

## Fortran source code of PROGRAM LCOAO, followed by sample input and output.

```
PROGRAM LCOAO
c-----GC-C-MCD--06.OCT.1983--Update-Dec.2001/Dec.2005-----JS-L
c
c  =====
c    Linear Combination of Orthogonalized Atomic Orbitals
c  =====
c
c  Jens Spanget-Larsen: "The alternant hydrocarbon pairing
c  theorem and all-valence electrons theory. An approximate LCOAO
c  theory for the electronic absorption and MCD spectra of
c  conjugated organic compounds"
c  Part 1. Croat. Chem. Acta 59, 711-717 (1986).
c  Part 2. Theor. Chem. Acc. 98, 137-153 (1997).
c
c  - Restricted Open Shell Formalism
c  - Grand Canonical/Canonical Monoexcited CI for Open Shell Systems
c
c  Development version, not user friendly!
c
c  Array Dimensions:
c          100 = Max. Number of atoms
c          300 = Max. Number of orbitals
c          101 = 100+1
c          201 = 2*100+1
c          301 = 3*100+1
c          400 = 4*100
c          10000 = 100*100
c          5050 = 100(100+1)/2
c          90000 = 300*300
c
c  INPUT FILE -
c
c  1) FORMAT(18(A4)): text heading
c  2) FORMAT(5I3):
c      NE      charge of the molecule
c      NPE     nr. of electrons in partly occupied MOs
c              (defaults: NPE=0 for even, NPE=1 for odd
c              number of electrons)
c      NPMO    nr. of partly occupied MOs
c              (defaults: NPMO=0 for even, NPMO=1 for odd
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c          number of electrons)
c      IPI      If IPI>0, only PI-PI* cfgs. included in CI
c              (molecular plane assumed to be X,Y)
c      IPRNT    print code (IPRNT=0-4 generates min-max printout)
c      NMOP     nr. of HOMOs and nr. of LUMOs printed (default 32)
c 3) One line per atom, FORMAT(I2,F13.6,2F15.6):
c      IQ       atomic number
c      X,Y,Z    atomic coordinates in Angstrom
c 4) One blank line, terminating input of atomic coordinates
c 5) FORMAT(6I3,F10.5):
c      IGCCI    CI calculation performed if IGCCI=1
c      NB       nr. of highest occ. valence MOs incl. in CI (default 10)
c      NA       nr. of lowest unocc. valence MOs incl. in CI (default 10)
c              (note that NB and NA define an all-valence MO 'window',
c              and in general, NB*NA singly excited cfgs. are generated;
c              but if IPI>0, only those cfgs. that are of PI-PI* type are
c              included in the CI)
c      ITRIP    triplet states computed if ITRIP=1
c      IDOB     dummy in this version of the program
c      MCD      MCD B-terms for PI-PI* states computed if MCD=>0 (only
c              if IPI>0; MCD=1-5 generates min-max printout)
c      EMAX     excited cfg. energy cutoff limit in eV (default 15)

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c-----JS-L

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implicit real*8(A-H,O-Z)
character*14 nin,nout
COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
1          EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB,
2          NB,NAB
COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300),C(400),
1          GAX(300),NTIT(20)
COMMON /C/ S(300,300),F(300,300)
COMMON /MOM/ SX(300),SY(300),SZ(300)
COMMON/E/NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN,NG,DAMP
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
COMMON /D/ V1(300),V2(300),V3(300),V4(300),V5(300),
1 INDEX(2,300),INZ(2,300),DIAG1(300),DIAG(400)
COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
.          DPI,DSIG,DDD(300),FPPPIM,FDM
COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),
.          XP(100),YP(100),BETA(5050),CPI(10000),

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.   CIPI(10000),IFROM(100),ITO(100),EP(100),POCC(100)
COMMON /SBIAS/ BIAS,IPI
105  FORMAT ((5X,16F8.4))
110  FORMAT (' SINGLET ENERGIES',/)
111  FORMAT (' TRIPLET ENERGIES',/)
112  FORMAT (//' CONFIGURATION INTERACTION: '// IGCCI=',I2,
.   ' NB=',I2,' NAB=',I2,' ITRIP=',I2,' IDOB=',I2,' MCD=',I2,
.   ' EMAX=',F6.2/)
113  FORMAT (//1X,18A4)
130  FORMAT (6I3,F10.5)
2002 FORMAT (/ ' SINGLET MATRIX',/)
2003 FORMAT (/ ' TRIPLET MATRIX',/)
2004 FORMAT (//' SINGLET STATE EIGENVECTORS (VERTICAL) ')
2005 FORMAT (//' TRIPLET STATE EIGENVECTORS (VERTICAL) ')
9999 format(4f20.10)
write(*,9)
9  format(' Name of input file: ')
read(*,11) NIN
write(*,12)
12 format(' Name of output file: ')
read(*,11) NOUT
11 format(a)
open(5,file=nin)
open(6,file=nout,status='new')
open(1,file='f1',status='unknown',form='formatted')
open(2,file='f2',status='unknown',form='formatted')
open(3,file='f3',status='unknown',form='formatted')
open(4,file='f4',status='unknown',form='formatted')
1  CALL READER
N2=N+N
N4=N2+N2
NT=N+NH
CALL GMATR(1)
CALL SMATR
CALL F0MATR
CALL LOWDIN
WRITE(6,3010)
3010 FORMAT(2X/10X,'G-, S-, AND F0-MATRICES'//)
CALL SCF
WRITE(6,3020)
3020 FORMAT(2X/10X,'SCF-CALCULATION')

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      DO 8 I=1,N5
      8 ET(I)=SUM(I)
c-----CI-CALCULATION; READ PARAMETERS, ASSIGN DEFAULTS:
      80 READ(5,130) IGCCI,NB,NAB,ITRIP,IDOB,MCD, EMAX
         IF(IGCCI.LE.0) GOTO 1
         DO 90 I=1,N5
      90 SUM(I)=ET(I)
         IF(NB.LE.0) NB =10
         IF(NAB.LE.0) NAB=10
         IF(IDOB.EQ.0) IDOB=2
         IF(NHOMO.GE.NLUMO) IDOB=-1
         IF(MCD.EQ.0) MCD=1
         MCD=MIN0(MCD,5)
         IF(IPI.LE.0) MCD=-1
         IF(MCD.GT.0) IDOB=-1
         IF(EMAX.LE..0) EMAX=15.0
         WRITE(6,113) (NTIT(II),II=1,18)
         WRITE(6,112) IGCCI,NB,NAB,ITRIP,IDOB,MCD,EMAX
         CALL GCCI
         IF(IPRNT.GE.2) WRITE(6,2002)
         IF(IPRNT.GE.2) CALL PRINT(S,JCOUNT,0,0,0,0,0)
         WRITE(6,3040)
3040  FORMAT(2X/10X,'SINGLET(+TRIPLET) SCI-MATRIX')
         NTEMP=N
         N=JCOUNT
         ICI=1
         CALL DIAGON
         WRITE(6,110)
         WRITE(6,105) (SUM(I),I=1,JCOUNT)
         WRITE(6,2004)
         CALL PRINT(F,JCOUNT,JCOUNT,1,32,0,0)
3050  FORMAT(2X/10X,'DIAG. SINGLET SCI-MATRIX')
         CALL DMOM (SX,SY,SZ,V3,V4,V5,F,ZCORE,SUM,JCOUNT)
         CALL SPRT1(0,DUMMY)
c-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD-B
         IR=0
         DO 1000 J=1,NST
         EP(J)=SUM(J)
         DO 1000 I=1,NST
         IR=IR+1
1000  CIPI(IR)=F(I,J) * SQRT( POCC(IFROM(I)) - POCC(ITO(I)) )

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SUBROUTINE STORE(A,IUN,K)
  implicit real*8(A-H,O-Z)
c-----STORE ARRAY A ON UNIT IUN      /JS-L
  DIMENSION A(300,300)
  REWIND IUN
  WRITE(IUN,9999) ((A(I,J),J=1,K),I=1,K)
  9999 format(4f20.10)
c  WRITE(6,100) K,K,IUN
c 100 FORMAT(2X/10X,I2,' BY ',I2,' ARRAY STORED ON UNIT',I2/)
  RETURN
  END
c#####
SUBROUTINE LOAD(A,IUN,K)
  implicit real*8(A-H,O-Z)
c-----LOAD UNIT IUN INTO ARRAY A    /JS-L
  DIMENSION A(300,300)
  REWIND IUN
  READ(IUN,9999) ((A(I,J),J=1,K),I=1,K)
  9999 format(4f20.10)
c  WRITE(6,100) K,K,IUN
c 100 FORMAT(2X/10X,I2,' BY ',I2,' ARRAY LOADED FROM UNIT',I2/)
  RETURN
  END
c#####
SUBROUTINE PRINT(H,NI,MI,MINI,MAXI,K1,K2)
  implicit real*8(A-H,O-Z)
c  PROGRAMMED BY P.A.STRAUB AND H.BAUMANN
c-----MODIFIED BY JS-L
c  THIS SUBROUTINE PRINTS A NI*MI MATRIX
c  FOR MI=0 ONLY THE SYMMETRIC PART BELOW DIAGONAL
c  FOR NI=0 ONLY THE SYMMETRIC PART ABOVE DIAGONAL
  DIMENSION H(300,300)
  DATA LINE/4H----/
  100 FORMAT(1X)
  103 FORMAT(1X,4H----,16(2A4))
  101 FORMAT(/,16(5X,I3))
  102 FORMAT(I3,1X,16F8.4)
  MIN=MINI
  MAX=MAXI
  L1=K1
  L2=K2

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IF(K1.EQ.0) L1=100000
IF(K2.EQ.0) L2=1000
M=MIN0(MI,NI)
N=MAX0(MI,NI)
M1 = M
IF(M1.LE.0) M1=N
IF(MIN.LE.0) MIN=1
IF(MAX.GT.0) M1=MIN0(M1,MAX)
DO 11 J=MIN,M1,16
JEND =MIN0(M1,J+15)
WRITE(6,101) (K,K=J,JEND)
WRITE(6,103) ((LINE,LL=1,2),K=J,JEND)
IA=1
IF(M.EQ.0) IA=J
DO 10 I=IA,N
IL2=I-1-L2
IF(IL2.LT.0) GOTO 8
IF(FLOAT(IL2)/FLOAT(L1)-FLOAT(IL2/L1).LT..000001) WRITE(6,100)
8 JIEND = JEND
IF (M.NE.0) GO TO 9
IF (JEND.GE.I) JIEND=I
IF (NI.EQ.0) GO TO 12
9 WRITE(6,102) I, (H(I,K),K=J,JIEND)
GO TO 10
12 WRITE(6,102) I, (H(K,I),K=J,JIEND)
10 CONTINUE
11 CONTINUE
RETURN
END

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c#####
SUBROUTINE DMOM (SX,SY,SZ,SCIX,SCIY,SCIZ,U,O,E,JC)
implicit real*8(A-H,O-Z)
c-----PRINTS EXC. ENERGIES, TRANSITION MOMENTS AND OSC. STRENGTHS /JS-L
COMMON /D/ XJSL(5,300),IQ(2,300)
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
DIMENSION SX(300),SY(300),SZ(300),SCIX(300),SCIY(300),
1 SCIZ(300),O(300),U(300,300),E(300)
101 FORMAT(1X,102(1H-))
103 FORMAT (I5,F12.6,F12.4,F12.1,5F12.6)
IF(ABS(U(1,1)).LT.SQRT(.5).AND.E(1).LT..0) WRITE(6,104)

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104 FORMAT(//' ----CAUTION----'// ' SCF GROUND STATE UNSTABLE'//
. ' TRANSITION MOMENTS AND OSC. STRENGTHS UNRELIABLE'//)
WRITE(6,102)
102 FORMAT (/,3X,2HNO,7X,2HEV,9X,2HKK,12X,2HNM,9X,2HSX,10X,2HSY,
. 10X,2HSZ,10X,3HOSC,7X,6HLOGEPS)
WRITE(6,101)
IF(NHOMO.GE.NLUMO) WRITE(6,105)
105 FORMAT(105X,'HOLE STATE CHARACTER')
DO 10 J=2,JC
E(J)=E(J)-E(1)
SCIX(J)=0.0
SCIY(J)=0.0
SCIZ(J)=0.0
HOLE=0.0
DO 5 I=2,JC
UIJ=U(I,J)
SCIX(J)=SCIX(J)+SX(I)*UIJ
SCIY(J)=SCIY(J)+SY(I)*UIJ
SCIZ(J)=SCIZ(J)+SZ(I)*UIJ
IF(IQ(2,I).LE.NHOMO) HOLE=HOLE+UIJ*UIJ
5 CONTINUE
EKK = E(J)*8.066
ENM = 10000./EKK
SCI2=SCIX(J)*SCIX(J)+SCIY(J)*SCIY(J)+SCIZ(J)*SCIZ(J)
O(J)=.00379277*E(J)*SCI2
ELOG=ABS(O(J))*5.43658E+4
IF (ELOG.LE.1.) ELOG=0.
IF (ELOG.NE.0.) ELOG=ALOG10(ELOG)
WRITE(6,103) J,E(J),EKK,ENM,SCIX(J),SCIY(J),SCIZ(J),O(J),ELOG
IF(NHOMO.GE.NLUMO) WRITE(6,106) HOLE,J
106 FORMAT(1H+,110X,F8.5,I5)
10 CONTINUE
RETURN
END
c#####
FUNCTION H(LX,IX,JX,MX)
implicit real*8(A-H,O-Z)
c INTEGRAL (LX,IX/JX,MX) IS COMPUTED BY THE GAMMA INTEGRALS STORED
c IN THE LOWER PART OF G AND THE VECTORS STORED IN U
c PROGRAMMED BY H. BAUMANN
c-----MODIFIED BY JS-L

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COMMON /B/ ES (300) ,ER (300) ,ZCORE (300) ,ET (300) ,SUM (300) ,
1      C (400) ,GAX (300)
COMMON /E/ NCYCL,EPREV,ITERR,N5
COMMON /C/ G (90000) ,U (90000)
DIMENSION W (300)
N4=N5-1
I1=300*(LX-1)
J1=300*(JX-1)
K1=300*(IX-1)
L1=300*(MX-1)
DO 93 NZ=1,N5
ES (NZ) =0.
93 W (NZ) =U (I1+NZ) *U (K1+NZ)
H=W (N5) *GAX (N5) *U (J1+N5) *U (L1+N5)
NZ1=-300
DO 90 NZ=1,N4
NZ1=NZ1+300
WN=W (NZ)
MI=NZ+1
H1=WN*GAX (NZ)
DO 94 MZ=MI,N5
ES (MZ) =ES (MZ) +WN*G (NZ1+MZ)
94 H1=W (MZ) *G (NZ1+MZ) +H1
90 H=H+U (J1+NZ) *U (L1+NZ) * (H1+ES (NZ) )
H=H+U (J1+N5) *U (L1+N5) *ES (N5)
RETURN
END
c#####
SUBROUTINE READER
implicit real*8 (A-H,O-Z)
c READ INPUT DATA
c PROGRAMMED BY H. BAUMANN
c-----NUMEROUS MODIFICATIONS BY JS-L
DIMENSION SDAT (36) ,ASDAT (36) ,APDAT (36) ,BDAT (36) ,ZDAT (36) ,GA (36) ,
. X (100) ,Y (100) ,Z (100) ,ZS (100) ,IQ (300) ,BSDAT (36) ,BPDAT (36) ,
. USDAT (36) ,UPDAT (36)
COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
. EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB
COMMON /B/ E (300) ,EE (300) ,ZCORE (300) ,ET (300) ,SUM (300) ,C (400) ,
. GAX (300) ,NTIT (20)
COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN,NG,DAMP

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COMMON /SPTERM/ SP(100)
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
.      DPI,DSIG,DDD(300),FPPPI,M,FDM
COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),
.  XP(100),YP(100),BETA(5050),CPI(10000),CIPI(10000),
.  IFROM(100),ITO(100),EP(100),POCC(100)
COMMON /SBIAS/ BIAS,IPI
COMMON /NMOP/ NMOP
EQUIVALENCE (C(1),X(1)),(C(101),Y(1)),(C(201),Z(1)),
.      (C(301),ZS(1)),(SUM(1),IQ(1))
DATA NQS /300/,IBLANK/4H /
DATA SDAT(1),ASDAT(1),BDAT(1),ZDAT(1),GA(1)
.  /1.2,-7.175,-12.,1.,12.85/
c -----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
DATA SDAT(2),ASDAT(2),APDAT(2),BDAT(2),ZDAT(2),GA(2)
.  / 10.0,99999.,99999.,0.01,0.000,12.85/
c -----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
DATA SDAT(3),ASDAT(3),APDAT(3),BDAT(3),ZDAT(3),GA(3)
.  /.65,-3.105,-2.05,-3.,1.,2.98/
DATA SDAT(4),ASDAT(4),APDAT(4),BDAT(4),ZDAT(4),GA(4)
1  /.975,-6.55,-3.035,-4.,2.,5.85/
DATA SDAT(5),ASDAT(5),APDAT(5),BDAT(5),ZDAT(5),GA(5)
1  /1.3,-10.305,-4.37,-5.,3.,8.10/
DATA SDAT(6),ASDAT(6),APDAT(6),BDAT(6),ZDAT(6),GA(6)
1  /1.625,-14.960,-5.805,-17.5,4.,10.93/
DATA SDAT(7),ASDAT(7),APDAT(7),BDAT(7),ZDAT(7),GA(7)
1  /1.950,-20.485,-8.480,-26.0,5.,13.10/
DATA SDAT(8),ASDAT(8),APDAT(8),BDAT(8),ZDAT(8),GA(8)
1  /2.275,-27.255,-10.965,-45.,6.,15.27/
DATA SDAT(9),ASDAT(9),APDAT(9),BDAT(9),ZDAT(9),GA(9)
1  /2.600,-28.48,-12.18,-50.,7.,17.36/
DATA SDAT(11),ASDAT(11),APDAT(11),BDAT(11),ZDAT(11),GA(11)
1  /1.1,-2.805,-1.565,-.5,1.,2.95/
DATA SDAT(12),ASDAT(12),APDAT(12),BDAT(12),ZDAT(12),GA(12)
1  /1.425,-5.875,-2.29,-1.,2.,4.46/
DATA SDAT(13),ASDAT(13),APDAT(13),BDAT(13),ZDAT(13),GA(13)
1  / 1.75,-8.595,-3.92,-1.5,3.,5.1/
DATA SDAT(14),ASDAT(14),APDAT(14),BDAT(14),ZDAT(14),GA(14)
1  /2.075,-12.125,-6.005,-5.25,4.,6.37/
DATA SDAT(15),ASDAT(15),APDAT(15),BDAT(15),ZDAT(15),GA(15)

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1      /2.4,-14.34,-7.235,-7.8,5.,9.31/
DATA SDAT(16),ASDAT(16),APDAT(16),BDAT(16),ZDAT(16),GA(16)
1      /1.817,-15.81,-7.385,-18.0,6.,10.01/
DATA SDAT(17),ASDAT(17),APDAT(17),BDAT(17),ZDAT(17),GA(17)
1      /3.05,-17.5,-9.38,-15.,7.,11.3/
DATA SDAT(34),ASDAT(34),APDAT(34),BDAT(34),ZDAT(34),GA(34)
1      /1.565,-15.425,-7.10,-14.0,6.,9.16/
99     FORMAT (18(A4))
100    FORMAT (1X,18(A4),//)
101    FORMAT (6I3,12F5.2)
104    FORMAT (I2,F13.6,2F15.6,5F5.2)
105    FORMAT(
.      '
.      '
.      '
.      ' "Linear Combination of Orthogonalized Atomic Orbitals" '/
.      ' J. Spanget-Larsen: Theor. Chem. Acc. 59, 137 (1997) '//
.      ' 100 atoms - 300 orbitals developement-vs.' /
.      ' Dec. 2005' /
.      '-----BKVH--' //)
106    FORMAT (' N=',I2,' NH=',I2,' NE=',I3,
1      ' NPE=',I2,' NPMO=',I2,' IPI=',I2,
2      ' IPRNT=',I2,' NMOP=',I2)
107    FORMAT(1X/' PP(PI)=' ,F6.3,' PP(SIG)=' ,F6.3,' PS=' ,F6.3,
.      ' SS=' ,F6.3,' D(PI)=' ,F6.3,' D(SIG)=' ,F6.3/
.      ' XG=' ,F6.3,' PEN(SS)=' ,F6.3,' PEN(SP)=' ,F6.3,' PEN(PP)=' ,F6.3/
.      ' PRM. FOR MAGN. DIPOLE INTEGRALS: PP(PI)=' ,F6.3,' FD=' ,F6.3/
.      ' SIGMA ORBITAL 'BIAS': ' ,F6.3,' ZDAT(2): ' ,F6.3)
698    FORMAT (I5,3F15.6,I11,2F10.3,10X,F10.3,10X,1F10.3)
699    FORMAT (I5,3F15.6,I11,6F10.3)
1000   FORMAT(1H )
7499   FORMAT(//4X,1HI,11X,1HX,14X,1HY,14X,1HZ,11X,4HN(Z),5X,3HEXP,6X,
.      4HX(S),6X,4HX(P),5X,7HBETA(S),3X,7HBETA(P),3X,5HGAMMA/
.      1X,130(1H-))
NQ=NQS
1      READ(5,99) (NTIT(I),I=1,18)
WRITE(6,1000)
WRITE(6,105)
WRITE(6,100) (NTIT(I),I=1,18)
IF (NTIT(1).EQ.IBLANK) STOP
READ(5,101) NE,NPE,NPMO,IPI,IPRNT,NMOP,FPPPI,FPPSIG,FPS,FSS,

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.          DPI,DSIG,XG,PENSS,PENSP,PENPP,BIAS,DAMP
C-----DEFAULTS
          ISCF   = 30
          IF(DAMP.LE..01)  DAMP   = 0.5
          IF(PENSS.LE..0)  PENSS  = 0.5
          IF(PENSP.LE..0)  PENSP  = 0.5
          IF(PENPP.LE..0)  PENPP  = 1.5
          IF(XG.LE..0)     XG     = 1.0
          IF(DPI.EQ..0)    DPI    = 0.23
          IF(DSIG.EQ..0)   DSIG   = 0.23
          IF(FPPPPI.LE..0) FPPPPI = 0.75
          IF(FPPSIG.LE..0) FPPSIG = 1.00
          IF(FPS.LE..0)    FPS    = 1.00
          IF(FSS.LE..0)    FSS    = 1.00
          IF(NMOP.EQ.0)    NMOP   = 32
                          FDM    = 0.0
                          FPPPIM = 1.50/EXP(-FDM*1.397*1.625/.529167)

          DO 990 I=1,36
          BSDAT(I)=ASDAT(I)
990      BPDAT(I)=APDAT(I)
          BSDAT(2)=0.001
          BPDAT(2)=0.001
          N=0
          NH=0
          DO 13 I=1,1000
C-----ASD, APD, BSD, BPD, SD ARE NEW ATOMIC PARAMETERS      /JS-L
          READ(5,104) IQ(I),X(I),Y(I),Z(I),ASD,APD,BSD,BPD,SD
          IQT=IQ(I)
          IF (IQT.LT.1) GO TO 14
C-----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
          IF (IQT.EQ.2) ZDAT(2) = ASD
          IF (IQT.EQ.2) GOTO 8888
C-----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
          IF (ABS (ASD) .GT..0) ASDAT (IQT)=-ABS (ASD)
          IF (ABS (APD) .GT..0) APDAT (IQT)=-ABS (APD)
8888    IF (ABS (BSD) .GT..0) BSDAT (IQT)=-ABS (BSD)
          IF (ABS (BPD) .GT..0) BPDAT (IQT)=-ABS (BPD)
          IF (ABS (SD) .GT..0) SDAT (IQT)= ABS (SD)
          IF (IQT.LE.2) NH=NH+1
          IF (IQT.GT.2) N=N+1
13      CONTINUE

