLIM(35),NELECS,JCCA,JCCB         CND12490
      COMMON/C4/EL(18)                                                  CND12480
      COMMON/C7/NATOMS,CHARGE,MULTIP,M,ITER,LIMEX                       CND12410
      COMMON/C9/OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN                 CND12440
      INTEGER AN,CHARGE,CZ,J,JLIM,CCCA,OCCB,Y,Z                        CND12500
      REAL YZ(9900)                                                     CND12510
      CHARACTER*4 EL,OPTION,OPNCLO,CNDO,INDO,CLOSED,OPEN,IAN*80,CARD    CND12450
      EQUIVALENCE (YZ,Y)                                                CND12520
      READ(5,5) CARD
      WRITE(6,5) CARD
    5 FORMAT(20A4)
      READ(5,20)NATOMS,CHARGE,LIMEX,ITER,MULTIP                         CND12850
   20 FORMAT(T11,5I4)                                                   5
      IF(LIMEX.EQ.0) LIMEX=5                                            CND12880
      EPS=10.**(-LIMEX)                                                 CND12890
      IF(ITER.EQ.0) ITER=25                                             CND12900
      IF(MULTIP.EQ.0) MULTIP=1                                          CND12970
      READ40,  (AN(I),I=1,NATOMS)                                       CND13010
      PRINT60,  (AN(I),I=1,NATOMS)                                      CND13013
   40 FORMAT(40I2)                                                      CND13020
      PRINT80,  OPTION,OPNCLO,NATOMS,CHARGE,LIMEX,ITER,MULTIP           CND14270
   80 FORMAT('0',A1,1X,A1,I4,' ATOMS     CHARGE=',I2,4X,'ENERGY CONSISTENCND14280
     *CY LIMIT=1.0E-',I2,4X,'ITERATION LIMIT=',I4,4X,'MULT=',I2)        CND14290
      CALL COORD                                                        CND14380
      PRINT514                                                          CND14390
  514 FORMAT('0',20X,'COORDINATES                                       CND14400
     5'/10X,3H*X*,12X,3H*Y*,12X,3H*Z*)                                  CND14410
      DO 10 I=1,NATOMS                                                  CND14420
      J=AN(I)                                                           CND14430
      PRINT70, EL(J),C(I,1),C(I,2),C(I,3)                               CND14440
   70 FORMAT(A1,3F15.7)                                                 CND14450
C      CONVERSION OF COORDINATES FROM ANGSTROM TO AT.                   CND14460
      DO 9 J=1,3                                                        CND14470
    9 C(I,J)=C(I,J)/.52916700                                           CND14480
   10 CONTINUE                                                          CND14490
C     Y(I)=0                  I=1,9135                                  CND14500
```

```
C       Z(1)=0                        I=1,765
        DO 2 I=1,9900
      2 YZ(I)=0.0
C       LOAD NON-ZERO Y COEFFICIENTS
        Y(7039)=     64
        Y(7040)=     64
        Y(7049)=    -64
        Y(7032)=   -128
        Y(7041)=    -64
        Y(7033)=   -128
        Y(7042)=    128
        Y(7025)=     64
        Y(7034)=    128
        Y(7026)=     64
        Y(7035)=    -64
        Y(7027)=    -64
        Y(6904)=    -96
        Y(6913)=     32
        Y(6896)=   -192
        Y(6905)=    192
        Y(6906)=    288
        Y(6915)=    -96
        Y(6887)=    192
        Y(6907)=   -192
        Y(6890)=     96
        Y(6899)=   -288
        Y(6891)=   -192
        Y(6900)=    192
        Y(6892)=    -32
        Y(6901)=     96
        Y(2854)=    -16
        Y(2863)=     16
        Y(2847)=     32
        Y(2856)=    -16
        Y(2865)=    -16
        Y(2840)=    -16
        Y(2849)=    -16
        Y(2858)=     32
        Y(2842)=     16
        Y(2851)=    -16
        Y(2710)=     48
        Y(2719)=    -48
        Y(2711)=     48
        Y(2720)=    -96
        Y(2729)=     48
        Y(2703)=    -48
        Y(2712)=    -48
        Y(2721)=     96
        Y(2704)=    -48
        Y(2713)=     48
        Y(2722)=     48
        Y(2731)=    -48
        Y(2705)=     96
        Y(2714)=    -48
        Y(2723)=    -48
        Y(2706)=     48
        Y(2715)=    -96
        Y(2724)=     48
        Y(2707)=    -48
        Y(2716)=     48
        Y(5329)=     64
        Y(5322)=   -128
        Y(5340)=    -64
        Y(5315)=     64
        Y(5333)=    128
        Y(5326)=    -64
        Y(5185)=    -96
        Y(5194)=     32
        Y(5136)=    -96
        Y(5195)=     64
        Y(5204)=     32
        Y(5178)=     96
        Y(5187)=     32
        Y(5196)=     64
        Y(5179)=     96
        Y(5188)=    -32
        Y(5197)=     32
        Y(5206)=    -96
        Y(5180)=    -64
        Y(5189)=    -32
        Y(5198)=    -96
        Y(5131)=    -32
```

```
Y(5190)=   -64                                                  CND15330
Y(5199)=    96                                                  CND15340
Y(5132)=   -32                                                  CND15350
Y(5191)=    96                                                  CND15360
Y(4375)=  -144                                                  CND15370
Y(4384)=    96                                                  CND15380
Y(4393)=   -16                                                  CND15390
Y(4368)=   144                                                  CND15400
Y(4386)=   -48                                                  CND15410