```

```

14 N2=N+N
   N4=N2+N2
   N5=N4+NH
   NTOTAL=NH+N
   DO 15 I=1,NTOTAL
   IQT=IQ(I)
   DO 16 J=I,NTOTAL
   IF (IQ(J).GE.IQT) GO TO 16
   XT=X(I)
   YT=Y(I)
   ZT=Z(I)
   IQ(I)=IQ(J)
   X(I)=X(J)
   Y(I)=Y(J)
   Z(I)=Z(J)
   IQ(J)=IQT
   X(J)=XT
   Y(J)=YT
   Z(J)=ZT
   IQT=IQ(I)
16 CONTINUE
15 CONTINUE
C-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
   NPI=NH+1
   NAT=NH+N
   IR=0
   DO 2000 IA=NPI,NAT
   IR=IR+1
   XP(IR)=X(IA)
2000 YP(IR)=Y(IA)
C-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
   N2S=NH+1
   N2P=NTOTAL+1
   NTN=NTOTAL+N
   N4=0
   TWOSQ3=2.*SQRT(3.)
   DO 52 I1=1,NTOTAL
   I2=I1+N
   I3=I2+N
   I4=I3+N
   IKI=IQ(I1)

```

```

c-----SP-TERMS FOR TRANSITION MOMENTS (SEE TRAMOM)          /JS-L
      SP(I1)=.0
      IF(IKI.LE.2) GO TO 999
      FN=5.
      IF(IKI.GT.10) FN=7.
      SP(I1)=FN/(SDAT(IKI)*TWOSQ3)
999  ET(I1)=BSDAT(IKI)
      DDD(I1)=ASDAT(IKI)
      ZCORE(I1)=ZDAT(IKI)
c-----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
      NESF = INT(ZDAT(IKI))
      IF(IKI.EQ.2) NESF = 0
c      N4=N4+INT(ZCORE(I1))          ( ORIGINAL VERSION )
      N4=N4+NESF
c-----ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF---ESF
      ZS(I1)=SDAT(IKI)
      GAX(I1)=GA(IKI)
      IF (IKI.GT.2) GOTO 51
      GO TO 52
51  DDD(I2)=APDAT(IKI)
      DDD(I3)=APDAT(IKI)
      DDD(I4)=APDAT(IKI)
      ET(I2)=BPDAT(IKI)
      ET(I3)=BPDAT(IKI)
      ET(I4)=BPDAT(IKI)
      GAX(I2)=GA(IKI)
      GAX(I3)=GA(IKI)
      GAX(I4)=GA(IKI)
52  CONTINUE
      GAH=GA(1)
      NE=N4-NE
      WRITE(6,106) N,NH,NE,NPE,NPMO,IPI,IPRNT,NMOP
      WRITE(6,107) FPPPI,FPPSIG,FPS,FSS,DPI,DSIG,
      .           XG,PENSS,PENSP,PENPP,FPPPIM,FDM,BIAS
      .           ,ZDAT(2)
      WRITE(6,7499)
      IF(NH.EQ.0) GO TO 33
      DO 30 I=1,NH
30  WRITE(6,698) I,X(I),Y(I),Z(I),IQ(I),ZS(I),DDD(I),ET(I),GAX(I)
33  IF(N.EQ.0) GO TO 34
      DO 50 I=1,N

```

```

      J=NH+I
      JJ=J+N
      IQJ=IQ(J)
50  WRITE(6,699) J,X(J),Y(J),Z(J),IQJ,ZS(J),DDD(J),DDD(JJ),
      .
      ET(J),ET(JJ),GAX(J)
34  RETURN
      END
c#####
      SUBROUTINE AUFBAU(NE,NMO,E,LOOK)
      implicit real*8(A-H,O-Z)
      DIMENSION E(300)
      COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
      IF(LOOK) 110,50,1
c-----DETERMINE OPEN SHELL DEGENERACY (NPMO) AND TOTAL OCCUPANCY (NPE)
      1  NPMO=0
      NPE=0
      NFMO=NE/2
      I=(NE+1)/2
      10  IF(I.GE.NMO) GOTO 20
      IF(ABS(E(I+1)-E(I)).GT..0001) GOTO 20
      I=I+1
      GOTO 10
      20  IF(NE.EQ.2*I) GOTO 60
      J=(NE+2)/2
      30  IF(J.EQ.1) GOTO 40
      IF(ABS(E(J)-E(J-1)).GT..0001) GOTO 40
      J=J-1
      GOTO 30
      40  NFMO=J-1
      NPMO=I-NFMO
      NPE=NE-2*NFMO
      GOTO 60
      50  LOOK=-1
      NFMO=(NE-NPE)/2
      IF(2*NFMO.NE.NE-NPE) NPE=NPE+1
      NPMO=MAX0(NPMO,(NPE+1)/2)
c-----ASSIGN GRAND CANONICALLY AVERAGED OCCUPATION NUMBERS
      60  NFMO1=NFMO+1
      DO 70 I=NFMO1,NMO
      70  OCC(I)=0.0
      DO 80 I=1,NFMO

```

```

80 OCC(I)=1.0
   IF(NPMO.EQ.0) GOTO 100
   OCCP=0.5*FLOAT(NPE)/FLOAT(NPMO)
   DO 90 I=1,NPMO
90  OCC(NFMO+I)=OCCP
100  NHOMO=NFMO+NPMO
     NLUMO=NFMO+1
110  RETURN
     END
c#####
   SUBROUTINE SPRT1(IFLAG,BTERM)
     implicit real*8(A-H,O-Z)
c     A PRINTPLOT OF THE ELECTRONIC TRANSITIONS IS PRODUCED
c     PROGRAMMED BY J.KELEMEN UND H.BAUMANN
c-----MODIFIED TO INDICATE POL. DIR.S AND MCD B-SIGNS BY JS-L
     COMMON /A/ NT
     COMMON /B/ ET(300),EE(300),OS(300),SO(300),E(300),C(400),
1      GX(300),LT(20)
     COMMON /D/ V1(300),V2(300),SCIX(300),SCIY(300),SCIZ(300)
     DIMENSION IPLT(100),BTERM(1)
     DATA HX/.5/,IBR/1H-/,IPL/1H+/,IPNT/1H:/,IBLNK/1H /
     DATA IX/1HX/,IY/1HY/,IZ/1HZ/,IO/1H0/
2  FORMAT (1H ,49X,21HL O G   E P S I L O N )
3  FORMAT (1H , 8X,3H1.0,7X,3H1.5, 7X,3H2.0, 7X,3H2.5, 7X, 3H3.0,7X,
.3H3.5, 7X, 3H4.0, 7X,3H4.5, 7X, 3H5.0, 7X, 3H5.5, 7X,3H6.0)
4  FORMAT (1H ,4X, 6HKK   :, 10(10H . . . . :),4X, 2HNM )
5  FORMAT (1H ,9X,101(1H-))
6  FORMAT (1H /)
7  FORMAT (1H )
8  FORMAT (1H ,F7.3,3H   :,99A1,1H:,F7.0)
9  FORMAT (1H )
     N=NT-1
     WRITE(6,9)
     WRITE(6,1000) (LT(I),I=1,18)
1000 FORMAT(//11X,18(A4))
     EP=1000.
     OMAX=0.
     DO 1 J=2,N
     E(J)=ABS(E(J))*8.066
     IF (OS(J).LE.1.E-5) OS(J)=1.E-5
     IF(IFLAG.NE.1) OS(J)=ALOG10(ABS(OS(J))*5.43658E+4)

```



```

EP=AMIN1 (E (J) ,EP)
IF (E (J) .LE.100.) OMAX=AMAX1 (OS (J) ,OMAX)
1 CONTINUE
SP=AMAX1 (EP,57.)
EP=AIN1 (EP)-5.
IF (EP.LE.0.) EP=1.
SP=AIN1 (SP)+5.
LIM=(SP-EP)/HX
WW=.36*BL**2
WRITE (6,6)
WRITE (6,2)
WRITE (6,7)
WRITE (6,3)
WRITE (6,4)
WRITE (6,5)
WN=SP+HX
DO 10 LL=1,LIM
WN=WN-HX
A=WN-0.5*HX
B=WN+0.5*HX
WL=(1.0E+4)/WN
DO 20 K=1,100
20 IPLT(K)=IBLNK
IPLT(20)=IPNT
IPLT(40)=IPNT
IPLT(60)=IPNT
IPLT(80)=IPNT
DO 30 J=1,N
IF (E (J) .LT.A.OR.E (J) .GE.B) GO TO 30
R=AMAX1 (AMAX1 (ABS (SCIX (J) ) ,ABS (SCIY (J) ) ) ,ABS (SCIZ (J) ) )
IR=IX
IF (ABS (SCIY (J) ) .GE.R) IR=IY
IF (ABS (SCIZ (J) ) .GE.R) IR=IZ
IF (R.LT..00001) IR=I0
M=1
IF (OS (J) .GT.1.) M=(OS (J) -1.) *20.
IF (M.GT.100) M=100
DO 40 K=1,M
ISYM=IBR
IF ( IFLAG.EQ.1 .AND. BTERM(J).GT..0 ) ISYM=IPL
IP=IPLT(K)

```

```

      IF(IP.NE.IX.AND.IP.NE.IY.AND.IP.NE.IZ.AND.IP.NE.IO) IPLT(K)=ISYM
40  CONTINUE
      IPLT(M)=IR
30  CONTINUE
      WRITE(6,8) WN,(IPLT(J),J=1,99),WL
10  CONTINUE
      WRITE(6,5)
      WRITE(6,4)
      WRITE(6,3)
      WRITE(6,7)
      WRITE(6,2)
      WRITE(6,9)
      DO 50 J=1,N
      E(J)=E(J)/8.066
50  CONTINUE
      RETURN
      END
c#####
      SUBROUTINE GMATR(IFLAG)
      implicit real*8(A-H,O-Z)
c      COMPUTES THE GAMMA INTEGRAL PARAMETERS
c-----PROGRAMMED BY H. BAUMANN, STRONGLY MODIFIED BY JS-L
      DIMENSION X(100),Y(100),Z(100),ZS(100)
      COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,
1          IGCCI,EATOM,ISCF,ITGT,ICI,GAH
      COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300),
1          C(400),GAX(300)
      COMMON /C/ S(300,300),G(300,300)
      COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN,NG
      COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
.          DPI,DSIG,DDD(300),FPPPIM,FDM
      EQUIVALENCE (C(1),X(1)),(C(101),Y(1)),(C(201),Z(1)),
.          (C(301),ZS(1))
101  FORMAT (//' DIATOMIC ELECTRON REPULSION INTEGRALS (EV) ')
102  FORMAT (//' INTERATOMIC DISTANCES (ANGSTROM) ')
c      GAMMA-MATRIX IN UPPER HALF OF G
c      DISTANCE-MATRIX IN LOWER HALF OF G
      XG=ABS(XG)
      XGINV=-1./XG
      DO 2 I=1,NTOTAL
      DO 2 J=1,NTOTAL

```

```

2 G(I,J)=0.
  IF (NH.LT.1) GO TO 8
  DO 7 I=1,NH
  DO 5 J=I,NH
  IF (I.EQ.J) GO TO 5
  D=SQRT((X(I)-X(J))**2+(Y(I)-Y(J))**2+(Z(I)-Z(J))**2)
  G(J,I)=D
  G(I,J)=14.3942*(D**XG+(14.3942/GAH)**XG)**XGINV
5 CONTINUE
  IF (N.LT.1) GO TO 7
  DO 6 J=1,N
  L=J+NH
  D=SQRT((X(I)-X(L))**2+(Y(I)-Y(L))**2+(Z(I)-Z(L))**2)
  G(L,I)=D
  GG = 1./GAX(L) + 1./GAH
  G(I,L)=14.3942 * (D**XG+(7.1971*GG)**XG) **XGINV
6 CONTINUE
7 CONTINUE
8 IF (N.LT.1) GO TO 18
  DO 10 I=1,N
  II=I+NH
  DO 10 J=I,N
  JJ=J+NH
  IF (I.EQ.J) GO TO 10
  D=SQRT((X(II)-X(JJ))**2+(Y(II)-Y(JJ))**2+(Z(II)-Z(JJ))**2)
  G(JJ,II)=D
  GG = 1./GAX(II) + 1./GAX(JJ)
  G(II,JJ)=14.3942 * (D**XG+(7.1971*GG)**XG) **XGINV
10 CONTINUE
  IF(IFLAG.EQ.1) WRITE(6,102)
  IF(IFLAG.EQ.1) CALL PRINT(G,NTOTAL,0,0,0,0,0)
  DO 4 I=1,NTOTAL
4 G(I,I)=GAX(I)
  IF(IPRNT.LT.1) GOTO 24
  WRITE(6,101)
  CALL PRINT(G,0,NTOTAL,0,0,0,0)
24 DO 11 J=N2S,NTOTAL
  DO 11 L=2,4
  I=J+N*(L-1)
  G(I,I)=G(J,J)
11 CONTINUE

```

```

DO 14 I=1,NH
DO 13 J=N2S,NTOTAL
DO 12 JJ=2,4
L=J+N*(JJ-1)
12 G(I,L)=G(I,J)
13 CONTINUE
14 CONTINUE
DO 17 K=N2S,NTOTAL
DO 17 M=N2S,NTOTAL
IG=MAX0(K,M)
IK=MIN0(K,M)
DO 16 II=1,4
I=IK+N*(II-1)
DO 15 JJ=1,4
J=IG+N*(JJ-1)
IMA=MAX0(I,J)
IMI=MIN0(I,J)
IF (J.NE.I) G(IMI, IMA)=G(IK, IG)
15 CONTINUE
16 CONTINUE
17 CONTINUE
18 ECORE=0.
NH1=NH-1
DO 20 I=1,NH1
I1=I+1
DO 20 J=I1,NH
ECORE=ECORE+ZCORE(I)*ZCORE(J)*G(I,J)
20 CONTINUE
IF (N.LT.1) GO TO 23
DO 21 I=1,NH
DO 21 JJ=N2S,NTOTAL
ECORE=ECORE+ZCORE(I)*ZCORE(JJ)*G(I, JJ)
21 CONTINUE
IF (N.LE.1) GO TO 23
N1=NTOTAL-1
DO 22 II=N2S,N1
I1=II+1
DO 22 JJ=I1,NTOTAL
ECORE=ECORE+ZCORE(II)*ZCORE(JJ)*G(II, JJ)
22 CONTINUE
23 CONTINUE

```

```

CALL STORE(G,2,N5)
RETURN
END
c#####
SUBROUTINE SMATR
implicit real*8(A-H,O-Z)
c-----COMPUTE OVERLAP MATRIX, SCALED OVERLAP MATRICES, ETC.      /JS-L
c  BASED ON:      QCPE 228, M.J.S. DEWAR AND P.J. STUDENT
COMMON/A/ NX,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,
.      IGCCI,EATOM,ISCF,ITGT
COMMON /B/ EK(300),EE(300),ZCORE(300),ET(300),SUM(300),C(400)
COMMON /C/ S(300,300),U(300,300)
COMMON /E/ NCYCL,EPREV,ITERR,N5,NUMAT,N2S
COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
.      DPI,DSIG,DDD(300),FPPIM,FDM
COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),XP(100),YP(100),BET(5050),
.      BETAM(100,100),CIPI(10000),IFROM(100),ITO(100),EP(100),POCC(100)
DIMENSION ZA(100),Z(5),A(7),B(7),T(3),X(100),
.      Y(100),Z1(100),IQ(300)
EQUIVALENCE (C(1),X(1)),(C(101),Y(1)),(C(201),Z1(1)),
.      (C(301),ZA(1)),(IQ(1),SUM(1))
101 FORMAT (//'OVERLAP MATRIX  ')
DO 9999 I=1,N5
DO 9997 J=1,I
U(J,I)=0.0
S(I,J)=0.0
9997 S(J,I)=0.0
9999 S(I,I)=1.0
DO 16 I1=1,NUMAT
NA=IQ(I1)
c-----NEXT STATEMENT CHANGED FROM IPLUS=NS2 TO AVOID REPETITION /JS-L
IPLUS=MIN0(NUMAT,I1+1)
DO 15 J1=IPLUS,NUMAT
IF (I1.EQ.J1) GO TO 15
IG=MAX0(I1,J1)
IK=MIN0(I1,J1)
NB=IQ(J1)
c  II=1 FIRST-FIRST
c  II=2 FIRST-SECOND
c  II=3 FIRST-THIRD
c  II=4 SECOND-SECOND

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```

c      II=5 SECOND-THIRD
c      II=6 THIRD-THIRD
      II=1
      IF ((NA.LT.3).AND.(NB.LT.3)) GO TO 14
      II=6
      IF ((NA.GT.10).AND.(NB.GT.10)) GO TO 14
      IF ((NA.GT.10).OR.(NB.GT.10)) GO TO 13
      II=4
      IF ((NA.LT.3).OR.(NB.LT.3)) II=2
      GO TO 14
13  II=3
c-----NEXT STATEMENT INSERTED BY JS-L
      IF ((NA.LT.3).OR.(NB.LT.3)) GOTO 14
      IF ((NA.GT.2).OR.(NB.GT.2)) II=5
14  RAB=U(IG,IK)/.529167
      IF(NA.GT.NB) GO TO 1
      ISP=2
      IPS=3
      FACTOR = +1.0
      SA=ZA(I1)
      SB=ZA(J1)
      GO TO 2
1  ISP=3
      IPS=2
      FACTOR = -1.0
      SA=ZA(J1)
      SB=ZA(I1)
2  J=II+2
      IF(II.GT.3) J=J-1
      ALPHA=0.5*RAB*(SA+SB)
      BETA=0.5*RAB*(SB-SA)
c-----PREPARE PARAMETERS FOR CONSTRUCTION OF F(0) MATRIX
      XPI =EXP(DPI *ALPHA)
      XSIG=EXP(DSIG*ALPHA)
      PPPI =(1.+FPPPPI * XPI )/2.
      PPSIG=(1.+FPPSIG* XSIG )/2.
      PS   =(1.+FPS   * XSIG )/2.
      SS   =(1.+FSS   * XSIG )/2.
      DO 3  I=1,J
      N=I-1
      A(I)=OA(ALPHA,N)

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      B(I)=OB(BETA ,N)
3  CONTINUE
      DO 4  I=1,5
4  Z(I)=0.0
      GO TO (5,6,7,8,9,10),II
C  -----
C  *** THE ORDERING OF THE ELEMENTS WITHIN Z IS
C  *** Z(1)=(S(B)/S(A))   Z(2)=(P-SIGMA(B)/S(A))   Z(3)=(S(B)/P-SIGMA(A))
C  *** Z(4)=(P-SIGMA(B)/P-SIGMA(A))   Z(5)=(P-PI(B)/P-PI(A))
C  -----
C  *** FIRST ROW - FIRST ROW OVERLAPS
      5  Z(1)=0.25*SQRT((SA*SB*RAB**2)**3)*(A(3)*B(1)-B(3)*A(1))
      GO TO 11
C  *** FIRST ROW - SECOND ROW OVERLAPS
      6  W=SQRT((SA**3)*(SB**5))*(RAB**4)*0.125
      Z(1)=W*SQRT(1.0/3.0)*(A(4)*B(1)-B(4)*A(1)+A(3)*B(2)-B(3)*A(2))
      Z(ISP)=W*(A(3)*B(1)-B(3)*A(1)+A(4)*B(2)-B(4)*A(2))*FACTOR
      GO TO 11
C  *** FIRST ROW - THIRD ROW OVERLAPS
      7  W=SQRT((SA**3)*(SB**7)/7.5)*(RAB**5)*0.0625
      Z(1)=W*(A(5)*B(1)-B(5)*A(1)+2.0*(A(4)*B(2)-B(4)*A(2)))/SQRT(3.0)
      Z(ISP)=W*FACTOR*(A(4)*(B(1)+B(3))-B(4)*(A(1)+A(3))
1      +B(2)*(A(3)+A(5))-A(2)*(B(3)+B(5)))
      GO TO 11
C  *** SECOND ROW - SECOND ROW OVERLAPS
      8  W=SQRT((SA*SB)**5)*(RAB**5)*0.0625
      RT3=1.0/SQRT(3.0)
      Z(1)=W*(A(5)*B(1)+B(5)*A(1)-2.0*A(3)*B(3))/3.0
      D=A(4)*(B(1)-B(3))-A(2)*(B(3)-B(5))
      E=B(4)*(A(1)-A(3))-B(2)*(A(3)-A(5))
      Z(ISP)=W*RT3*FACTOR*(D+E)
      Z(IPS)=W*RT3*FACTOR*(E-D)
      Z(4)=W*(B(3)*(A(5)+A(1))-A(3)*(B(5)+B(1)))
      Z(5)=0.5*W*(A(5)*(B(1)-B(3))-B(5)*(A(1)-A(3))-A(3)*B(1)+B(3)*A(1))
      GO TO 11
C  *** SECOND ROW - THIRD ROW OVERLAPS
      9  W=SQRT((SA**5)*(SB**7)/7.5)*(RAB**6)*0.03125
      RT3=1.0/SQRT(3.0)
      Z(1)=W*(A(6)*B(1)+A(5)*B(2)-2.0*(A(4)*B(3)+A(3)*B(4))+A(2)*B(5)
1      +A(1)*B(6))/3.0
      Z(ISP)=W*RT3*FACTOR*(A(6)*B(2)+A(5)*B(1)-2.0*(A(4)*B(4)+A(3)*B(3))

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1          +A(2)*B(6)+A(1)*B(5))
Z(IPS)=W*RT3*FACTOR*(A(5)*(2.0*B(3)-B(1))-B(5)*(2.0*A(3)-A(1))
1          -A(2)*(B(6)-2.0*B(4))+B(2)*(A(6)-2.0*A(4)))
Z(4)=W*(B(4)*(A(1)+A(5))-A(4)*(B(1)+B(5))+B(3)*(A(2)+A(6))
1          -A(3)*(B(2)+B(6)))
Z(5)=0.5*W*(A(6)*(B(1)-B(3))-B(6)*(A(1)-A(3))+A(5)*(B(2)-B(4))
1          -B(5)*(A(2)-A(4))-A(4)*B(1)+B(4)*A(1)-A(3)*B(2)+B(3)*A(2))
GO TO 11
C *** THIRD ROW - THIRD ROW OVERLAPS
10 W=SQRT((SA*SB*RAB**2)**7)/480.0
RT3=1.0/SQRT(3.0)
Z(1)=W*(A(7)*B(1)-3.0*(A(5)*B(3)-A(3)*B(5))-A(1)*B(7))/3.0
D=A(6)*(B(1)-B(3))-2.0*A(4)*(B(3)-B(5))+A(2)*(B(5)-B(7))
E=B(6)*(A(1)-A(3))-2.0*B(4)*(A(3)-A(5))+B(2)*(A(5)-A(7))
Z(ISP)=W*RT3*FACTOR*(D-E)
Z(IPS)=W*RT3*FACTOR*(-D-E)
Z(4)=W*(A(3)*(B(7)+2.0*B(3))-A(5)*(B(1)+2.0*B(5))-B(5)*A(1)
1          +A(7)*B(3))
Z(5)=0.5*W*(A(7)*(B(1)-B(3))+B(7)*(A(1)-A(3))
1          +A(5)*(B(5)-B(3)-B(1))+B(5)*(A(5)-A(3)-A(1))+2.0*A(3)*B(3))
11 U(IK,IG)= Z(1) * PENSS
S(IK,IG)= Z(1) * SS
S(IG,IK)= Z(1)
IF (II.EQ.1) GO TO 15
C COMPUTE THE BOND-DIRECTION COSINES
IG=MAX0(I1,J1)
IK=MIN0(I1,J1)
T(1)=(X(I1)-X(J1))/U(IG,IK)
T(2)=(Y(I1)-Y(J1))/U(IG,IK)
T(3)=(Z1(I1)-Z1(J1))/U(IG,IK)
IF (NA.LT.3) GO TO 17
C S-PX, S-PY, S-PZ
C-----ERROR CORRECTED: J2-->I2, J1-->I1 /JS-L
I2=I1
DO 18 K=1,3
I2=I2+NX
IG=MAX0(J1,I2)
IK=MIN0(J1,I2)
SH=T(K)*Z(3)
U(IK,IG)= SH * PENSP
S(IK,IG)= SH * PS

```



```

18 S(IG,IK) = SH
17 IF (NB.LT.3) GO TO 19
c   PX-S, PY-S, PZ-S
    J2=J1
    DO 20 K=1,3
    J2=J2+NX
    IG=MAX0(I1,J2)
    IK=MIN0(I1,J2)
    SH=T(K)*Z(2)
    U(IK,IG) = SH * PENSP
    S(IK,IG) = SH * PS
20 S(IG,IK) = SH
19 IF (II.LT.4) GO TO 15
c   XX-, XY-, XZ-, YY-, YZ-, ZZ-WECHSELWIRKUNG
    I2=I1
    DO 21 K=1,3
    I2=I2+NX
    J2=J1
    DO 21 L=1,3
    J2=J2+NX
    IG=MAX0(I2,J2)
    IK=MIN0(I2,J2)
    FF=0.
    IF (K.EQ.L) FF=1.
    SH1=T(K)*T(L)*Z(4)
    SH2=(FF-T(K)*T(L))*Z(5)
    U(IK,IG) = (SH1 + SH2) * PENPP
    S(IK,IG) = SH1 * PPSIG + SH2 * PPPI
    S(IG,IK) = SH1          + SH2
c-MCD- -MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD-
    IF (K*L.NE.9) GO TO 21
    BETAM(I1-NH,J1-NH) = SH2 * ( 1.+ FPPPIM * EXP(FDM*ALPHA) ) / 2.
    BETAM(J1-NH,I1-NH) = BETAM(I1-NH,J1-NH)
c-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD-
21 CONTINUE
15 CONTINUE
16 CONTINUE
    IF (IPRNT.LT.3) RETURN
    WRITE(6,101)
    CALL PRINT(S,N5,0,0,0,NX,NH)
    RETURN

```

```

      END
c#####
      FUNCTION OA(A,K)
      implicit real*8(A-H,O-Z)
c      THIS QCPE 228 FUNCTION EVALUATES THE A INTEGRALS
      B=1./A
      S=1.
      OA=1.
      IF (K.LT.1) GO TO 2
      DO 1 M=1,K
      L=K-M+1
      S=L*S*B
1      OA=OA+S
2      OA=OA*B*EXP(-A)
      RETURN
      END
c#####
      FUNCTION OB(BETA,N)
      implicit real*8(A-H,O-Z)
c      THIS QCPE 228 FUNCTION EVALUATES THE B INTEGRALS
      B=BETA**2
      FN=N
      J=MOD(N,2)
      IF (J.EQ.0) GO TO 2
      FNUMER=FN+2.
      SUM=BETA/FNUMER
      FACTOR=-2.
      FI=3.0
      GO TO 3
2      FNUMER=FN+1.
      SUM=1./FNUMER
      FACTOR=2.
      FI=2.
3      T=SUM
4      DENOM=FNUMER+2.
      T=(T/FI)*(B/(FI-1.))*(FNUMER/DENOM)
      IF (T.LE.1.E-10) GO TO 5
      SUM=T+SUM
      FI=FI+2.
      FNUMER=DENOM
      GO TO 4

```

```

5 OB=FACTOR*SUM
RETURN
END
c#####
SUBROUTINE F0MATR
implicit real*8(A-H,O-Z)
c-----COMPUTE F0 IN AO BASIS; DIAGONAL IN DDD(*)
c ON ENTRY: F0( S ) SF ) , SP( R ) SP )
c J. Spanget-Larsen, Theor. Chem. Acc. 98, 137-153 (1997)
COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT
COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300)
COMMON /C/ F0(300,300),SP(300,300)
COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL
COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
. DPI,DSIG,DDD(300),FPPIM,FDM
COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),XP(100),YP(100),BET(5050),
1 BETAM(100,100),CIPI(10000),IFROM(100),ITO(100),EP(100),POCC(100)
DO 10 I=1,N5
DO 10 J=1,I
10 SP(I,J)=0.0
c-----COMPUTE PENETRATION TERMS FOR ONE-CENTER F0 ELEMENTS
DO 40 I=1,NTOTAL
J=1
IF(I.GT.NH) J=4
DO 40 I1=1,J
IG=I+(I1-1)*N
DO 40 I2=1,I1
IK=I+(I2-1)*N
TEMP=0.0
DO 30 L=1,N5
IG1=MAX0(IK,L)
IK1=MIN0(IK,L)
IG2=MAX0(L,IG)
IK2=MIN0(L,IG)
30 TEMP=TEMP + SP(IK1,IG1) * DDD(L) * SP(IK2,IG2)
IF(IK.LT.IG) SP(IG,IK)=TEMP
40 IF(IK.EQ.IG) SUM(IK) =TEMP
c-----OFF-DIAGONAL F0 ELEMENTS (IN UPPER HALF OF F0)
DO 50 IG=1,N5
DO 50 IK=1,IG
50 IF(IK.LT.IG) F0(IK,IG) = SP(IG,IK) + F0(IK,IG)*(ET(IK)+ET(IG))

```

```

c-----DIAGONAL F0 ELEMENTS (IN DDD)
      DO 60 I=1,N5
      60 DDD(I)=DDD(I)+SUM(I)
c-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
      DO 6000 I=1,N
      BETAM(I,I)=DDD(N+NH+I)-SUM(N+NH+I)
      DO 6000 J=1,I
      IF(I.NE.J) BETAM(I,J)=BETAM(I,J)*(BETAM(I,I)+BETAM(J,J))
      6000 BETAM(J,I)=BETAM(I,J)
c-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
      WRITE(6,1000) (SUM(I),I=1,N5)
      1000 FORMAT(//' DIAGONAL PENETRATION TERMS'//(10F13.8))
      RETURN
c      ON EXIT:  F0( S ) F0* ), SP( - ! SP )
      END
c#####
      SUBROUTINE LOWDIN
      implicit real*8(A-H,O-Z)
c-----LOWDIN TRANSFORM F0 MATRIX /JS-L
      COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
      1      EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB
      COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300)
      COMMON /C/ H(300,300),W(300,300)
      COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN
      COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
      .      DPI,DSIG,DDD(300),FPPPIM,FDM
      COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),XP(100),YP(100),
      1      BETA(5050),BETAM(100,100),CIPI(10000),
      2      IFROM(100),ITO(100),EP(100),POCC(100)
      COMMON /SBIAS/ BIAS,IPI
c-----COMPUTE INVERSE SQUARE ROOT OF OVERLAP-MATRIX
      20 NTEMP=N
      N=N5
      HBIAS = BIAS
      BIAS = 0.0
      CALL DIAGON
      BIAS = HBIAS
      N=NTEMP
      IF(IPRNT.LT.4) GOTO 30
      WRITE(6,1000) (SUM(I),I=1,N5)
      1000 FORMAT(//' EIGENVALUES OF OVERLAP-MATRIX'//(10F13.8))

```

```

WRITE(6,1100)
1100 FORMAT(//' EIGENVECTORS OF OVERLAP-MATRIX')
CALL PRINT(W,N5,N5,0,0,N,NH)
30 DO 40 I=1,N5
IF(SUM(I).GE..0001) GOTO 40
WRITE(6,1200) I,SUM(I)
1200 FORMAT(//I4,'. EIGENVALUE OF OVERLAP-MATRIX =',F13.8,
. // ' MATRIX NOT POSITIVE DEFINITE, CALCULATION INTERRUPTED')
STOP
40 SUM(I)=1./SQRT(SUM(I))
DO 60 I=1,N5
DO 60 J=1,I
TEMP=0.0
DO 50 K=1,N5
50 TEMP=TEMP+W(I,K)*SUM(K)*W(J,K)
60 H(I,J)=TEMP
IF(IPRNT.LT.3) GOTO 70
WRITE(6,1300)
1300 FORMAT(//' INVERSE SQUARE ROOT OF OVERLAP-MATRIX')
CALL PRINT(H,N5,0,0,0,N,NH)
C- - -REARRANGE
70 DO 90 I=1,N5
DO 80 J=1,I
W(I,J)=H(I,J)
80 W(J,I)=W(I,J)
90 H(I,I)=DDD(I)
C- - -PRINT
IF(IPRNT.GT.2) WRITE(6,1350)
1350 FORMAT(//'F(0) MATRIX IN AO BASIS (EV)')
IF(IPRNT.GT.2) CALL PRINT(H,0,N5,0,0,N,NH)
C-----LOWDIN TRANSFORM F(0) MATRIX
DO 150 I=1,N5
DO 130 L=1,N5
TEMP=0.0
IF(L.EQ.1) GOTO 110
L1=L-1
DO 100 K=1,L1
100 TEMP=TEMP+H(K,L)*W(I,K)
110 DO 120 K=L,N5
120 TEMP=TEMP+H(L,K)*W(I,K)
130 SUM(L)=TEMP

```

```

      DO 150 J=1,I
      TEMP=0.0
      DO 140 L=1,N5
140  TEMP=TEMP+SUM(L)*W(L,J)
      IF(I.EQ.J) EE(I) =TEMP
      IF(I.NE.J) H(I,J)=TEMP
150  CONTINUE
      DO 160 I=1,N5
160  H(I,I)=EE(I)
C- - -PRINT
      180 IF(IPRNT.GT.1) WRITE(6,1400)
1400  FORMAT(//'F(0) MATRIX IN LOWDIN BASIS (EV) ')
      IF(IPRNT.GT.1) CALL PRINT(H,N5,0,0,0,N,NH)
C- - -STORE
      190 CALL STORE(H,1,N5)
C-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
      IR=0
      NP=NH+3*N
      DO 3002 I=1,N
      DO 3001 L=1,N
      SUM(L)=.0
      DO 3001 K=1,N
3001  SUM(L)=SUM(L)+BETAM(K,L)*W(NP+I,NP+K)
      DO 3002 J=1,I
      IR=IR+1
      BETA(IR)=.0
      DO 3002 L=1,N
3002  BETA(IR)=BETA(IR)+SUM(L)*W(NP+L,NP+J)
C-MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--MCD--
      RETURN
      END
C#####
      SUBROUTINE SCF
      implicit real*8(A-H,O-Z)
C-----SCF PROCEDURE /JS-L
      COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
1      EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB,NB,NAB
      COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300),
1      C(400),GAX(300),NTIT(20)
      COMMON /C/ S(300,300),U(300,300)
      COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN,NG,DAMP

```

```

COMMON /MOM/ SX(300),SY(300)
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
COMMON /F/ PENSS,PENSP,PENPP,XG,FPPPI,FPPSIG,FPS,FSS,
.
      DPI,DSIG,DDD(300),FPPPIM,FDM
COMMON /SBIAS/ BIAS,IPI
COMMON /NMOP/ NMOP
72 FORMAT (I4,5X,'D=',F4.2,5X,'DE =',F15.8,' EV',5X,
.
      'DP=',F12.8,5X)
73 FORMAT (I4,5X,'D=',F4.2,5X,'DE =',F15.8,' EV',5X,
.
      'DP=',F12.8,5X,' ENERGIES SATISFIED')
74 FORMAT (I4,5X,'D=',F4.2,5X,'DE =',F15.8,' EV',5X,
.
      'DP=',F12.8,5X,' DENSITIES SATISFIED')
75 FORMAT (I4,5X,'D=',F4.2,5X,'DE =',F15.8,' EV',5X,
.
      'DP=',F12.8,5X,' ENERGIES AND DENSITIES SATISFIED')
820 FORMAT (10X,I3,' : ',F12.6,F12.6)
1961 FORMAT (//' MO ENERGIES (EV) AND HALF OCCUPATION NUMBERS'/)
3002 FORMAT (//' MO COEFFICIENTS STORED COLUMNWISE (LOWDIN BASIS)')
3003 FORMAT (//' DENSITY MATRIX (LOWDIN BASIS)')
      NTEMP=N
      LOOK=1
      IF(NPMO+NPE.NE.0) LOOK=0
      ETOT1=0.
      CALL LOAD(S,1,N5)
      DO 1 I=1,N5
      ET(I)=0.0
1 SX(I)=0.0
      DAMP=ALOG(DAMP)
      DD=1.
C-----SCF LOOP
      WRITE(6,3009) (NTIT(I),I=1,18)
3009 FORMAT(1H //1X,18(A4)//' INITIAL DENSITIES AND CHARGES: '/')
      DO 10 NCYCL=1,ISCF
      N=N5
      CALL DIAGON
      N=NTEMP
      CALL AUFBAU(NE,N5,SUM,LOOK)
      IF(ITERR.NE.0) GOTO 30
      CALL FMATR(DE,DP,NCYCL,DD)
      IF(NCYCL.EQ.1) WRITE(6,3050)
3050 FORMAT(//' SCF PROCEDURE: '/')
      IF(DP.LT.1.E-4 .AND. DE.LT.5.E-4) WRITE(6,75) NCYCL,DD,DE,DP