Y(4395)=    96                                                  CND15420
Y(4370)=   -96                                                  CND15430
Y(4379)=    48                                                  CND15440
Y(4397)=  -144                                                  CND15450
Y(4372)=    16                                                  CND15460
Y(4381)=   -96                                                  CND15470
Y(4390)=   144                                                  CND15480
Y(1900)=   144                                                  CND15490
Y(1909)=  -144                                                  CND15500
Y(1893)=  -144                                                  CND15510
Y(1920)=   144                                                  CND15520
Y(1895)=   144                                                  CND15530
Y(1922)=  -144                                                  CND15540
Y(1906)=  -144                                                  CND15550
Y(1915)=   144                                                  CND15560
Y( 955)=   -16                                                  CND15570
Y( 964)=    32                                                  CND15580
Y( 973)=   -16                                                  CND15590
Y( 948)=    16                                                  CND15600
Y( 956)=   -48                                                  CND15610
Y( 975)=    32                                                  CND15620
Y( 950)=   -32                                                  CND15630
Y( 959)=    48                                                  CND15640
Y( 977)=   -16                                                  CND15650
Y( 952)=    16                                                  CND15660
Y( 961)=   -32                                                  CND15670
Y( 970)=    16                                                  CND15680
Y(8155)=    64                                                  CND15690
Y(8156)=   -64                                                  CND15700
Y(8165)=   -64                                                  CND15710
Y(8148)=   -64                                                  CND15720
Y(8157)=    64                                                  CND15730
Y(8149)=    64                                                  CND15740
Y(8158)=    64                                                  CND15750
Y(8150)=   -64                                                  CND15760
Y(8020)=   -96                                                  CND15770
Y(8029)=    32                                                  CND15780
Y(8021)=   128                                                  CND15790
Y(8013)=    96                                                  CND15800
Y(8031)=   -96                                                  CND15810
Y(8014)=  -128                                                  CND15820
Y(8015)=   -32                                                  CND15830
Y(8024)=    96                                                  CND15840
Y(7034)=   -64                                                  CND15850
Y(7075)=  -128                                                  CND15860
Y(7035)=    64                                                  CND15870
Y(7066)=   128                                                  CND15880
Y(7069)=   128                                                  CND15890
Y(7070)=    64                                                  CND15900
Y(7079)=  -128                                                  CND15910
Y(7071)=   -64                                                  CND15920
Y(3205)=   -16                                                  CND15930
Y(3214)=    16                                                  CND15940
Y(3206)=    16                                                  CND15950
Y(3215)=   -16                                                  CND15960
Y(3198)=    16                                                  CND15970
Y(3216)=   -16                                                  CND15980
Y(3199)=   -16                                                  CND15990
Y(3217)=    16                                                  CND16000
Y(3200)=   -16                                                  CND16010
Y(3209)=    16                                                  CND16020
Y(3201)=    16                                                  CND16030
Y(3210)=   -16                                                  CND16040
Y(7579)=    64                                                  CND16050
Y(7560)=   -64                                                  CND16060
Y(7572)=  -128                                                  CND16070
Y(7573)=   128                                                  CND16080
Y(7565)=    64                                                  CND16090
Y(7565)=   -64                                                  CND16100
Y(5660)=    64                                                  CND16110
Y(5661)=   -64                                                  CND16120
Y(5673)=   -64                                                  CND16130
Y(5671)=   -64                                                  CND16140
Y(5674)=    64                                                  CND16150