```

```

        IF(DP.LT.1.E-4 .AND. DE.LT.5.E-4) GO TO 20
    IF(DP.LT.1.E-4) WRITE(6,74) NCYCL,DD,DE,DP
        IF(DP.LT.1.E-4) GO TO 10
    IF(DE.LT.5.E-4) WRITE(6,73) NCYCL,DD,DE,DP
    IF(DE.LT.5.E-4) GO TO 10
    WRITE(6,72) NCYCL,DD,DE,DP
10 CONTINUE
    WRITE(6,3006)
3006 FORMAT(//' SCF PROCEDURE INTERRUPTED, CONVERGENCE NOT ATTAINED'//)
c-----TOTAL ENERGY
    20 N=N5
        CALL DIAGON
        N=NTEMP
        BIAS=0.0
        IF(IPRNT.LT.2) GOTO 30
        WRITE(6,3001)
3001 FORMAT(//' GROUND STATE FOCK MATRIX IN LOWDIN BASIS (EV) ')
        CALL PRINT(S,N5,0,0,0,N,NH)
    30 CALL LOAD(S,2,N5)
        CALL SHIFT(S,N5)
        CALL ENERGY(1,ECORE,SUM)
        WRITE(6,1961)
c-----PRINT MO ENERGIES AND OCCUPATION NUMBERS
        DO 40 I=1,N5
            J=N5+1-I
            WRITE(6,820) J,SUM(J),OCC(J)
            IF(J.EQ.1) GOTO 40
            IF(ABS(OCC(J)-OCC(J-1)).GT.0.001) WRITE(6,3010)
3010 FORMAT(1X)
        40 CONTINUE
            WRITE(6,3002)
            MIN=MAX0(1,NLUMO-NMOP)
            MAX=MIN0(N5,NHOMO+NMOP)
            CALL PRINT(U,N5,N5,MIN,MAX,N,NH)
            CALL STORE(U,4,N5)
            IF (IPRNT.LT.2) GO TO 83
            WRITE(6,3003)
            CALL PMATR (S,U,N5)
            CALL PRINT(S,N5,0,0,0,N,NH)
        83 WRITE(6,3005)
3005 FORMAT(//' ATOMIC POPULATIONS'//)

```



```
CALL PRATP(SX,N,NH,ZCORE)
CALL PI
RETURN
END
```

```
c#####
```

```
      SUBROUTINE PI
      implicit real*8(A-H,O-Z)
      COMMON /A/ NC,NH
      COMMON /C/ S(300,300),U(300,300)
      COMMON /PIMCD/ MCD,N,NOCC,NST,LPI(300),XP(100),YP(100),BETA(5050),
1     CPI(10000),CIPI(10000),IFROM(100),ITO(100),EP(100),POCC(100)
      COMMON /MOM/ Q(300)
      COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
      COMMON /SBIAS/ BIAS,IPI
      REAL NEL
      N=NC
      NPI=NH+3*NC+1
      NORB=NH+4*NC
      IP=0
      IR=0
      NEL=0.0
      DO 20 MO=1,NORB
      LPI(MO)=1
      IF(IPI.LE.0) GO TO 20
      SPI=0.0
      IX=0
      DO 10 MY=NPI,NORB
      IX=IX+1
10     SPI=SPI+ABS(U(MY,MO))
      IF(SPI.LT.0.1) LPI(MO)=0
      IF(SPI.LT.0.1) GO TO 20
      IP=IP+1
      POCC(IP)=OCC(MO)
      IF(OCC(MO).GT.0.01) NOCC=IP
      LPI(MO)=IP
      NEL=NEL + 2.0 * OCC(MO)
      IX=0
      DO 15 MY=NPI,NORB
      IX=IX+1
      C=0.0
      C=U(MY,MO)
```

```

      IR=IR+1
15  CPI(IR)=C
20  CONTINUE
      IF(IPI.LE.0) RETURN
c-----DETERMINE CENTER OF CHARGE
      IF( NEL .GT. 0.1 ) GO TO 25
      WRITE(6,500) NEL
500  FORMAT(//1X,'  ERROR   NO. OF PI ELECTRONS',F6.2//)
      NEL=1.0
25  X0=.0
      Y0=.0
      IR=0
      DO 30 MY=NPI,NORB
      IR=IR+1
      X0=X0+XP(IR)*Q(MY)/NEL
      Y0=Y0+YP(IR)*Q(MY)/NEL
30  CONTINUE
      WRITE(6,1000) X0,Y0
1000 FORMAT(' PI ELECTRON CENTER OF CHARGE:   X,Y   =',F8.4,' ',F8.4)
c-----SHIFT TO CHARGE CENTERED COORDINATE SYSTEM
      WRITE(6,2000)
2000 FORMAT(/1X,'CHARGE CENTERED X,Y-COORDINATES FOR PI SYSTEM:')
      DO 40 MY=1,N
      XP(MY)=XP(MY)-X0
      YP(MY)=YP(MY)-Y0
40  WRITE(6,3000) MY,XP(MY),YP(MY)
3000 FORMAT(I5,2F9.4)
      RETURN
      END
c#####
      SUBROUTINE PRATP(PAO,NC,NH,ZCORE)
      implicit real*8(A-H,O-Z)
      DIMENSION PAO(1),ZCORE(1),PA(300),CHARGE(300)
c-----COMPUTE ATOMIC POPULATIONS AND NET CHARGES
      SPA=0.0
      SCH=0.0
      NT=NC+NH
      DO 20 I=1,NT
      PA(I)=PAO(I)
      IF(I.LE.NH) GOTO 10
      PA(I)=PAO(I)+PAO(I+NC)+PAO(I+2*NC)+PAO(I+3*NC)

```

```

10 CHARGE(I)=ZCORE(I)-PA(I)
   SPA=SPA+PA(I)
20 SCH=SCH+CHARGE(I)
c-----PRINT
   WRITE(6,1000)
1000 FORMAT(' POSITION',11X,'AO POPULATIONS',16X,'ATOMIC      NET',
.         /13X,'S',8X,'PX',7X,'PY',7X,'PZ',6X,'POPULATION  CHARGE',
.         /1X,67('-'))
   IF(NH.EQ.0) GOTO 40
   DO 30 I=1,NH
30 WRITE(6,2000) I,PAO(I),PA(I),CHARGE(I)
2000 FORMAT(I5,4X,F9.4,27X,2F11.4)
40 IF(NC.EQ.0) GOTO 60
   DO 50 J=1,NC
   I=NH+J
50 WRITE(6,3000) I,PAO(I),PAO(I+NC),PAO(I+2*NC),PAO(I+3*NC),PA(I),
.         CHARGE(I)
3000 FORMAT(I5,4X,4F9.4,2F11.4)
60 WRITE(6,4000) SPA,SCH
4000 FORMAT(/42X,'SUM',2F11.4/1X)
   RETURN
   END
c#####
SUBROUTINE ENERGY(IFLAG,ECORE,EMO)
  implicit real*8(A-H,O-Z)
  DIMENSION EMO(1)
  COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
c-----HUECKEL ENERGY
  EHUECK=0.0
  DO 10 I=1,NHOMO
10 EHUECK = EHUECK + 2.0 * OCC(I) * EMO(I)
  WRITE(6,1000) EHUECK
1000 FORMAT('// ' HUECKEL ENERGY                      ',F15.6,' EV')
  IF(IFLAG.LT.1) RETURN
c-----ROOTHAAN CLOSED SHELL ELECTRONIC ENERGY
  ER=EHUECK
c- - -DIAGONAL CONTRIBUTIONS
  DO 20 I=1,NHOMO
20 ER = ER - OCC(I)**2 * H(I,I,I,I)
c- - -OFF-DIAGONAL CONTRIBUTIONS
  NHOMO1=NHOMO-1

```

```

DO 30 I=1,NHOMO1
I1=I+1
DO 30 J=I1,NHOMO
30 ER = ER - 4.0 * OCC(I) * OCC(J) * ( H(I,I,J,J) - H(I,J,J,I)/2.0 )
E = ER + E CORE
WRITE(6,2000) ER,ECORE,E
2000 FORMAT( /' Roothaan Closed Shell Energy      ',F15.6,' EV',
.          //' Core Repulsion                    ',F15.6,' EV',
.          //' Total Valence Shell Energy        ',F15.6,' EV')
IF(NHOMO.LT.NLUMO) RETURN
c-----PROJECTION OF OPEN SHELL STATES
WRITE(6,3000)
3000 FORMAT(//' PROJECTION OF OPEN SHELL STATES:')
IF(NPMO-2) 40,50,80
c- - -A SINGLE UNPAIRED ELECTRON IN ONE SPACE-ORBITAL
40 E = E - H(NHOMO,NHOMO,NHOMO,NHOMO)/4.
WRITE(6,4000) E
4000 FORMAT( /' Doublet                          ',F15.6,' EV')
RETURN
50 A = H(NHOMO,NHOMO,NHOMO,NHOMO)
B = H(NLUMO,NLUMO,NLUMO,NLUMO)
C = H(NHOMO,NHOMO,NLUMO,NLUMO)
D = H(NHOMO,NLUMO,NLUMO,NHOMO)
IF(NPE-2) 70,60,70
c- - -TWO ELECTRONS IN TWO DEGENERATE SPACE-ORBITALS
60 E1 = E - A/4. - B/4.      - 0.5*D
E2 = E - A/4. - B/4.      + 1.5*D
E3 = E + A/4. + B/4. - C - 0.5*D
E4 = E + A/4. + B/4. - C + 1.5*D
X1 = 0.
X2 = E2 - E1
X3 = E3 - E1
X4 = E4 - E1
WRITE(6,5000) E1,X1,E2,X2,E3,X3,E4,X4
5000 FORMAT( /' Triplet          U V          ',2F15.6,' EV',
.          //'          ( U V          ',2F15.6,' EV',
.          /'          (' ,
.          /' Singlets          ( U U - V V          ',2F15.6,' EV',
.          /'          (' ,
.          /'          ( U U + V V          ',2F15.6,' EV')
RETURN

```

```

c- - -ONE OR THREE ELECTRONS IN TWO DEGENERATE SPACE-ORBITALS
 70 E = E - A/16. - B/16. - C/4. + D/8.
    WRITE(6,4000) E
    RETURN
 80 WRITE(6,6000)
6000 FORMAT(//' (PRESENT VERSION DOES NOT TREAT SPACE DEGENERACIES',
.          ' LARGER THAN TWO)')
    RETURN
    END
c#####
SUBROUTINE PMATR (W,U,N)
  implicit real*8(A-H,O-Z)
c-----RETURNS BOND ORDERS IN LOWER HALF OF W
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
DIMENSION W(300,300),U(300,300)
DO 20 I=1,N
DO 20 J=1,I
TEMP=0.0
DO 10 K=1,NHOMO
 10 TEMP=TEMP+OCC(K)*U(I,K)*U(J,K)
 20 W(I,J)=TEMP+TEMP
    RETURN
    END
c#####
SUBROUTINE FMATR(DE,DP,NCYC,DD)
  implicit real*8(A-H,O-Z)
c-----CONSTRUCT CLOSED SHELL OR PSEUDO-CLOSED SHELL CNDO FOCK MATRIX
COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
1      EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1
COMMON /B/ E(300),EE(300),ZCORE(300),ET(300),SUM(300),
1      C(400),GAX(300)
COMMON /C/ S(300,300),U(300,300)
COMMON /E/ NCYCL,EPREV,ITERR,N5,NTOTAL,N2S,N2P,NTN,NG,DAMP
COMMON /MOM/ SX(300),SY(300),SZ(300)
c-----COMPUTE BOND ORDER MATRIX
CALL PMATR(S,U,N5)
c- - -DAMPING /JS-L
IF(DD.GT..05) GOTO 2
DD=0.0
GOTO 4
 2 IF(NCYC.NE.1) CALL LOAD(U,3,N5)

```

```

      CALL STORE(S,3,N5)
      IF(NCYC.EQ.1) GOTO 4
      DD = EXP( DAMP * (NCYC-1) )
      DD1= 1.0 - DD
      DO 3 I=1,N5
      DO 3 J=1,I
3     S(I,J) = DD1 * S(I,J) + DD * U(I,J)
c-----EVALUATE CONVERGENCE PARAMETERS DE AND DP
4     DE=0.0
      DP=0.0
      DO 10 I=1,N5
      DE=AMAX1(DE,ABS(ET(I)-SUM(I)))
      ET(I)=SUM(I)
      DP=AMAX1(DP,ABS(SX(I)-S(I,I)))
10    SX(I)=S(I,I)
      IF(NCYC.EQ.1) CALL PRATP(SX,N,NH,ZCORE)
c-----COMPUTE GROSS ATOMIC ORBITAL AND ATOMIC CHARGES
      DO 30 I=1,NTOTAL
      L=1
      IF(I.GT.NH) L=4
      ZC=ZCORE(I)/FLOAT(L)
      TEMP=0.0
      DO 20 J=1,L
      K=I+(J-1)*N
      SY(K)=SX(K)-ZC
      TEMP=TEMP+SY(K)
c- - - GROSS AO CHARGE REDEFINED AS *P(K,K)-1* FOR USE OF TRAD. PRM*S:
20    SY(K)=SY(K)+ZC-1.
c 20 CONTINUE
30    SZ(I)=TEMP
c- - -ENTER F(0)
      CALL LOAD(U,1,N5)
      DO 40 I=1,N5
      DO 40 J=1,I
40    S(J,I)=U(I,J)
c- - -ENTER GAMMA MATRIX
      CALL LOAD(U,2,N5)
c-- ---CONSTRUCT DIAGONAL CNDO FOCK MATRIX ELEMENTS
      N3=N*3
      DO 60 I=1,NTOTAL
      TEMP=0.0

```

```

      DO 50 J=1,NTOTAL
      MIN=MIN0(I,J)
      MAX=MAX0(I,J)
50  IF(I.NE.J)  TEMP = TEMP + SZ(J) * U(MIN,MAX)
60  SUM(I)=TEMP
      DO 80 I=1,NTOTAL
      U(I,I) = S(I,I) + ( SZ(I) - SY(I)/2. ) * GAX(I)  +  SUM(I)
      IF(I.LE.NH) GOTO 80
      DO 70 K=N,N3,N
      L=I+K
70  U(L,L) = S(L,L) + ( SZ(I) - SY(L)/2. ) * GAX(I)  +  SUM(I)
80  CONTINUE
c-----CONSTRUCT OFF-DIAGONAL CNDO FOCK MATRIX ELEMENTS
      DO 90 I=2,N5
      I1=I-1
      DO 90 J=1,I1
90  U(I,J) = S(J,I) - 0.5 * S(I,J) * U(J,I)
c      PRESENT STORAGE:  U( FOCK ) GAMMA ) ,  S( P ( HCORE )
c- ----RETURN FOCK MATRIX IN LOWER HALF OF S
      DO 110 I=1,N5
      DO 110 J=1,I
110 S(I,J)=U(I,J)
      RETURN
      END
c#####
      SUBROUTINE DIAGON
      implicit real*8(A-H,O-Z)
c      EISPACK PROGRAM TRED2 CALCULATES OF THE SYMMETRIC MATRIX A
c      THE TRIDIAGONAL MATRIX. VECTOR D CONTAINS THE DIAGONAL ELEMENTS
c      OF THE TRIDIAGONAL MATRIX. VECTOR E CONTAINS IN HIS LAST N-1
c      POSITIONS THE SUBDIAGONAL ELEMENTS OF THE TRIDIAGONAL MATRIX.
c      THE ELEMENT E(1) IS SET TO ZERO. Z CONTAINS THE ORTHOGONAL
c      TRANSFORMATION MATRIX, PRODUCED IN THE REDUCTION TO THE
c      TRIDIAGONAL FORM.
      COMMON /A/ N,NH,NE,NM
      COMMON /B/ EL(300),EE(300),ZCORE(300),ET(300),D(300)
      COMMON /C/ A(300,300),Z(300,300)
      COMMON /D/ E(300)
      DO 100 I = 1,N
      DO 100 J=1,I
      Z(I,J) = A(I,J)

```

```

100 CONTINUE
    IF (N.EQ.1) GO TO 320
C-----FOR I=N STEP -1 UNTIL 2 DO--
    DO 300 II = 2,N
    I = N+2-II
    L=I-1
    H=0.0
    SCALE = 0.0
    IF (L.LT.2) GO TO 130
C-----SCALE ROW
    DO 120 K=1,L
120 SCALE = SCALE + ABS(Z(I,K))
    IF (SCALE.NE.0.0) GO TO 140
130 E(I) = Z(I,L)
    GO TO 290
140 DO 150 K = 1, L
    Z(I,K) = Z(I,K)/SCALE
    H = H + Z(I,K)*Z(I,K)
150 CONTINUE
    F = Z(I,L)
    G = -SIGN(SQRT(H),F)
    E(I) = SCALE*G
    H = H-F*G
    Z(I,L) = F-G
    F = 0.0
    DO 240 J = 1,L
    Z(J,I) = Z(I,J)/(SCALE*H)
    G = 0.0
C-----FORM ELEMENT OF A*U
    DO 180 K = 1,J
180 G = G+Z(J,K)*Z(I,K)
    JP1 = J+1
    IF (L.LT.JP1) GO TO 220
    DO 200 K = JP1, L
200 G=G+Z(K,J)*Z(I,K)
C-----FORM ELEMENT OF P
220 E(J) = G/H
    F = F + E(J)*Z(I,J)
240 CONTINUE
    HH = F/(H+H)
C-----FORM REDUCED A

```



```

      DO 260 J = 1,L
      F = Z(I,J)
      G = E(J) - HH*F
      E(J) = G
      DO 260 K = 1,J
      Z(J,K) = Z(J,K) -F*E(K)-G*Z(I,K)
260 CONTINUE
      DO 280 K = 1,L
280 Z(I,K) = SCALE*Z(I,K)
290 D(I) = H
300 CONTINUE
320 D(1) = 0.0
      E(1) = 0.0
c-----ACCUMULATION OF TRANSFORMATION MATRICES
      DO 500 I=1,N
      L = I-1
      IF (D(I).EQ.0.0) GO TO 380
      DO 360 J = 1,L
      G = 0.0
      DO 340 K = 1,L
340 G = G + Z(I,K)*Z(K,J)
      DO 360 K = 1,L
      Z(K,J) = Z(K,J) - G*Z(K,I)
360 CONTINUE
380 D(I) = Z(I,I)
      Z(I,I) = 1.0
      IF (L.LT.1) GO TO 500
      DO 400 J = 1,L
      Z(I,J) = 0.0
      Z(J,I) = 0.0
400 CONTINUE
500 CONTINUE
      CALL IMTQL2
      RETURN
      END
c#####
      SUBROUTINE IMTQL2
      implicit real*8(A-H,O-Z)
c      EISPACK PROGRAM IMTQL2 CALCULATESOF A TRIDIAGONAL MATRIX THE EIGEN
c      AND EIGENVALUES. THE DIAGONAL OF THE TRIDIAGONAL MATRIX
c      IS GIVEN IN D AND THE OFF-DIAGONAL IN E. ON ENTRY Z CONTAINS

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C      THE TRANSFORMATION-MATRIX. AT THE END THE VECTORS AND D
C      THE EIGENVALUES ARE GIVEN IN D IN ASCENDING ORDER.
COMMON /A/ N,NH,NE,NM
COMMON /B/ EL(300),EE(300),ZCORE(300),ET(300),D(300)
COMMON /C/ A(300,300),Z(300,300)
COMMON /D/ E(300)
COMMON /E/ NCYCL,EPREV,IERR
C-----ACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING
C      THE RELATIVE PRECISION OF FLOATING POINT ARITHMETIC.
ACHEP=2.**(-47)
IERR=0
IF (N.EQ.1) GO TO 1001
DO 100 I=2,N
100 E(I-1)=E(I)
E(N)=0.
DO 240 L=1,N
J=0
C-----LOOK FOR SMALL SUB-DIAGONAL ELEMENT
105 DO 110 MX=L,N
M=MX
IF (M.EQ.N) GO TO 120
IF (ABS(E(M)) .LE. ACHEP*(ABS(D(M))+ABS(D(M+1))))
.      GO TO 120
110 CONTINUE
120 P=D(L)
IF (M.EQ.L) GO TO 240
IF (J.EQ.30) GO TO 1000
J=J+1
C-----FORM SHIFT
G=(D(L+1)-P)/(2.0*E(L))
R=SQRT(G**2+1.)
G=D(M)-P+E(L)/(G+SIGN(R,G))
S=1.
C=1.
P=0.
MML=M-L
C-----FOR I=M-1 STEP -1 UNTIL L DO --
DO 200 II=1,MML
I=M-II
F=S*E(I)
B=C*E(I)

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      IF (ABS(F).LT.ABS(G)) GO TO 150
      C=G/F
      R=SQRT(C**2+1.)
      E(I+1)=F*R
      S=1./R
      C=C*S
      GO TO 160
150  S=F/G
      R=SQRT(S**2+1.)
      E(I+1)=G*R
      C=1./R
      S=S*C
160  G=D(I+1)-P
      R=(D(I)-G)*S+2.*C*B
      P=S*R
      D(I+1)=G+P
      G=C*R-B
C-----FORM VECTOR
      DO 180 K=1,N
      F=Z(K,I+1)
      Z(K,I+1)=S*Z(K,I)+C*F
      Z(K,I)=C*Z(K,I)-S*F
180  CONTINUE
200  CONTINUE
      D(L)=D(L)-P
      E(L)=G
      E(M)=0.
      GO TO 105
240  CONTINUE
C-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-N
C   SIGMA BIAS FOR SPECIAL PURPOSES:
      CALL SIGMA
C-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-NB-N
C-----ORDER EIGENVALUES AND EIGENVECTORS
      DO 300 II=2,N
      I=II-1
      K=I
      P=D(I)
      DO 260 J=II,N
      IF (D(J).GT.P) GO TO 260
      K=J

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```

      P=D(J)
260 CONTINUE
      IF (K.EQ.I) GO TO 300
      D(K)=D(I)
      D(I)=P
      DO 280 J=1,N
      P=Z(J,I)
      Z(J,I)=Z(J,K)
      Z(J,K)=P
280 CONTINUE
300 CONTINUE
      GO TO 1001
c-----SET ERROR FLAG: NO CONVERGENCE AFTER 30 ITERATIONS
1000 IERR=L
      WRITE(6,101) IERR
      101 FORMAT (' MORE THAN',I3,' IMTQL2 ITERATIONS')
1001 CONTINUE
      RETURN
      END
c#####
      SUBROUTINE SIGMA
      implicit real*8(A-H,O-Z)
c-----SHIFT ALL SIGMA MO ENERGIES BY AN AMOUNT *BIAS*
      COMMON /A/ N,NH
      COMMON /B/ EP(300),EE(300),ZC(300),ET(300),D(300)
      COMMON /C/ A(300,300),Z(300,300)
      COMMON /SBIAS/ BIAS,IPI
      IF(ABS(BIAS).LT.0.1) RETURN
      NPI=N-(N-NH)/4+1
      DO 20 MO=1,N
      SPI=0.0
      DO 10 MY=NPI,N
10 SPI=SPI+ABS(Z(MY,MO))
      IF(SPI.LT.0.1) D(MO)=D(MO)-BIAS
20 CONTINUE
      RETURN
      END
c#####
      SUBROUTINE GCCI
      implicit real*8(A-H,O-Z)
c SINGLY EXCITED CONFIGURATIONS

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c      PROGRAMMED BY H.BAUMANN
      DIMENSION X(100),Y(100),Z(100),ZS(100),INDIZ(5,300)
      EQUIVALENCE (C(1),X(1)),(C(101),Y(1)),(C(201),Z(1)),
1         (C(301),ZS(1)),(XJSL(1,1),INDIZ(1,1))
      COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
      COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
1         EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB,
2         NB,NAB
      COMMON /ZE/ N4
      COMMON /B/ ES(300),ER(300),EQ(300),SUM(300),ET(300),C(400)
1 ,GAX(300)
      COMMON /C/ ESING(300,300),U(300,300)
      COMMON /D/ XJSL(5,300),IQ(2,300),INZ(2,300),W(300)
      COMMON /MOM/ S1(300),S2(300),S3(300)
      COMMON /E/ NCYCL,EPREV,ITERR,N5
      COMMON /PIMCD/ MCD,NC,NOCC,NST,LPI(300),XP(100),
1  YP(100),BETA(5050),CPI(10000),
2  CIPI(10000),IFROM(100),ITO(100),EP(100),POCC(100)
101 FORMAT (//38X,' CONFIGURATION ENERGY',37X,'TRANSITION MOMENT')
102 FORMAT (' OCC.ORB.',8X,9HVIRT.ORB.,18X,5HIN EV,20X,5HCONF.)
120 FORMAT (5X,3HNO.,13X,3HNO.,14X,7HSINGLET,6X,7HTRIPLET,14X,3HNO.,
.      18X,2HSX,8X,2HSY,8X,2HSZ,7X,3HOSC/1X,132(1H-))
121 FORMAT (4X,I3,1X,11H ----> ,1X,I3,14X,F8.4,5X,F8.4,13X,I3,13X,
.      4F10.5)
9999 format(4f20.10)
c-----LOAD GROUND CFG. INTO IQ(*,1)
      IQ(1,1)=0
      IQ(2,1)=0
      DO 8 I=1,110
      DO 8 J=I,110
      ESING(I,J)=0.
8 ESING(J,I)=0.
      CALL LOAD(ESING,2,N5)
      CALL LOAD(U,4,N5)
      JCOUNT=1
      JCO=0
      IF (NLUMO.GT.N5.OR.NHOMO.LT.1) GO TO 21
      WRITE(6,101)
      WRITE(6,102)
      WRITE(6,120)
      IF(NHOMO.GE.NLUMO) WRITE(6,1000)

```

```

1000 FORMAT(/' GRAND CANONICAL ENSEMBLE AVERAGING PROCEDURE:'/)
      NMIN=MAX0(1,NLUMO-NB)
      NMAX=MIN0(N5,NHOMO+NAB)
      NB=NB/IDOB
      NAB=NAB/IDOB
      NMI=MAX0(2,NLUMO-NB)
      NMA=MIN0(N5-1,NHOMO+NAB)
      TEST=ABS(SUM(NMA)-SUM(NMA+1))
      IF (TEST.LT.1.E-4) NAB=NAB-1
      TEST=ABS(SUM(NMI)-SUM(NMI-1))
      IF (TEST.LT.1.E-4) NB=NB-1
      IF (NMAX.EQ.N5) GO TO 5
      TEST=ABS(SUM(NMAX)-SUM(NMAX+1))
      IF (TEST.LT.1.E-4) NMAX=NMAX-1
5     IF (NMIN.EQ.1) GO TO 6
      TEST=ABS(SUM(NMIN)-SUM(NMIN-1))
      IF (TEST.LT.1.E-4) NMIN=NMIN+1
6     CALL SHIFT(ESING,N5)
      DO 3 I=NLUMO,NMAX
      IF(LPI(I).LT.1) GO TO 3
      JJJ=0
      DO 12 JJ=NMIN,NHOMO
      J=NHOMO-JJJ
      JJJ=JJJ+1
      IF(LPI(J).LT.1) GO TO 12
      IF(I.LE.J) GOTO 12
      DOCC=OCC(J)-OCC(I)
      IF(ABS(DOCC).LE..00001) GOTO 12
      ERI=SUM(I)-SUM(J)-DOCC*H(I,I,J,J)
      ESI=ERI+DOCC*2.*H(I,J,J,I)
      JCO=JCO+1
      IF (ESI.GE.EMAX) GO TO 12
      CALL TRAMOM (SX,SY,SZ,I,J,U,X,Y,Z)
16    JCOUNT=JCOUNT+1
      ESING(JCOUNT,JCOUNT)=ESI
      IQ(1,JCOUNT)=J
      IQ(2,JCOUNT)=I
      O=.00379277*ESI*(SX*SX+SY*SY+SZ*SZ)
      S1(JCOUNT)=SX
      S2(JCOUNT)=SY
      S3(JCOUNT)=SZ

```



```

c#####
SUBROUTINE CCI(E,IQ,N)
  implicit real*8(A-H,O-Z)
c-----CONV. SINGLET GRAND CANONICAL CI-MATRIX TO CANONICAL CI-MATRIX
DIMENSION E(300,300),IQ(2,300)
INTEGER O
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
COMMON /MOM/ S1(300),S2(300),S3(300)
c-----RETURN IF NOT THE CASE OF A SINGLE HALF FILLED ORBITAL
IF(NHOMO.NE.NLUMO) RETURN
WRITE(6,1000)
1000 FORMAT(/' CANONICAL ENSEMBLE AVERAGING PROCEDURE: '/')
O=NHOMO
DO 20 J=2,N
L =IQ(1,J)
K =IQ(2,J)
OCCLK=OCC(L)-OCC(K)
DO 10 I=2,J
L1=IQ(1,I)
K1=IQ(2,I)
C = 0.0
IF( L .EQ.O .AND. L1.EQ.O ) C = C - H(K1,O,O,K)
IF( K .EQ.O .AND. K1.EQ.O ) C = C - H(L1,O,O,L)
IF( L1.EQ.O .AND. K .EQ.O ) C = C + H(L,O,K1,O)
IF( K1.EQ.O .AND. L .EQ.O ) C = C + H(K,O,L1,O)
10 E(I,J)=E(I,J)+0.25*C/SQRT(OCCLK*(OCC(L1)-OCC(K1)))
OSC=0.00379277*E(J,J)*(S1(J)**2+S2(J)**2+S3(J)**2)
20 WRITE(6,2000) L,K,E(J,J),J,S1(J),S2(J),S3(J),OSC
2000 FORMAT(4X,I3,' ----> ',I3,14X,F8.4,26X,I3,13X,4F10.5)
RETURN
END
c#####
SUBROUTINE TRAMOM(SX,SY,SZ,I,J,U,X,Y,Z)
  implicit real*8(A-H,O-Z)
c PROGRAMMED BY H.BAUMANN
c TRANSITION MOMENT BETWEEN GROUND CFG. AND SINGLY EXC. CFG. J->I
c-----MODIFIED TO INCLUDE SP-TERMS BY JS-L
DIMENSION X(100),Y(100),Z(100),U(300,300)
COMMON /A/ N,NH,NE,NQ,ECORE,ICOUNT,JCOUNT,EMAX,IPRNT,IGCCI,
1 EATOM,ISCF,ITGT,ICI,GAH,ITRIP,IPEN,ETOT,ETOT1,IDOB
COMMON /E/ NCYCL,EPREV,ITERR,N5,NT,N2S

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```

COMMON /SPTERM/ SP(100)
COMMON /OCCDAT/ NHOMO,NLUMO,NPE,NPMO,OCC(300)
FACTOR=4.8033*SQRT(2.)
SX=0.
SY=0.
SZ=0.
IF (1.GT.NH) GO TO 16
DO 14 K=1,NH
UIJ=U(K,I)*U(K,J)
SX=SX+UIJ*X(K)
SY=SY+UIJ*Y(K)
SZ=SZ+UIJ*Z(K)
14 CONTINUE
16 IF (1.GT.N) GO TO 17
DO 15 NMULT=1,4
DO 15 K=N2S,NT
KK=K+N*(NMULT-1)
UIJ=U(KK,I)*U(KK,J)
SX=SX+UIJ*X(K)
SY=SY+UIJ*Y(K)
SZ=SZ+UIJ*Z(K)
15 CONTINUE
C-----ADD SP-CONTRIBUTIONS
DO 99 IN=1,N
NS=NH+IN
NPX=NS+N
NPY=NPX+N
NPZ=NPY+N
USI=U(NS,I)
USJ=U(NS,J)
SPN=SP(NS)
SX=SX + (USI*U(NPX,J)+USJ*U(NPX,I)) * SPN
SY=SY + (USI*U(NPY,J)+USJ*U(NPY,I)) * SPN
99 SZ=SZ + (USI*U(NPZ,J)+USJ*U(NPZ,I)) * SPN
17 FAC=SQRT(OCC(J)-OCC(I))*FACTOR
SX=SX*FAC
SY=SY*FAC
SZ=SZ*FAC
RETURN
END
C#####

```

```

SUBROUTINE MCDB(IFLAG)
  implicit real*8(A-H,O-Z)
  COMMON /PIMCD/ MCD,N,NOCC,NST,LPI(300),X(100),Y(100),BETA(5050),
1  C(10000),CI(10000),FROM(100),TO(100),E(100),OCC(100)
  LOGICAL P(5)
  INTEGER FROM,TO
  EXTERNAL MATPRT
  IF(MCD.LT.0) RETURN
  DO 10 I=1,5
10  P(I)=.FALSE.
  IF(IFLAG.EQ.2) GOTO 100
  DO 15 I=1,MCD
15  P(6-I)=.TRUE.
  WRITE(6,1000)
1000 FORMAT(/' -----',
.         /' CALCULATION OF MCD B TERMS FOR PI-PI* TRANSITIONS',
.         /' -----',
.         //' PI MOLECULAR ORBITAL COEFFICIENTS')
  CALL MATPRT(C,N,0)
  WRITE(6,1500) (OCC(I),I=1,N)
1500 FORMAT(1X//' OCCUPATION NUMBERS'//5X,16F8.4)
  WRITE(6,2000)
2000 FORMAT(1X//' PI TYPE BETA MATRIX FOR MAGNETIC DIPOLE INTEGRALS')
  CALL MATPRT(BETA,N,1)
  100 CALL BTERM(N,NOCC,NST,X,Y,BETA,C,CI,FROM,TO,E,MATPRT,P,OCC)
  RETURN
  END
c#####
c  SUBROUTINE BTERM(N,NOCC,NST,X,Y,BETA,C,CI,FROM,TO,E,MATPRT,P,OCC)
c  Adapted from Computer Program BTERM, QCPE Bull. 1, 37 (1981).
c  This routine was originally developed for use with a
c  PPP program operating with one-dimensional arrays. (JS-L)
  implicit real*8(A-H,O-Z)
  LOGICAL P(5)
  INTEGER FROM(1),TO(1),F,FI,FF,GF
  DIMENSION X(1),Y(1),BETA(1),C(1),CI(1),E(1),OCC(1),
1  DEXMO(1),DEYMO(1),DMZMO(1),DEXCFG(1),DEYCFG(1),DMZAO(1),
1  AXI(1),AYI(1)
  COMMON/C/ INDEX(100,100),BG(10000),BF(10000),B(100),AI(100),
1  AZI(100),SBG(100),SBF(100),DEXST(5050),DEYST(5050),
1  DMZST(5050),DMZCFG(5050)

```

```

EQUIVALENCE (DEXST(1),DEXMO(1)),(DEYST(1),DEYMO(1)),
.      (DMZST(1),DMZMO(1)),(BG(1),DEXCFG(1)),(BF(1),DEYCFG(1)),
.      (DMZCFG(1),DMZAO(1)),(SBG(1),AXI(1)),(SBF(1),AYI(1))
DATA F1/0.13124/,F2/4.8033/,F3/8.0658/,F4/0.00379277/
S(I,J)=SIGN(1.,FLOAT(I-J))
PI180 = 3.141592654/180.0
IF(N.GT.100.OR.NST.GT.100)GOTO 260
MAX=MAX0(N,NST)
DO 10 J=1,MAX
DO 10 I=1,J
INDEX(I,J)=I+(J*(J-1))/2
10 INDEX(J,I)=INDEX(I,J)
SQR2=SQRT(2.0)

```

```

C-----
C  ELEMENTS OF MAGNETIC DIPOLE MOMENT OPERATOR OVER AO*S, Z-COMPONENT
C  (ACCORDING TO LINDERBERG*S FORMULA)
C-----

```

```

MYNY=0
DO 20 MY=1,N
      DO 20 NY=1,MY
            MYNY=MYNY+1
20      DMZAO(MYNY)=-BETA(MYNY)*(X(MY)*Y(NY)-X(NY)*Y(MY))*F1
      IF(P(1)) WRITE(6,1000)
1000 FORMAT(//'Z-COMPONENT OF MAGNETIC DIPOLE OPERATOR',
.          /' IN AO BASIS (BOHR-MAGNETONS)')
      IF(P(1)) CALL MATPRT(DMZAO,N,1)

```

```

C-----
C  ELEMENTS OF DIPOLE OPERATORS OVER MO*S
C  (ELECTRIC DIPOLE OPERATOR ACCORDING TO DIPOLE LENGTH EXPRESSION)
C-----

```

```

DO 70 I=1,N
      II=N*(I-1)
      DO 40 NY=1,N
            A=0.0
            DO 30 MY=1,N
                  MYNY=INDEX(MY,NY)
30      A=A+DMZAO(MYNY)*S(MY,NY)*C(MY+II)
40      AI(NY)=A
      DO 60 J=1,I
            JJ=N*(J-1)
            AX=0.0

```

```

        AY=0.0
        AZ=0.0
        DO 50 MY=1,N
            CC=C(MY+II)*C(MY+JJ)
            AX=AX-CC*X(MY)
            AY=AY-CC*Y(MY)
50          AZ=AZ+C(MY+JJ)*AI(MY)
            JI=INDEX(J,I)
            DEXMO(JI)=AX * F2
            DEYMO(JI)=AY * F2
60          DMZMO(JI)=AZ
70          CONTINUE
            IF(P(2)) WRITE(6,1100)
1100        FORMAT(//'X-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.            /' IN MO BASIS (DEBYES)')
            IF(P(2)) CALL MATPRT(DEXMO,N,1)
            IF(P(2)) WRITE(6,1200)
1200        FORMAT(//' Y-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.            /' IN MO BASIS (DEBYES)')
            IF(P(2)) CALL MATPRT(DEYMO,N,1)
            IF(P(2)) WRITE(6,1300)
1300        FORMAT(//' Z-COMPONENT OF MAGNETIC DIPOLE OPERATOR'
.            /' IN MO BASIS (BOHR-MAGNETONS)')
            IF(P(2)) CALL MATPRT(DMZMO,N,1)
C-----
C  ELEMENTS OF DIPOLE OPERATORS OVER GROUND AND SINGLY EXCITED
C  CONFIGURATIONS (AS DEFINED BY THE LISTS *FROM* AND *TO*)
C-----
        DO 150 I=1,NST
            I1=FROM(I)
            I2=TO(I)
            DO 150 J=1,I
                IF(J.LT.I) GO TO 110
C-----DIAGONAL ELEMENTS
                IF(J.GT.1) GO TO 90
C- - -GROUND CONFIGURATION
                DEXCFG(1)=0.0
                DEYCFG(1)=0.0
                DMZCFG(1)=0.0
                DO 80 K=1,NOCC
                    KK=INDEX(K,K)

```

```

      DEXCFG(1)=DEXCFG(1)+2.0*DEXMO(KK)*OCC(K)
80      DEYCFG(1)=DEYCFG(1)+2.0*DEYMO(KK)*OCC(K)
      GO TO 150
c- - -EXCITED CONFIGURATION
90      II=INDEX(I,I)
      I1I1=INDEX(I1,I1)
      I2I2=INDEX(I2,I2)
      DEXCFG(II)=DEXCFG(1)-DEXMO(I1I1)+DEXMO(I2I2)
      DEYCFG(II)=DEYCFG(1)-DEYMO(I1I1)+DEYMO(I2I2)
100     DMZCFG(II)=.0
      GO TO 150
c-----OFF-DIAGONAL ELEMENTS
110     IF(J.GT.1) GO TO 120
c- - -EXCITED CONFIGURATION / GROUND CONFIGURATION
      I1I2=INDEX(I1,I2)
      AX=SQR2*DEXMO(I1I2)
      AY=SQR2*DEYMO(I1I2)
      AZ=SQR2*DMZMO(I1I2)
      GO TO 140
c- - -EXCITED CONFIGURATION / EXCITED CONFIGURATION
120     J1=FROM(J)
      J2=TO(J)
      AX=.0
      AY=.0
      AZ=.0
      IF(I1.NE.J1) GO TO 130
      I2J2=INDEX(I2,J2)
      AX=DEXMO(I2J2)
      AY=DEYMO(I2J2)
      AZ=DMZMO(I2J2)*S(I2,J2)
      GO TO 140
130     IF(I2.NE.J2) GO TO 140
      J1I1=INDEX(J1,I1)
      AX=-DEXMO(J1I1)
      AY=-DEYMO(J1I1)
      AZ=-DMZMO(J1I1)*S(J1,I1)
140     IJ=INDEX(I,J)
      DEXCFG(IJ)=AX
      DEYCFG(IJ)=AY
      DMZCFG(IJ)=AZ
150     CONTINUE