```

```
Y(5692)=    64                                                  CND16160
Y(5684)=    64                                                  CND16170
Y(5685)=   -64                                                  CND16180
Y(7435)=   -96                                                  CND16190
Y(7444)=    32                                                  CND16200
Y(7436)=   -96                                                  CND16210
Y(7445)=   160                                                  CND16220
Y(7428)=    96                                                  CND16230
Y(7437)=   128                                                  CND16240
Y(7446)=   -96                                                  CND16250
Y(7429)=    96                                                  CND16260
Y(7438)=  -128                                                  CND16270
Y(7447)=   -96                                                  CND16280
Y(7430)=  -160                                                  CND16290
Y(7439)=    96                                                  CND16300
Y(7431)=   -32                                                  CND16310
Y(7440)=    96                                                  CND16320
Y(5545)=   -96                                                  CND16330
Y(5554)=    32                                                  CND16340
Y(5546)=    32                                                  CND16350
Y(5555)=    32                                                  CND16360
Y(5538)=    96                                                  CND16370
Y(5556)=    32                                                  CND16380
Y(5539)=   -32                                                  CND16390
Y(5557)=   -96                                                  CND16400
Y(5540)=   -32                                                  CND16410
Y(5549)=   -32                                                  CND16420
Y(5541)=   -32                                                  CND16430
Y(5530)=    96                                                  CND16440
Y(3070)=    48                                                  CND16450
Y(3079)=   -48                                                  CND16460
Y(3071)=   -48                                                  CND16470
Y(3080)=    48                                                  CND16480
Y(3063)=   -48                                                  CND16490
Y(3081)=    48                                                  CND16500
Y(3064)=    48                                                  CND16510
Y(3082)=   -48                                                  CND16520
Y(3065)=    48                                                  CND16530
Y(3074)=   -48                                                  CND16540
Y(3066)=   -48                                                  CND16550
Y(3075)=    48                                                  CND16560
Y(8230)=   -64                                                  CND16570
Y(8201)=    64                                                  CND16580
Y(8193)=    64                                                  CND16590
Y(8194)=   -64                                                  CND16600
Y(7615)=   -64                                                  CND16610
Y(7616)=   -64                                                  CND16620
Y(7625)=    64                                                  CND16630
Y(7608)=    64                                                  CND16640
Y(7617)=    64                                                  CND16650
Y(7609)=    64                                                  CND16660
Y(7618)=   -64                                                  CND16670
Y(7610)=   -64                                                  CND16680
Y(3250)=    16                                                  CND16690
Y(3259)=   -16                                                  CND16700
Y(3243)=   -16                                                  CND16710
Y(3251)=    16                                                  CND16720
Y(3245)=    16                                                  CND16730
Y(3254)=   -16                                                  CND16740
Y(5725)=   -64                                                  CND16750
Y(5718)=    64                                                  CND16760
Y(5736)=    64                                                  CND16770
Y(5729)=   -64                                                  CND16780
Z(341)=    -1                                                   CND16790
Z(343)=     3                                                   CND16800
Z(345)=    -3                                                   CND16810
Z(347)=     1                                                   CND16820
Z(664)=    -1                                                   CND16830
Z(665)=     5                                                   CND16840
Z(666)=   -10                                                   CND16850
Z(667)=    10                                                   CND16860
Z(668)=    -5                                                   CND16870
Z(669)=     1                                                   CND16880
Z(154)=    -1                                                   CND16890
Z(156)=     5                                                   CND16900
Z(158)=   -10                                                   CND16910
Z(160)=    10                                                   CND16920
Z(162)=    -5                                                   CND16930
Z(164)=     1                                                   CND16940
Z(222)=    -1                                                   CND16950
Z(223)=     1                                                   CND16960
Z(224)=     4                                                   CND16970
Z(225)=    -4                                                   CND16980
```

```
      Z(2260) =     -6                                                  CND16390
      Z(2270) =      6                                                  CND17000
      Z(2280) =      4                                                  CND17010
      Z(2290) =     -4                                                  CND17020
      Z(2300) =     -1                                                  CND17030
      Z(2310) =      1                                                  CND17040
      Z(3070) =     -1                                                  CND17050
      Z(3080) =      2                                                  CND17060
      Z(3090) =      2                                                  CND17070
      Z(3100) =     -6                                                  CND17080
      Z(3120) =      6                                                  CND17090
      Z(3130) =     -2                                                  CND17100
      Z(3140) =     -2                                                  CND17110
      Z(3150) =      1                                                  CND17120
      Z(4090) =     -1                                                  CND17130
      Z(4100) =      3                                                  CND17140
      Z(4110) =     -1                                                  CND17150
      Z(4120) =     -5                                                  CND17160
      Z(4130) =      5                                                  CND17170
      Z(4140) =      1                                                  CND17180
      Z(4150) =     -3                                                  CND17190
      Z(4160) =      1                                                  CND17200
      Z(5280) =     -1                                                  CND17210
      Z(5290) =      4                                                  CND17220
      Z(5300) =     -5                                                  CND17230
      Z(5320) =      5                                                  CND17240
      Z(5330) =     -4                                                  CND17250
      Z(5340) =      1                                                  CND17260
      Z(5620) =     -1                                                  CND17270
      Z(5630) =      2                                                  CND17280
      Z(5650) =     -2                                                  CND17290
      Z(5660) =      1                                                  CND17300
      Z(7320) =     -1                                                  CND17310
      Z(7330) =      1                                                  CND17320
      Z(5450) =      1                                                  CND17330
      Z(5460) =     -3                                                  CND17340
      Z(5470) =      2                                                  CND17350
      Z(5480) =      2                                                  CND17360
      Z(5490) =     -3                                                  CND17370
      Z(5500) =      1                                                  CND17380
      Z(5790) =      1                                                  CND17390
      Z(5800) =     -1                                                  CND17400
      Z(5810) =     -1                                                  CND17410
      Z(5820) =      1                                                  CND17420
      Z(5960) =     -1                                                  CND17430
      Z(5980) =      1                                                  CND17440
      Z(4430) =     -1                                                  CND17450
      Z(4440) =      1                                                  CND17460
      Z(4450) =      2                                                  CND17470
      Z(4460) =     -2                                                  CND17480
      Z(4470) =     -1                                                  CND17490
      Z(4480) =      1                                                  CND17500
      Z(5980) =     -1                                                  CND17510
      Z(5990) =      3                                                  CND17520
      Z(7000) =     -3                                                  CND17530
      Z(7010) =      1                                                  CND17540
      Z(3240) =      1                                                  CND17550
      Z(3250) =     -1                                                  CND17560