```

```

      IF(P(3)) WRITE(6,1400)
1400 FORMAT(//'X-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.         /' IN CONFIGURATION BASIS (DEBYES)')
      IF(P(3)) CALL MATPRT(DEXCFG,NST,1)
      IF(P(3)) WRITE(6,1500)
1500 FORMAT(//' Y-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.         /' IN CONFIGURATION BASIS (DEBYES)')
      IF(P(3)) CALL MATPRT(DEYCFG,NST,1)
      IF(P(3)) WRITE(6,1600)
1600 FORMAT(//' Z-COMPONENT OF MAGNETIC DIPOLE OPERATOR',
.         /' IN CONFIGURATION BASIS (BOHR-MAGNETONS)')
      IF(P(3)) CALL MATPRT(DMZCFG,NST,1)

```

```

c-----
c  ELEMENTS OF DIPOLE OPERATORS OVER CI-STATES
c-----

```

```

      DO 190 I=1,NST
          II=NST*(I-1)
          DO 170 L=1,NST
              AX=.0
              AY=.0
              AZ=.0
              DO 160 K=1,NST
                  KL=INDEX(K,L)
                  AX=AX+DEXCFG(KL)*CI(K+II)
                  AY=AY+DEYCFG(KL)*CI(K+II)
160                 AZ=AZ+DMZCFG(KL)*S(K,L)*CI(K+II)
                  AXI(L)=AX
                  AYI(L)=AY
170                 AZI(L)=AZ
              DO 190 J=1,I
                  JJ=NST*(J-1)
                  AX=.0
                  AY=.0
                  AZ=.0
                  DO 180 L=1,NST
                      AX=AX+CI(L+JJ)*AXI(L)
                      AY=AY+CI(L+JJ)*AYI(L)
180                     AZ=AZ+CI(L+JJ)*AZI(L)
                  IJ=INDEX(I,J)
                  DEXST(IJ)=AX
                  DEYST(IJ)=AY

```

```

          DMZST(IJ)=AZ
190          CONTINUE
          IF(P(4)) WRITE(6,1700)
1700 FORMAT(//'X-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.           /' IN STATE BASIS (DEBYES)')
          IF(P(4)) CALL MATPRT(DEXST,NST,1)
          IF(P(4)) WRITE(6,1800)
1800 FORMAT(//' Y-COMPONENT OF ELECTRIC DIPOLE OPERATOR',
.           /' IN STATE BASIS (DEBYES)')
          IF(P(4)) CALL MATPRT(DEYST,NST,1)
          IF(P(4)) WRITE(6,1900)
1900 FORMAT(//' Z-COMPONENT OF MAGNETIC DIPOLE OPERATOR',
.           /' IN STATE BASIS (BOHR-MAGNETONS)')
          IF(P(4)) CALL MATPRT(DMZST,NST,1)
C-----
C  EXPANSION OF B-TERMS  B(F) = SUMMA(I) ( BG(I,F) + BF(I,F) )
C-----
          DO 240 F=1,NST
              FF=NST*(F-1)
              GF=INDEX(1,F)
              SBG(F)=.0
              SBF(F)=.0
              DO 230 I=1,NST
                  FI=INDEX(F,I)
                  IG=INDEX(I,1)
C- - -CONTRIBUTION DUE TO MIXING OF I*TH STATE WITH GROUND STATE
                  IF(I.NE.1) GO TO 200
                  BG(1+FF)=.0
                  GO TO 210
200                  EIE1=E(I)-E(1)
                  IF(ABS(EIE1).LT.0.000001) GOTO 270
                  BG(I+FF)= DMZST(IG)
.                   * (DEXST(GF)*DEYST(FI)-DEXST(FI)*DEYST(GF))
.                   / ( EI E1 * F3)
                  SBG(F)=SBG(F)+BG(I+FF)
C- - -CONTRIBUTION DUE TO MIXING OF I*TH STATE WITH EXC.STATE F
210                  IF(I.NE.F) GO TO 220
                  BF(F+FF)=.0
                  GO TO 230
220                  EIEF=E(I)-E(F)
                  IF(ABS(EIEF).LT.0.000001) GOTO 270

```

```

          BF(I+FF) = DMZST(FI) * S(F, I)
          * (DEXST(GF) * DEYST(IG) - DEXST(IG) * DEYST(GF))
          / ( EI EF * F3)
          SBF(F) = SBF(F) + BF(I+FF)
230      CONTINUE
240      B(F) = SBG(F) + SBF(F)
          IF(P(5)) WRITE(6,2000)
2000     FORMAT(// ' CONTRIBUTIONS TO MCD B-TERMS B(F) DUE TO MIXING',
          .      ' OF I''TH STATE WITH GROUNDSTATE'/' I/F')
          IF(P(5)) CALL MATPRT(BG, NST, 0)
          IF(P(5)) WRITE(6,2100)
2100     FORMAT(// ' CONTRIBUTIONS TO MCD B-TERMS B(F) DUE TO MIXING',
          .      ' OF I''TH STATE WITH F''TH STATE'/' I/F')
          IF(P(5)) CALL MATPRT(BF, NST, 0)
C-----PRINT B-TERMS
          WRITE(6,2200)
2200     FORMAT(// ' WAVENUMBERS IN KK = 1000CM-1, '/
          .      ' MCD B-TERMS IN (BOHR-MAGNETON DEBYE**2)/KK, '/
          .      ' ELECTRIC TRANSITION MOMENTS IN DEBYES'/'
          .      ' TRANSITION MOMENT ANGLES IN DEG'/'
          .      ' OSCILLATOR STRENGTHS OSC'//
          .      ' F      W      BG      +      BF      =      B      M(X) ',
          .      '      M(Y)      PHI(X-->Y)      OSC'/1X,100(' - '))
          DO 250 F=2, NST
              GF=INDEX(1, F)
              W= F3 * (E(F)-E(1))
              DE2= DEXST(GF)**2 + DEYST(GF)**2
              O= F4 * (E(F)-E(1)) * DE2
              PHI= 0.0
              IF ( SQRT(DE2) .LE. 0.00001 ) GOTO 250
              PHI= 90.0
              IF ( ABS(DEXST(GF)) .LE. 0.0000001 ) GOTO 250
              PHI= ATAN(DEYST(GF)/DEXST(GF)) / PI180
          250      WRITE(6,2500) F, W, SBG(F), SBF(F), B(F), DEXST(GF),
          .          DEYST(GF), PHI, O
          2500     FORMAT(1X, I3, F8.3, 65F12.6)
C-----PLOT SPECTRUM WITH INDICATION OF MCD B-SIGNS
          CALL SPRT1(1, B)
          RETURN
C-----
C   TROUBLE SECTION

```



```

C-----
  260 WRITE(6,3000) N,NST
 3000 FORMAT(1X// ' N =', I3, ', NST=', I3,
.          /' DIMENSIONS TOO LARGE FOR SUBROUTINE BTERM',
.          /' RECOMPILE WITH APPROPRIATE ARRAY DIMENSIONS'/1H1)
      RETURN
  270 WRITE(6,4000) I,F
 4000 FORMAT(1X// ' TERMINATION DUE TO NEAR DEGENERACY OF STATES NO.',
.          I3, ' AND', I3/1H1)
      RETURN
      END
C#####
      SUBROUTINE MATPRT(A,N,MS)
      implicit real*8(A-H,O-Z)
C-----
C   PRINT N * N MATRIX  A,  STORAGE MODE MS ( 0 OR 1 )
C-----
      DIMENSION A(1)
      DATA LINE/4H----/
      DO 20 J1=1,N,16
          J2=MIN0(N,J1+15)
          WRITE(6,1000) (J,J=J1,J2)
          WRITE(6,1500) ((LINE,L=1,2),J=J1,J2)
          I1=1
          IF(MS.EQ.1) I1=J1
          DO 20 I=I1,N
              IF(MS.EQ.1) GO TO 10
              K1=N*(J1-1)+I
              K2=N*(J2-1)+I
              WRITE(6,2000) I, (A(K),K=K1,K2,N)
              GO TO 20
10          II=I*(I-1)/2
              K1=II+I1
              K2=II+MIN0(I,J2)
              WRITE(6,2000) I, (A(K),K=K1,K2)
20          CONTINUE
1000 FORMAT(/16(5X,I3))
1500 FORMAT(1X,4H----,16(2A4))
2000 FORMAT(I4,16F8.4)
      RETURN
      END

```

### Sample input

TERRYLENE, 15pi x 15pi\* CIS

```
0 0 0 1 0 0 . . . . .
1 -1.182756 -3.352135 0.000000
1 -1.182739 3.352136 0.000000
1 1.182756 -3.352135 0.000000
1 1.182739 3.352136 0.000000
1 -6.798507 -1.212935 0.000000
1 -6.798468 1.213008 0.000000
1 6.798507 -1.212935 0.000000
1 6.798468 1.213008 0.000000
1 -3.170793 -3.361339 0.000000
1 -3.170708 3.361325 0.000000
1 3.170793 -3.361339 0.000000
1 3.170708 3.361325 0.000000
1 -5.582218 -3.334393 0.000000
1 -5.582117 3.334435 0.000000
1 5.582218 -3.334393 0.000000
1 5.582117 3.334435 0.000000
6 0.710472 0.000000 0.000000
6 -0.710472 0.000000 0.000000
6 -1.427097 -1.218037 0.000000
6 -1.427064 1.218042 0.000000
6 1.427097 -1.218037 0.000000
6 1.427064 1.218042 0.000000
6 -0.699663 -2.421796 0.000000
6 -0.699657 2.421764 0.000000
6 0.699663 -2.421796 0.000000
6 0.699657 2.421764 0.000000
6 -2.914267 -1.224578 0.000000
6 -2.914284 1.224552 0.000000
6 2.914267 -1.224578 0.000000
6 2.914284 1.224552 0.000000
6 -3.617841 0.000000 0.000000
6 3.617841 0.000000 0.000000
6 -5.032374 0.000000 0.000000
6 5.032374 0.000000 0.000000
6 -5.747035 -1.209951 0.000000
6 -5.747016 1.209973 0.000000
6 5.747035 -1.209951 0.000000
6 5.747016 1.209973 0.000000
6 -3.650575 -2.429048 0.000000
6 -3.650512 2.429009 0.000000
6 3.650575 -2.429048 0.000000
6 3.650512 2.429009 0.000000
6 -5.053112 -2.426264 0.000000
6 -5.053026 2.426326 0.000000
6 5.053112 -2.426264 0.000000
6 5.053026 2.426326 0.000000
. . . . .
1 90 90 0 0 1 20.
```

## Sample output

>-----<  
L C O A O  
>-----<

"Linear Combination of Orthogonalized Atomic Orbitals"

J. Spanget-Larsen: Theor. Chem. Acc. 59, 137 (1997)

100 atoms - 300 orbitals development-vs.

Dec. 2005

-----BKVH--

TERRYLENE, 15pi x 15pi\* CIS

N=30 NH=16 NE=136 NPE= 0 NPMO= 0 IPI= 1 IPRNT= 0 NMOP=32

PP(PI)= 0.750 PP(SIG)= 1.000 PS= 1.000 SS= 1.000 D(PI)= 0.230 D(SIG)= 0.230

XG= 1.000 PEN(SS)= 0.500 PEN(SP)= 0.500 PEN(PP)= 1.500

PRM. FOR MAGN. DIPOLE INTEGRALS: PP(PI)= 1.500 FD= 0.000

SIGMA ORBITAL 'BIAS': 0.000 ZDAT(2): 0.000

I	X	Y	Z	N (Z)	EXP	X (S)	X (P)	BETA (S)	BETA (P)	GAMMA
1	-1.182756	-3.352135	0.000000	1	1.200	-7.175		-7.175		12.850
2	-1.182739	3.352136	0.000000	1	1.200	-7.175		-7.175		12.850
3	1.182756	-3.352135	0.000000	1	1.200	-7.175		-7.175		12.850
4	1.182739	3.352136	0.000000	1	1.200	-7.175		-7.175		12.850
5	-6.798507	-1.212935	0.000000	1	1.200	-7.175		-7.175		12.850
6	-6.798468	1.213008	0.000000	1	1.200	-7.175		-7.175		12.850
7	6.798507	-1.212935	0.000000	1	1.200	-7.175		-7.175		12.850
8	6.798468	1.213008	0.000000	1	1.200	-7.175		-7.175		12.850
9	-3.170793	-3.361339	0.000000	1	1.200	-7.175		-7.175		12.850
10	-3.170708	3.361325	0.000000	1	1.200	-7.175		-7.175		12.850
11	3.170793	-3.361339	0.000000	1	1.200	-7.175		-7.175		12.850
12	3.170708	3.361325	0.000000	1	1.200	-7.175		-7.175		12.850
13	-5.582218	-3.334393	0.000000	1	1.200	-7.175		-7.175		12.850
14	-5.582117	3.334435	0.000000	1	1.200	-7.175		-7.175		12.850
15	5.582218	-3.334393	0.000000	1	1.200	-7.175		-7.175		12.850
16	5.582117	3.334435	0.000000	1	1.200	-7.175		-7.175		12.850
17	0.710472	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
18	-0.710472	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
19	-1.427097	-1.218037	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
20	-1.427064	1.218042	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
21	1.427097	-1.218037	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
22	1.427064	1.218042	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
23	-0.699663	-2.421796	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
24	-0.699657	2.421764	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930

25	0.699663	-2.421796	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
26	0.699657	2.421764	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
27	-2.914267	-1.224578	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
28	-2.914284	1.224552	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
29	2.914267	-1.224578	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
30	2.914284	1.224552	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
31	-3.617841	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
32	3.617841	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
33	-5.032374	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
34	5.032374	0.000000	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
35	-5.747035	-1.209951	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
36	-5.747016	1.209973	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
37	5.747035	-1.209951	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
38	5.747016	1.209973	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
39	-3.650575	-2.429048	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
40	-3.650512	2.429009	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
41	3.650575	-2.429048	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
42	3.650512	2.429009	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
43	-5.053112	-2.426264	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
44	-5.053026	2.426326	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
45	5.053112	-2.426264	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930
46	5.053026	2.426326	0.000000	6	1.625	-14.960	-5.805	-14.960	-5.805	10.930

INTERATOMIC DISTANCES (ANGSTROM)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0.0000															
2	6.7043	0.0000														
3	2.3655	7.1093	0.0000													
4	7.1093	2.3655	6.7043	0.0000												
5	6.0094	7.2372	8.2630	9.1946	0.0000											
6	7.2372	6.0093	9.1946	8.2629	2.4259	0.0000										
7	8.2630	9.1946	6.0094	7.2372	13.5970	13.8117	0.0000									
8	9.1946	8.2629	7.2372	6.0093	13.8117	13.5969	2.4259	0.0000								
9	1.9881	7.0017	4.3536	8.0015	4.2162	5.8382	10.1982	10.9686	0.0000							
10	7.0016	1.9880	8.0014	4.3535	5.8382	4.2161	10.9686	10.1980	6.7227	0.0000						
11	4.3536	8.0015	1.9881	7.0017	10.1982	10.9686	4.2162	5.8382	6.3416	9.2417	0.0000					
12	8.0014	4.3535	7.0016	1.9880	10.9686	10.1980	5.8382	4.2161	9.2417	6.3414	6.7227	0.0000				
13	4.3995	8.0041	6.7650	9.5118	2.4454	4.7072	12.5612	13.1894	2.4116	7.1167	8.7531	11.0203	0.0000			
14	8.0040	4.3994	9.5118	6.7649	4.7072	2.4454	13.1893	12.5610	7.1167	2.4116	11.0203	8.7529	6.6688	0.0000		
15	6.7650	9.5118	4.3995	8.0041	12.5612	13.1894	2.4454	4.7072	8.7531	11.0203	2.4116	7.1167	11.1644	13.0044	0.0000	
16	9.5118	6.7649	8.0040	4.3994	13.1893	12.5610	4.7072	2.4454	11.0203	8.7529	7.1167	2.4116	13.0044	11.1642	6.6688	0.0000
17	3.8498	3.8498	3.3852	3.3852	7.6063	7.6063	6.2077	6.2077	5.1345	5.1344	4.1655	4.1655	7.1215	7.1215	5.9036	5.9035
18	3.3852	3.3852	3.8498	3.8498	6.2077	6.2077	7.6063	7.6063	4.1655	4.1655	5.1345	5.1344	5.9036	5.9035	7.1215	7.1215
19	2.1480	4.5767	3.3713	5.2629	5.3714	5.8959	8.2256	8.5773	2.7630	4.9001	5.0729	6.4893	4.6630	6.1635	7.3218	8.3579
20	4.5767	2.1480	5.2629	3.3713	5.8959	5.3714	8.5773	8.2255	4.9001	2.7630	6.4893	5.0728	6.1636	4.6630	8.3579	7.3217
21	3.3713	5.2629	2.1480	4.5767	8.2256	8.5773	5.3714	5.8959	5.0729	6.4893	2.7630	4.9001	7.3218	8.3579	4.6630	6.1635
22	5.2629	3.3713	4.5767	2.1480	8.5773	8.2255	5.8959	5.3714	6.4893	5.0728	4.9001	2.7630	8.3579	7.3217	6.1636	4.6630
23	1.0483	5.7941	2.0998	6.0730	6.2175	7.0998	7.5950	8.3327	2.6437	6.2889	3.9829	6.9588	4.9671	7.5480	6.3478	8.5203

24	5.7941	1.0483	6.0730	2.0998	7.0998	6.2174	8.3327	7.5949	6.2889	2.6436	6.9588	3.9828	7.5480	4.9670	8.5203	6.3477
25	2.0998	6.0730	1.0483	5.7941	7.5950	8.3327	6.2175	7.0998	3.9829	6.9588	2.6437	6.2889	6.3478	8.5203	4.9671	7.5480
26	6.0730	2.0998	5.7941	1.0483	8.3327	7.5949	7.0998	6.2174	6.9588	3.9828	6.2889	2.6436	8.5203	6.3477	7.5480	4.9670
27	2.7431	4.8933	4.6165	6.1426	3.8843	4.5857	9.7128	10.0139	2.1521	4.5931	6.4493	7.6195	3.4014	5.2822	8.7545	9.6423
28	4.8933	2.7431	6.1426	4.6165	4.5857	3.8842	10.0140	9.7128	4.5931	2.1521	7.6196	6.4493	5.2822	3.4013	9.6423	8.7545
29	4.6165	6.1426	2.7431	4.8933	9.7128	10.0139	3.8843	4.5857	6.4493	7.6195	2.1521	4.5931	8.7545	9.6423	3.4014	5.2822
30	6.1426	4.6165	4.8933	2.7431	10.0140	9.7128	4.5857	3.8842	7.6196	6.4493	4.5931	2.1521	9.6423	8.7545	5.2822	3.4013
31	4.1432	4.1433	5.8551	5.8551	3.4041	3.4041	10.4867	10.4867	3.3909	3.3909	7.5752	7.5752	3.8700	3.8700	9.7857	9.7856
32	5.8551	5.8551	4.1432	4.1433	10.4867	10.4867	3.4041	3.4041	7.5752	7.5752	3.3909	3.3909	9.7857	9.7856	3.8700	3.8700
33	5.1045	5.1046	7.0615	7.0615	2.1425	2.1425	11.8929	11.8929	3.8424	3.8424	8.8651	8.8650	3.3794	3.3794	11.1260	11.1259
34	7.0615	7.0615	5.1045	5.1046	11.8929	11.8929	2.1425	2.1425	8.8651	8.8650	3.8424	3.8424	11.1260	11.1259	3.3794	3.3794
35	5.0420	6.4533	7.2533	8.2967	1.0515	2.6413	12.5455	12.7773	3.3564	5.2473	9.1737	10.0211	2.1308	4.5474	11.5267	12.2066
36	6.4533	5.0420	8.2967	7.2533	2.6412	1.0515	12.7773	12.5455	5.2473	3.3564	10.0212	9.1736	4.5474	2.1309	12.2067	11.5266
37	7.2533	8.2967	5.0420	6.4533	12.5455	12.7773	1.0515	2.6413	9.1737	10.0211	3.3564	5.2473	11.5267	12.2066	2.1308	4.5474
38	8.2967	7.2533	6.4533	5.0420	12.7773	12.5455	2.6412	1.0515	10.0212	9.1736	5.2473	3.3564	12.2067	11.5266	4.5474	2.1309
39	2.6348	6.2859	4.9207	7.5355	3.3747	4.8139	10.5196	11.0656	1.0485	5.8102	6.8848	8.9475	2.1333	6.0785	9.2771	10.8839
40	6.2858	2.6348	7.5354	4.9206	4.8139	3.3747	11.0655	10.5195	5.8102	1.0485	8.9475	6.8846	6.0785	2.1333	10.8839	9.2769
41	4.9207	7.5355	2.6348	6.2859	10.5196	11.0656	3.3747	4.8139	6.8848	8.9475	1.0485	5.8102	9.2771	10.8839	2.1333	6.0785
42	7.5354	4.9206	6.2858	2.6348	11.0655	10.5195	4.8139	3.3747	8.9475	6.8846	5.8102	1.0485	10.8839	9.2769	6.0785	2.1333
43	3.9796	6.9548	6.3042	8.5015	2.1257	4.0362	11.9136	12.3978	2.1018	6.0860	8.2769	10.0562	1.0510	5.7849	10.6740	12.0952
44	6.9548	3.9795	8.5015	6.3041	4.0362	2.1257	12.3977	11.9134	6.0860	2.1017	10.0563	8.2767	5.7850	1.0510	12.0952	10.6738
45	6.3042	8.5015	3.9796	6.9548	11.9136	12.3978	2.1257	4.0362	8.2769	10.0562	2.1018	6.0860	10.6740	12.0952	1.0510	5.7849
46	8.5015	6.3041	6.9548	3.9795	12.3977	11.9134	4.0362	2.1257	10.0563	8.2767	6.0860	2.1017	12.0952	10.6738	5.7850	1.0510

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17	0.0000															
18	1.4209	0.0000														
19	2.4602	1.4132	0.0000													
20	2.4602	1.4132	2.4361	0.0000												
21	1.4132	2.4602	2.8542	3.7524	0.0000											
22	1.4132	2.4602	3.7524	2.8541	2.4361	0.0000										
23	2.8024	2.4218	1.4065	3.7118	2.4438	4.2156	0.0000									
24	2.8024	2.4218	3.7118	1.4064	4.2156	2.4437	4.8436	0.0000								
25	2.4218	2.8024	2.4438	4.2156	1.4065	3.7118	1.3993	5.0416	0.0000							
26	2.4218	2.8024	4.2156	2.4437	3.7118	1.4064	5.0416	1.3993	4.8436	0.0000						
27	3.8260	2.5212	1.4872	2.8597	4.3414	4.9813	2.5175	4.2662	3.8071	5.1338	0.0000					
28	3.8260	2.5212	2.8597	1.4872	4.9813	4.3414	4.2662	2.5175	5.1339	3.8071	2.4491	0.0000				
29	2.5212	3.8260	4.3414	4.9813	1.4872	2.8597	3.8071	5.1338	2.5175	4.2662	5.8285	6.3222	0.0000			
30	2.5212	3.8260	4.9813	4.3414	2.8597	1.4872	5.1339	3.8071	4.2662	2.5175	6.3222	5.8286	2.4491	0.0000		
31	4.3283	2.9074	2.5066	2.5066	5.1899	5.1899	3.7922	3.7922	4.9503	4.9503	1.4123	1.4123	6.6459	6.6459	0.0000	
32	2.9074	4.3283	5.1899	5.1899	2.5066	2.5066	4.9503	4.9503	3.7922	3.7922	6.6459	6.6459	1.4123	1.4123	7.2357	0.0000
33	5.7428	4.3219	3.8055	3.8055	6.5733	6.5733	4.9636	4.9636	6.2226	6.2226	2.4466	2.4466	8.0404	8.0405	1.4145	8.6502
34	4.3219	5.7428	6.5733	6.5733	3.8055	3.8055	6.2226	6.2226	4.9636	4.9636	8.0404	8.0405	2.4466	2.4466	8.6502	1.4145
35	6.5699	5.1799	4.3199	4.9555	7.1741	7.5738	5.1908	6.2181	6.5596	7.3993	2.8328	3.7351	8.6613	8.9970	2.4490	9.4427
36	6.5699	5.1798	4.9555	4.3200	7.5738	7.1741	6.2182	5.1908	7.3993	6.5596	3.7352	2.8328	8.9969	8.6613	2.4490	9.4427
37	5.1799	6.5699	7.1741	7.5738	4.3199	4.9555	6.5596	7.3993	5.1908	6.2181	8.6613	8.9970	2.8328	3.7351	9.4427	2.4490
38	5.1798	6.5699	7.5738	7.1741	4.9555	4.3200	7.3993	6.5596	6.2182	5.1908	8.9969	8.6613	3.7352	2.8328	9.4427	2.4490
39	4.9919	3.8137	2.5319	4.2714	5.2201	6.2517	2.9509	5.6779	4.3502	6.5157	1.4117	3.7271	6.6744	7.5131	2.4293	7.6636
40	4.9918	3.8136	4.2714	2.5318	6.2516	5.2200	5.6778	2.9509	6.5157	4.3502	3.7270	1.4116	7.5130	6.6744	2.4292	7.6635
41	3.8137	4.9919	5.2201	6.2517	2.5319	4.2714	4.3502	6.5157	2.9509	5.6779	6.6744	7.5131	1.4117	3.7271	7.6636	2.4293

42	3.8136	4.9918	6.2516	5.2200	4.2714	2.5318	6.5157	4.3502	5.6778	2.9509	7.5130	6.6744	3.7270	1.4116	7.6635	2.4292
43	6.2535	4.9745	3.8220	5.1409	6.5919	7.4346	4.3535	6.5158	5.7528	7.5231	2.4533	4.2312	8.0575	8.7640	2.8190	9.0040
44	6.2534	4.9744	5.1409	3.8220	7.4346	6.5918	6.5158	4.3534	7.5231	5.7527	4.2312	2.4533	8.7640	8.0574	2.8190	9.0039
45	4.9745	6.2535	6.5919	7.4346	3.8220	5.1409	5.7528	7.5231	4.3535	6.5158	8.0575	8.7640	2.4533	4.2312	9.0040	2.8190
46	4.9744	6.2534	7.4346	6.5918	5.1409	3.8220	7.5231	5.7527	6.5158	4.3534	8.7640	8.0574	4.2312	2.4533	9.0039	2.8190

33	34	35	36	37	38	39	40	41	42	43	44	45	46
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33	0.0000															
34	10.0647	0.0000														
35	1.4052	10.8471	0.0000													
36	1.4053	10.8471	2.4199	0.0000												
37	10.8471	1.4052	11.4941	11.7460	0.0000											
38	10.8471	1.4053	11.7460	11.4940	2.4199	0.0000										
39	2.7946	9.0163	2.4251	4.1997	9.4764	10.0776	0.0000									
40	2.7946	9.0162	4.1997	2.4252	10.0775	9.4763	4.8581	0.0000								
41	9.0163	2.7946	9.4764	10.0776	2.4251	4.1997	7.3011	8.7696	0.0000							
42	9.0162	2.7946	10.0775	9.4763	4.1997	2.4252	8.7696	7.3010	4.8581	0.0000						
43	2.4264	10.3732	1.4003	3.7019	10.8684	11.3958	1.4025	5.0538	8.7037	9.9663	0.0000					
44	2.4264	10.3732	3.7019	1.4004	11.3958	10.8683	5.0539	1.4025	9.9663	8.7035	4.8526	0.0000				
45	10.3732	2.4264	10.8684	11.3958	1.4003	3.7019	8.7037	9.9663	1.4025	5.0538	10.1062	11.2108	0.0000			
46	10.3732	2.4264	11.3958	10.8683	3.7019	1.4004	9.9663	8.7035	5.0539	1.4025	11.2108	10.1061	4.8526	0.0000		

DIAGONAL PENETRATION TERMS

-1.72302029	-1.72296620	-1.72302029	-1.72296620	-1.66894465	-1.66898529	-1.66894465	-1.66898529	-1.71808545	-1.71802153
-1.71808545	-1.71802153	-1.65481058	-1.65487079	-1.65481058	-1.65487079	-2.78162438	-2.78162438	-2.64907904	-2.64912074
-2.64907904	-2.64912074	-2.42590066	-2.42599826	-2.42590066	-2.42599826	-2.64021465	-2.64029960	-2.64021465	-2.64029960
-2.80002431	-2.80002431	-2.80522693	-2.80522693	-2.42405298	-2.42392710	-2.42405298	-2.42392710	-2.40722989	-2.40734963
-2.40722989	-2.40734963	-2.40806992	-2.40800904	-2.40806992	-2.40800904	-5.15146736	-5.15146736	-5.09753707	-5.09763783
-5.09753707	-5.09763783	-3.82169414	-3.82182302	-3.82169414	-3.82182302	-5.09026748	-5.09036360	-5.09026748	-5.09036360
-5.16156196	-5.16156196	-4.83864655	-4.83864655	-3.19719945	-3.19707007	-3.19719945	-3.19707007	-3.81066605	-3.81077811
-3.81066605	-3.81077811	-3.59818767	-3.59810363	-3.59818767	-3.59810363	-5.20899538	-5.20899538	-4.69860887	-4.69861561
-4.69860887	-4.69861561	-3.38578943	-3.38591815	-3.38578943	-3.38591815	-4.68925384	-4.68932790	-4.68925384	-4.68932790
-5.23930711	-5.23930711	-5.14375196	-5.14375196	-4.01323219	-4.01313768	-4.01323219	-4.01313768	-3.36657223	-3.36676098
-3.36657223	-3.36676098	-3.33124559	-3.33118330	-3.33124559	-3.33118330	-2.30139903	-2.30139903	-2.15290330	-2.15295730
-2.15290330	-2.15295730	-1.58766990	-1.58782396	-1.58766990	-1.58782396	-2.14151790	-2.14163413	-2.14151790	-2.14163413
-2.32309855	-2.32309855	-2.33723334	-2.33723334	-1.59101354	-1.59081189	-1.59101354	-1.59081189	-1.56608656	-1.56628505
-1.56608656	-1.56628505	-1.58249793	-1.58237897	-1.58249793	-1.58237897				

G-, S-, AND F0-MATRICES

TERRYLENE, 15pi x 15pi\* CIS

INITIAL DENSITIES AND CHARGES:

POSITION	AO POPULATIONS				ATOMIC POPULATION	NET CHARGE
	S	PX	PY	PZ		
1	0.8656				0.8656	0.1344
2	0.8656				0.8656	0.1344
3	0.8656				0.8656	0.1344
4	0.8656				0.8656	0.1344
5	0.8747				0.8747	0.1253
6	0.8747				0.8747	0.1253
7	0.8747				0.8747	0.1253
8	0.8747				0.8747	0.1253
9	0.8659				0.8659	0.1341
10	0.8659				0.8659	0.1341
11	0.8659				0.8659	0.1341
12	0.8659				0.8659	0.1341
13	0.8779				0.8779	0.1221
14	0.8779				0.8779	0.1221
15	0.8779				0.8779	0.1221
16	0.8779				0.8779	0.1221
17	0.7498	1.1259	1.1402	1.0048	4.0207	-0.0207
18	0.7498	1.1259	1.1402	1.0048	4.0207	-0.0207
19	0.7609	1.1182	1.1461	0.9999	4.0251	-0.0251
20	0.7609	1.1182	1.1461	0.9999	4.0251	-0.0251
21	0.7609	1.1182	1.1461	0.9999	4.0251	-0.0251
22	0.7609	1.1182	1.1461	0.9999	4.0251	-0.0251
23	0.8421	1.1453	1.1138	1.0004	4.1016	-0.1016
24	0.8421	1.1453	1.1138	1.0004	4.1016	-0.1016
25	0.8421	1.1453	1.1138	1.0004	4.1016	-0.1016
26	0.8421	1.1453	1.1138	1.0004	4.1016	-0.1016
27	0.7617	1.1186	1.1448	1.0012	4.0263	-0.0263
28	0.7617	1.1186	1.1448	1.0012	4.0264	-0.0264
29	0.7617	1.1186	1.1448	1.0012	4.0263	-0.0263
30	0.7617	1.1186	1.1448	1.0012	4.0264	-0.0264
31	0.7494	1.1350	1.1373	1.0060	4.0277	-0.0277
32	0.7494	1.1350	1.1373	1.0060	4.0277	-0.0277
33	0.7555	1.1278	1.1799	1.0033	4.0666	-0.0666
34	0.7555	1.1278	1.1799	1.0033	4.0666	-0.0666
35	0.8412	1.1156	1.1361	0.9906	4.0836	-0.0836
36	0.8412	1.1156	1.1361	0.9906	4.0836	-0.0836
37	0.8412	1.1156	1.1361	0.9906	4.0836	-0.0836
38	0.8412	1.1156	1.1361	0.9906	4.0836	-0.0836
39	0.8432	1.1450	1.1130	0.9961	4.0973	-0.0973
40	0.8432	1.1450	1.1130	0.9961	4.0973	-0.0973
41	0.8432	1.1450	1.1130	0.9961	4.0973	-0.0973
42	0.8432	1.1450	1.1130	0.9961	4.0973	-0.0973
43	0.8497	1.1445	1.1256	1.0047	4.1245	-0.1245
44	0.8497	1.1444	1.1256	1.0047	4.1245	-0.1245
45	0.8497	1.1445	1.1256	1.0047	4.1245	-0.1245
46	0.8497	1.1444	1.1256	1.0047	4.1245	-0.1245
				SUM	136.0000	0.0000

## SCF PROCEDURE:

1	D=1.00	DE =	126.03173595 EV	DP=	1.17991637	
2	D=0.50	DE =	4.37634904 EV	DP=	0.00980255	
3	D=0.25	DE =	0.10466108 EV	DP=	0.01023161	
4	D=0.13	DE =	0.12447295 EV	DP=	0.00289083	
5	D=0.06	DE =	0.03396496 EV	DP=	0.00205039	
6	D=0.03	DE =	0.01715356 EV	DP=	0.00094896	
7	D=0.00	DE =	0.00978533 EV	DP=	0.00053590	
8	D=0.00	DE =	0.00508226 EV	DP=	0.00026559	
9	D=0.00	DE =	0.00270364 EV	DP=	0.00014753	
10	D=0.00	DE =	0.00139074 EV	DP=	0.00007801	DENSITIES SATISFIED
11	D=0.00	DE =	0.00074562 EV	DP=	0.00004430	DENSITIES SATISFIED
12	D=0.00	DE =	0.00039184 EV	DP=	0.00002425	ENERGIES AND DENSITIES SATISFIED

HUECKEL ENERGY -2553.905569 EV

ROOTHAAN CLOSED SHELL ENERGY -27736.452827 EV

CORE REPULSION 22937.183984 EV

TOTAL VALENCE SHELL ENERGY -4799.268843 EV

## MO ENERGIES (EV) AND HALF OCCUPATION NUMBERS

136:	130.242248	0.000000
135:	129.414555	0.000000
134:	127.518761	0.000000
133:	119.749509	0.000000
132:	118.372479	0.000000
131:	117.329359	0.000000
130:	117.279904	0.000000
129:	113.088191	0.000000
128:	109.127642	0.000000
127:	108.547495	0.000000
126:	107.770710	0.000000
125:	106.412546	0.000000
124:	105.816098	0.000000
123:	102.571240	0.000000
122:	98.519542	0.000000
121:	91.134343	0.000000
120:	86.614324	0.000000
119:	84.964100	0.000000
118:	84.896142	0.000000
117:	83.609940	0.000000
116:	83.381296	0.000000
115:	82.402008	0.000000



114:	78.553370	0.000000
113:	74.357646	0.000000
112:	64.303060	0.000000
111:	62.510745	0.000000
110:	60.914434	0.000000
109:	51.492124	0.000000
108:	44.066320	0.000000
107:	35.696550	0.000000
106:	35.608998	0.000000
105:	35.084532	0.000000
104:	31.764982	0.000000
103:	31.034316	0.000000
102:	30.562170	0.000000
101:	30.512033	0.000000
100:	29.442446	0.000000
99:	28.628707	0.000000
98:	28.087536	0.000000
97:	27.383412	0.000000
96:	27.015863	0.000000
95:	25.852343	0.000000
94:	25.261742	0.000000
93:	25.249949	0.000000
92:	24.558318	0.000000
91:	24.262440	0.000000
90:	24.039015	0.000000
89:	24.013565	0.000000
88:	23.610536	0.000000
87:	23.606475	0.000000
86:	23.444594	0.000000
85:	22.297341	0.000000
84:	22.221832	0.000000
83:	4.472093	0.000000
82:	3.900980	0.000000
81:	3.029219	0.000000
80:	2.429670	0.000000
79:	1.950389	0.000000
78:	1.399049	0.000000
77:	1.284140	0.000000
76:	0.084223	0.000000
75:	-0.431110	0.000000
74:	-0.620592	0.000000
73:	-0.793287	0.000000
72:	-1.010693	0.000000
71:	-1.185655	0.000000
70:	-1.578192	0.000000
69:	-2.988610	0.000000
68:	-7.318976	1.000000
67:	-8.832815	1.000000
66:	-9.439048	1.000000
65:	-9.604447	1.000000

64:	-9.717216	1.000000
63:	-9.886933	1.000000
62:	-10.180995	1.000000
61:	-10.839699	1.000000
60:	-11.334736	1.000000
59:	-11.512978	1.000000
58:	-11.744267	1.000000
57:	-11.815913	1.000000
56:	-11.964396	1.000000
55:	-12.001938	1.000000
54:	-12.024620	1.000000
53:	-12.061715	1.000000
52:	-12.187290	1.000000
51:	-12.360616	1.000000
50:	-12.478566	1.000000
49:	-12.681473	1.000000
48:	-12.754032	1.000000
47:	-12.763073	1.000000
46:	-12.764859	1.000000
45:	-12.951142	1.000000
44:	-13.165047	1.000000
43:	-13.336981	1.000000
42:	-13.348554	1.000000
41:	-13.474668	1.000000
40:	-13.522955	1.000000
39:	-13.547546	1.000000
38:	-13.939530	1.000000
37:	-14.122658	1.000000
36:	-14.439953	1.000000
35:	-14.617422	1.000000
34:	-14.923588	1.000000
33:	-15.151726	1.000000
32:	-15.316026	1.000000
31:	-15.879871	1.000000
30:	-15.891238	1.000000
29:	-15.924347	1.000000
28:	-16.142589	1.000000
27:	-16.359892	1.000000
26:	-17.041947	1.000000
25:	-17.294768	1.000000
24:	-17.919890	1.000000
23:	-18.402377	1.000000
22:	-18.746646	1.000000
21:	-20.167376	1.000000
20:	-20.365752	1.000000
19:	-20.953874	1.000000
18:	-22.027939	1.000000
17:	-22.155467	1.000000
16:	-22.506520	1.000000
15:	-22.688088	1.000000
14:	-26.417255	1.000000

13:	-26.640238	1.000000
12:	-27.208456	1.000000
11:	-28.934966	1.000000
10:	-30.145622	1.000000
9:	-30.502174	1.000000
8:	-32.100485	1.000000
7:	-36.157080	1.000000
6:	-37.818797	1.000000
5:	-39.288734	1.000000
4:	-41.672644	1.000000
3:	-44.237376	1.000000
2:	-48.953750	1.000000
1:	-52.278231	1.000000

MO COEFFICIENTS STORED COLUMNWISE (LOWDIN BASIS)