      Z(3260) =     -3                                                  CND17570
      Z(3270) =      3                                                  CND17580
      Z(3280) =      3                                                  CND17590
      Z(3290) =     -3                                                  CND17600
      Z(3300) =     -1                                                  CND17610
      Z(3310) =      1                                                  CND17620
      Z(4600) =      1                                                  CND17630
      Z(4520) =     -2                                                  CND17640
      Z(4540) =      1                                                  CND17650
      RETURN                                                            CND17660
      END                                                               CND17670
/*
//GO.SYSIN DD *                                                         CND17680
WATER MOLECULE                                                          A8110240
CNDO CLSD     3          100                                            CND17710
 8 1 1
    2.0000     0.0000     0.0000
    2.5860     0.0000     0.7568
    2.5860     0.0000    -0.7568
/*                                                                      CND17960
//
```

APPENDIX C

This program was written for generating cartesian coordinates of glycine zwitterion and water as the input for CNDO and ab initio programs. The program consists of 3 main subroutines for tranformation of any vector around a cartesian axis. All of the needed parameters for glycine and water are added to the program by the data statement. The following is the listing of the programe.

```
/FILE , NEWDATA) LREC(132) NEW(REPL)
/LOAD WATFIV
/OPT SOURCE
      IMPLICIT REAL*8(A-H,O-Z)
      WRITE(6,10)
   10 FORMAT(T4,'*** THE COORDINATE OF GLYCINE-ZWITTERION ***'//)
C
C     CALCULATE THE COORDINATE OF H1
      DATA XHA1,YHA1,ZHA1/ 0.0000, 1.0300, 0.0000/
      CALL XROTA(XHA2,YHA2,ZHA2,XHA1,YHA1,ZHA1,(109.4700-90.0000))
      CALL XROTA(XH1,YH1,ZH1,XHA2,YHA2,(ZHA2+1.4700),(109.4700-90.0000))
      WRITE(6,20)XH1,YH1,ZH1
C
C     CALCULATE THE COORDINATE OF H2
      CALL ZROTA(XH3,YH3,ZHB,XHA2,YHA2,(ZHA2+1.4700),120.0000)
      CALL XROTA(XH2,YH2,ZH2,XHB,YHB,ZHB,(109.4700-90.0000))
      WRITE(6,30)XH2,YH2,ZH2
C
C     CALCULATE THE COORDINATE OF H3
      CALL ZROTA(XHC,YHC,ZHC,XHA2,YHA2,(ZHA2+1.4700),240.0000)
      CALL XROTA(XH3,YH3,ZH3,XHC,YHC,ZHC,(109.4700-90.0000))
      WRITE(6,40)XH3,YH3,ZH3
C
C     CALCULATE THE COORDINATE OF H4
      DATA XHD,YHD,ZHD/ 1.0900, 0.0000, 0.0000/
      CALL ZROTA(XHD1,YHD1,ZHD1,XHD,YHD,ZHD,-(109.4700-90.0000))
      CALL YROTA(XH4,YH4,ZH4,XHD1,YHD1,ZHD1, 30.0000)
      WRITE(6,50)XH4,YH4,ZH4
C
C     CALCULATE THE COORDINATE OF H5
      CALL ZROTA(XHD1,YHD1,ZHD1,XHD,YHD,ZHD,-(109.4700-90.0000))
      CALL YROTA(XH5,YH5,ZH5,XHD1,YHD1,ZHD1,150.0000)
      WRITE(6,60)XH5,YH5,ZH5
C
C     CALCULATE THE COORDINATE OF N
      DATA XN1,YN1,ZN1/ 0.0000, 0.0000, 1.4700/
      CALL XROTA(XN,YN,ZN,XN1,YN1,ZN1,(109.4700-90.0000))
      WRITE(6,70)XN,YN,ZN
C
C     CALCULATE THE COORDINATE OF C1
      DATA XC1,YC1,ZC1/ 0.0000, 0.0000, 0.0000/
      WRITE(6,80)XC1,YC1,ZC1
C
C     CALCULATE THE COORDINATE OF C2
      DATA XC2,YC2,ZC2/ 0.0000, 1.5200, 0.0000/
      WRITE(6,90)XC2,YC2,ZC2
C
C     CALCULATE THE COORDINATE OF O1
      DATA XOA,YOA,ZOA/ 0.0000, 1.2700, 0.0000/
      CALL XROTA(XO1,YO1,ZO1,XCA,YCA,ZOA, (122.000/2.0000))
      YO1=YO1+1.5200
      WRITE(6,100)XO1,YO1,ZO1
C
C     CALCULATE THE COORDINATE OF O2
      DATA XOB,YOB,ZOB/ 0.0000, 1.2700, 0.0000/
```

```
      CALL XRDTA(X02,Y02,Z02,XC8,YC8,ZC8,-(122.000/2.000))
           Y02=Y02+1.52
      WRITE(6,110)X02,Y02,Z02
   20 FORMAT(T2,'H1',1X,3(F10.4))
   30 FORMAT(T2,'H2',1X,3(F10.4))
   40 FORMAT(T2,'H3',1X,3(F10.4))
   50 FORMAT(T2,'H4',1X,3(F10.4))
   60 FORMAT(T2,'H5',1X,3(F10.4))
   70 FORMAT(T2,'N ',1X,3(F10.4))
   80 FORMAT(T2,'C1',1X,3(F10.4))
   90 FORMAT(T2,'C2',1X,3(F10.4))
  100 FORMAT(T2,'O1',1X,3(F10.4))
  110 FORMAT(T2,'O2',1X,3(F10.4))
      STOP
      END
C
      SUBROUTINE XRDTA(XP,YP,ZP,XR,YR,ZR,D)
      IMPLICIT REAL*8(A-H,O-Z)
      DATA RA/0.0174532D252/
      XP=XR
      YP=YR*DCOS(D*RA)-ZR*DSIN(D*RA)
      ZP=ZR*DCOS(D*RA)+YR*DSIN(D*RA)
      RETURN
      END
C
      SUBROUTINE YRDTA(XP,YP,ZP,XR,YR,ZR,D)
      IMPLICIT REAL*8(A-H,O-Z)
      DATA RA/0.0174532D252/
      YP=YR
      ZP=ZR*DCOS(D*RA)-XR*DSIN(D*RA)
      XP=XR*DCOS(D*RA)+ZR*DSIN(D*RA)
      RETURN
      END
C
      SUBROUTINE ZRDTA(XP,YP,ZP,XR,YR,ZR,D)
      IMPLICIT REAL*8(A-H,O-Z)
      DATA RA/0.0174532D252/
      ZP=ZR
      XP=XR*DCOS(D*RA)-YR*DSIN(D*RA)
      YP=YR*DCOS(D*RA)+XR*DSIN(D*RA)
      RETURN
      END
```

About The Author

Mr. Prayong Doungdee was born on September, 21, 1955. He received his B. Ed. in Chemistry from Srinakharinwirot University (Prasarnmit campus). Two publications have come out of his master's degree work. They are "A Comparative Study of the Hydration of Aliphatic Amino Acids" in J. Sc. Soc. Thailand., forthcoming, and "The Influence of Hydration on the Rotational Barriers of Glycine" in Inor. Thero. Chim. Acta., forthcoming. He has received a grant from the Austrian government to study for a doctorate at Innsbruck University.