	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52
1	0.0000	0.0582	-0.1344	-0.0855	0.0965	0.0000	0.0099	-0.0895	-0.0086	0.0340	0.0702	0.0000	0.1164	0.1106	0.0000	-0.1009
2	0.0000	-0.0582	-0.1344	0.0855	0.0965	0.0000	0.0099	0.0896	0.0086	0.0351	-0.0697	0.0000	-0.1163	0.1106	0.0000	0.1009
3	0.0000	0.0582	0.1344	-0.0855	-0.0965	0.0000	0.0099	0.0895	0.0086	0.0340	0.0702	0.0000	0.1164	-0.1106	0.0000	0.1009
4	0.0000	-0.0582	0.1344	0.0855	-0.0965	0.0000	0.0099	-0.0896	-0.0086	0.0351	-0.0697	0.0000	-0.1163	-0.1106	0.0000	-0.1009
5	0.0000	-0.1731	0.1033	-0.0590	-0.0528	0.0000	0.1045	-0.0482	0.1443	-0.0895	-0.0879	0.0000	-0.1218	-0.1004	0.0000	0.1307
6	0.0000	0.1732	0.1033	0.0590	-0.0528	0.0000	0.1045	0.0482	-0.1444	-0.0909	0.0866	0.0000	0.1217	-0.1004	0.0000	-0.1307
7	0.0000	-0.1731	-0.1033	-0.0590	0.0528	0.0000	0.1045	0.0482	-0.1443	-0.0895	-0.0879	0.0000	-0.1218	0.1004	0.0000	-0.1307
8	0.0000	0.1732	-0.1033	0.0590	0.0528	0.0000	0.1045	-0.0482	0.1444	-0.0909	0.0866	0.0000	0.1217	0.1004	0.0000	0.1307
9	0.0000	-0.0489	-0.1341	-0.0994	-0.0429	0.0000	0.1166	-0.1143	0.0111	0.0630	-0.0562	0.0000	0.0530	-0.0997	0.0000	-0.0912
10	0.0000	0.0489	-0.1341	0.0994	-0.0429	0.0000	0.1166	0.1143	-0.0111	0.0622	0.0571	0.0000	-0.0530	-0.0997	0.0000	0.0912
11	0.0000	-0.0489	0.1341	-0.0994	0.0429	0.0000	0.1166	0.1143	-0.0111	0.0630	-0.0562	0.0000	0.0530	0.0997	0.0000	0.0912
12	0.0000	0.0489	0.1341	0.0994	0.0429	0.0000	0.1166	-0.1143	0.0111	0.0622	0.0571	0.0000	-0.0530	0.0997	0.0000	-0.0912
13	0.0000	-0.0280	0.0421	0.0141	-0.1547	0.0000	-0.1758	-0.0579	0.0013	-0.1027	-0.0888	0.0000	0.0926	0.1545	0.0000	0.0529
14	0.0000	0.0280	0.0421	-0.0140	-0.1547	0.0000	-0.1759	0.0579	-0.0013	-0.1040	0.0872	0.0000	-0.0927	0.1545	0.0000	-0.0529
15	0.0000	-0.0280	-0.0421	0.0141	0.1547	0.0000	-0.1758	0.0579	-0.0013	-0.1027	-0.0888	0.0000	0.0926	-0.1545	0.0000	-0.0529
16	0.0000	0.0280	-0.0421	-0.0140	0.1547	0.0000	-0.1759	-0.0579	0.0013	-0.1040	0.0872	0.0000	-0.0927	-0.1545	0.0000	0.0529
17	0.0000	0.0000	0.0172	0.0000	0.0411	0.0000	-0.0247	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0000	-0.0438	0.0000	0.0000
18	0.0000	0.0000	-0.0172	0.0000	-0.0411	0.0000	-0.0247	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0000	0.0438	0.0000	0.0000
19	0.0000	0.0498	0.0421	-0.0368	-0.0124	0.0000	0.0285	-0.0010	0.0094	-0.0179	0.0178	0.0000	-0.0095	-0.0361	0.0000	-0.0107
20	0.0000	-0.0498	0.0421	0.0368	-0.0124	0.0000	0.0285	0.0009	-0.0094	-0.0177	-0.0180	0.0000	0.0095	-0.0361	0.0000	0.0107
21	0.0000	0.0498	-0.0421	-0.0368	0.0124	0.0000	0.0285	0.0010	-0.0094	-0.0179	0.0178	0.0000	-0.0095	0.0361	0.0000	0.0107
22	0.0000	-0.0498	-0.0421	0.0368	0.0124	0.0000	0.0285	-0.0009	0.0094	-0.0177	-0.0180	0.0000	0.0095	0.0361	0.0000	-0.0107
23	0.0000	0.0146	0.0237	0.0348	0.0596	0.0000	-0.0016	-0.0050	0.0202	0.0016	-0.0259	0.0000	-0.0189	0.0325	0.0000	0.0193
24	0.0000	-0.0146	0.0237	-0.0348	0.0596	0.0000	-0.0016	0.0051	-0.0202	0.0012	0.0260	0.0000	0.0189	0.0325	0.0000	-0.0193
25	0.0000	0.0146	-0.0237	0.0348	-0.0596	0.0000	-0.0016	0.0050	-0.0202	0.0016	-0.0259	0.0000	-0.0189	-0.0325	0.0000	-0.0193
26	0.0000	-0.0146	-0.0237	-0.0348	-0.0596	0.0000	-0.0016	-0.0051	0.0202	0.0012	0.0260	0.0000	0.0189	-0.0325	0.0000	0.0193
27	0.0000	-0.0428	0.0119	-0.0198	-0.0091	0.0000	-0.0645	-0.0290	0.0028	-0.0035	-0.0162	0.0000	-0.0120	0.0332	0.0000	0.0035
28	0.0000	0.0429	0.0120	0.0198	-0.0091	0.0000	-0.0645	0.0290	-0.0028	-0.0038	0.0161	0.0000	0.0120	0.0332	0.0000	-0.0035
29	0.0000	-0.0428	-0.0119	-0.0198	0.0091	0.0000	-0.0645	0.0290	-0.0028	-0.0035	-0.0162	0.0000	-0.0120	-0.0332	0.0000	-0.0035
30	0.0000	0.0429	-0.0120	0.0198	0.0091	0.0000	-0.0645	-0.0290	0.0028	-0.0038	0.0161	0.0000	0.0120	-0.0332	0.0000	0.0035
31	0.0000	0.0000	0.0303	0.0000	-0.0182	0.0000	0.0430	0.0000	0.0000	0.0134	0.0001	0.0000	0.0000	-0.0282	0.0000	0.0000

32	0.0000	0.0000	-0.0303	0.0000	0.0182	0.0000	0.0430	0.0000	0.0000	0.0134	0.0001	0.0000	0.0000	0.0282	0.0000	0.0000
33	0.0000	0.0000	-0.0336	0.0000	-0.0559	0.0000	-0.0479	0.0000	0.0000	-0.0255	-0.0002	0.0000	0.0000	0.0094	0.0000	0.0000
34	0.0000	0.0000	0.0336	0.0000	0.0559	0.0000	-0.0479	0.0000	0.0000	-0.0255	-0.0002	0.0000	0.0000	-0.0094	0.0000	0.0000
35	0.0000	-0.0087	-0.0252	-0.0339	0.0280	0.0000	0.0295	-0.0266	-0.0057	0.0325	-0.0231	0.0000	-0.0281	-0.0192	0.0000	0.0197
36	0.0000	0.0087	-0.0252	0.0339	0.0280	0.0000	0.0295	0.0266	0.0057	0.0321	0.0236	0.0000	0.0282	-0.0192	0.0000	-0.0197
37	0.0000	-0.0087	0.0252	-0.0339	-0.0280	0.0000	0.0295	0.0266	0.0057	0.0325	-0.0231	0.0000	-0.0281	0.0192	0.0000	-0.0197
38	0.0000	0.0087	0.0252	0.0339	-0.0280	0.0000	0.0295	-0.0266	-0.0057	0.0321	0.0236	0.0000	0.0282	0.0192	0.0000	0.0197
39	0.0000	-0.0547	0.0060	0.0045	-0.0078	0.0000	0.0335	0.0325	0.0315	-0.0169	0.0175	0.0000	-0.0348	-0.0188	0.0000	-0.0010
40	0.0000	0.0547	0.0060	-0.0045	-0.0078	0.0000	0.0335	-0.0325	-0.0315	-0.0166	-0.0178	0.0000	0.0348	-0.0187	0.0000	0.0010
41	0.0000	-0.0547	-0.0060	0.0045	0.0078	0.0000	0.0335	-0.0325	-0.0315	-0.0169	0.0175	0.0000	-0.0348	0.0188	0.0000	0.0010
42	0.0000	0.0547	-0.0060	-0.0045	0.0078	0.0000	0.0335	0.0325	0.0315	-0.0166	-0.0178	0.0000	0.0348	0.0187	0.0000	-0.0010
43	0.0000	0.0381	0.0057	0.0267	0.0184	0.0000	-0.0338	0.0300	-0.0272	0.0123	0.0323	0.0000	0.0034	0.0184	0.0000	-0.0136
44	0.0000	-0.0381	0.0057	-0.0266	0.0185	0.0000	-0.0338	-0.0300	0.0272	0.0128	-0.0321	0.0000	-0.0034	0.0184	0.0000	0.0136
45	0.0000	0.0381	-0.0057	0.0267	-0.0184	0.0000	-0.0338	-0.0300	0.0272	0.0123	0.0323	0.0000	0.0034	-0.0184	0.0000	0.0136
46	0.0000	-0.0381	-0.0057	-0.0266	-0.0185	0.0000	-0.0338	0.0300	-0.0272	0.0128	-0.0321	0.0000	-0.0034	-0.0184	0.0000	-0.0136
47	0.0000	0.0000	0.0186	0.0000	0.0407	0.0000	0.3040	0.0000	0.0000	-0.2884	-0.0021	0.0000	-0.0001	-0.0461	0.0000	0.0000
48	0.0000	0.0000	0.0186	0.0000	0.0407	0.0000	-0.3040	0.0000	0.0000	0.2884	0.0021	0.0000	0.0001	-0.0461	0.0000	0.0000
49	0.0000	-0.0908	0.1242	0.0744	0.0096	0.0000	0.1427	0.0527	0.2451	-0.0341	-0.0210	0.0000	0.1701	0.0924	0.0000	-0.0072
50	0.0000	0.0908	0.1242	-0.0744	0.0097	0.0000	0.1427	-0.0527	-0.2451	-0.0343	0.0205	0.0000	-0.1701	0.0924	0.0000	0.0072
51	0.0000	0.0908	0.1242	-0.0744	0.0096	0.0000	-0.1427	0.0527	0.2451	0.0341	0.0210	0.0000	-0.1701	0.0924	0.0000	-0.0072
52	0.0000	-0.0908	0.1242	0.0744	0.0097	0.0000	-0.1427	-0.0527	-0.2451	0.0343	-0.0205	0.0000	0.1701	0.0924	0.0000	0.0072
53	0.0000	-0.1524	-0.0255	-0.0492	-0.0593	0.0000	-0.0868	-0.0002	-0.0176	-0.1179	0.0105	0.0000	-0.2319	-0.0307	0.0000	-0.0257
54	0.0000	0.1523	-0.0255	0.0492	-0.0593	0.0000	-0.0868	0.0002	0.0176	-0.1179	-0.0122	0.0000	0.2319	-0.0307	0.0000	0.0257
55	0.0000	0.1524	-0.0255	0.0492	-0.0593	0.0000	0.0868	-0.0002	-0.0176	0.1179	-0.0105	0.0000	0.2319	-0.0307	0.0000	-0.0257
56	0.0000	-0.1523	-0.0255	-0.0492	-0.0593	0.0000	0.0868	0.0002	0.0176	0.1179	0.0122	0.0000	-0.2319	-0.0307	0.0000	0.0257
57	0.0000	0.1855	-0.0923	-0.0903	-0.0081	0.0000	-0.0537	-0.0249	-0.2397	0.0238	0.0564	0.0000	-0.1639	-0.1581	0.0000	-0.0034
58	0.0000	-0.1855	-0.0923	0.0903	-0.0081	0.0000	-0.0537	0.0249	0.2397	0.0245	-0.0560	0.0000	0.1640	-0.1582	0.0000	0.0034
59	0.0000	-0.1855	-0.0923	0.0903	-0.0081	0.0000	0.0537	-0.0249	-0.2397	-0.0238	-0.0564	0.0000	0.1639	-0.1581	0.0000	-0.0034
60	0.0000	0.1855	-0.0923	-0.0903	-0.0081	0.0000	0.0537	0.0249	0.2397	-0.0245	0.0560	0.0000	-0.1640	-0.1582	0.0000	0.0034
61	0.0000	0.0000	0.0644	0.0000	0.2938	0.0000	-0.0632	0.0000	0.0000	0.2511	0.0019	0.0000	0.0001	0.1821	0.0000	0.0000
62	0.0000	0.0000	0.0644	0.0000	0.2938	0.0000	0.0632	0.0000	0.0000	-0.2511	-0.0019	0.0000	-0.0001	0.1821	0.0000	0.0000
63	0.0000	0.0000	0.0012	0.0000	-0.2519	0.0000	0.1625	0.0000	0.0000	-0.2105	-0.0015	0.0000	-0.0001	-0.2231	0.0000	0.0000
64	0.0000	0.0000	0.0012	0.0000	-0.2519	0.0000	-0.1625	0.0000	0.0000	0.2105	0.0015	0.0000	0.0001	-0.2231	0.0000	0.0000
65	0.0000	0.2329	-0.1520	0.0481	0.0892	0.0000	-0.0998	0.0381	-0.1983	0.1358	0.0929	0.0000	0.1350	0.0980	0.0000	-0.1494
66	0.0000	-0.2329	-0.1519	-0.0481	0.0892	0.0000	-0.0999	-0.0381	0.1983	0.1372	-0.0909	0.0000	-0.1349	0.0980	0.0000	0.1494
67	0.0000	-0.2329	-0.1520	-0.0481	0.0892	0.0000	0.0998	0.0381	-0.1983	-0.1358	-0.0929	0.0000	-0.1350	0.0980	0.0000	-0.1494
68	0.0000	0.2329	-0.1519	0.0481	0.0892	0.0000	0.0999	-0.0381	0.1983	-0.1372	0.0909	0.0000	0.1349	0.0980	0.0000	0.1494
69	0.0000	-0.1611	-0.1306	0.0326	-0.1861	0.0000	-0.0119	0.0068	0.0528	-0.0586	-0.0061	0.0000	0.1374	0.0684	0.0000	-0.0953
70	0.0000	0.1610	-0.1306	-0.0326	-0.1861	0.0000	-0.0119	-0.0068	-0.0528	-0.0586	0.0053	0.0000	-0.1374	0.0685	0.0000	0.0953
71	0.0000	0.1611	-0.1306	-0.0326	-0.1861	0.0000	0.0119	0.0068	0.0528	0.0586	0.0061	0.0000	-0.1374	0.0684	0.0000	-0.0953
72	0.0000	-0.1610	-0.1306	0.0326	-0.1861	0.0000	0.0119	-0.0068	-0.0528	0.0586	-0.0053	0.0000	0.1374	0.0685	0.0000	0.0953
73	0.0000	0.0693	0.1313	-0.0505	0.1591	0.0000	0.0758	0.0003	0.0028	0.0285	-0.0099	0.0000	-0.1799	-0.1043	0.0000	0.1148
74	0.0000	-0.0692	0.1313	0.0505	0.1591	0.0000	0.0758	-0.0003	-0.0028	0.0282	0.0104	0.0000	0.1799	-0.1043	0.0000	-0.1148
75	0.0000	-0.0693	0.1313	0.0505	0.1591	0.0000	-0.0758	0.0003	0.0028	-0.0285	0.0099	0.0000	0.1799	-0.1043	0.0000	0.1148
76	0.0000	0.0692	0.1313	-0.0505	0.1591	0.0000	-0.0758	-0.0003	-0.0028	-0.0282	-0.0104	0.0000	-0.1799	-0.1043	0.0000	-0.1148
77	0.0000	0.0973	0.0000	0.2504	0.0000	0.0000	0.0000	-0.0492	0.2185	0.0015	-0.1942	0.0000	-0.1158	0.0000	0.0000	-0.2413
78	0.0000	0.0973	0.0000	0.2504	0.0000	0.0000	0.0000	0.0492	-0.2185	0.0015	-0.1942	0.0000	-0.1158	0.0000	0.0000	0.2413
79	0.0000	-0.1010	-0.1584	-0.2507	-0.0628	0.0000	0.0292	-0.0770	0.0672	-0.1315	0.1837	0.0000	0.0304	0.0696	0.0000	-0.2214
80	0.0000	-0.1010	0.1583	-0.2507	0.0628	0.0000	-0.0293	-0.0770	0.0672	0.1287	0.1856	0.0000	0.0305	-0.0696	0.0000	-0.2214

81	0.0000	-0.1010	0.1584	-0.2507	0.0628	0.0000	0.0292	0.0770	-0.0672	-0.1315	0.1837	0.0000	0.0304	-0.0696	0.0000	0.2214
82	0.0000	-0.1010	-0.1583	-0.2507	-0.0628	0.0000	-0.0293	0.0770	-0.0672	0.1287	0.1856	0.0000	0.0305	0.0696	0.0000	0.2214
83	0.0000	-0.0057	0.2192	0.1732	-0.0576	0.0000	0.0466	0.1094	0.0518	0.0228	-0.1388	0.0000	-0.0530	-0.1209	0.0000	0.1569
84	0.0000	-0.0056	-0.2192	0.1732	0.0576	0.0000	-0.0466	0.1094	0.0518	-0.0207	-0.1391	0.0000	-0.0530	0.1209	0.0000	0.1569
85	0.0000	-0.0057	-0.2192	0.1732	-0.0576	0.0000	0.0466	-0.1094	-0.0518	0.0228	-0.1388	0.0000	-0.0530	0.1209	0.0000	-0.1569
86	0.0000	-0.0056	0.2192	0.1732	-0.0576	0.0000	-0.0466	-0.1094	-0.0518	-0.0207	-0.1391	0.0000	-0.0530	-0.1209	0.0000	-0.1569
87	0.0000	0.0687	0.0049	-0.1564	0.1554	0.0000	0.0649	-0.2585	0.0242	0.1801	-0.1702	0.0000	0.0677	-0.0605	0.0000	-0.0046
88	0.0000	0.0686	-0.0049	-0.1564	-0.1554	0.0000	-0.0649	-0.2585	0.0242	-0.1777	-0.1728	0.0000	0.0676	0.0605	0.0000	-0.0046
89	0.0000	0.0687	-0.0049	-0.1564	-0.1554	0.0000	0.0649	0.2585	-0.0242	0.1801	-0.1702	0.0000	0.0677	0.0605	0.0000	0.0046
90	0.0000	0.0686	0.0049	-0.1564	0.1554	0.0000	-0.0649	0.2585	-0.0242	-0.1777	-0.1728	0.0000	0.0676	-0.0605	0.0000	0.0046
91	0.0000	0.0850	0.0000	0.1269	0.0000	0.0000	0.0000	0.2773	-0.1625	-0.0016	0.2203	0.0000	-0.1514	0.0000	0.0000	-0.0028
92	0.0000	0.0850	0.0000	0.1269	0.0000	0.0000	0.0000	-0.2773	0.1625	-0.0016	0.2203	0.0000	-0.1514	0.0000	0.0000	0.0028
93	0.0000	-0.1976	0.0000	0.1231	0.0000	0.0000	0.0000	0.1750	0.1766	-0.0012	0.1634	0.0000	-0.0154	0.0000	0.0000	-0.1102
94	0.0000	-0.1976	0.0000	0.1231	0.0000	0.0000	0.0000	-0.1750	-0.1766	-0.0012	0.1634	0.0000	-0.0154	0.0000	0.0000	0.1102
95	0.0000	0.0734	0.0878	-0.1082	-0.0057	0.0000	-0.1251	-0.1603	-0.0538	-0.0310	-0.1819	0.0000	-0.0301	0.1035	0.0000	0.1688
96	0.0000	0.0734	-0.0878	-0.1083	0.0057	0.0000	0.1251	-0.1603	-0.0539	0.0337	-0.1814	0.0000	-0.0301	-0.1035	0.0000	0.1687
97	0.0000	0.0734	-0.0878	-0.1082	-0.0057	0.0000	-0.1251	0.1603	0.0538	-0.0310	-0.1819	0.0000	-0.0301	-0.1035	0.0000	-0.1688
98	0.0000	0.0734	0.0878	-0.1083	-0.0057	0.0000	0.1251	0.1603	0.0539	0.0337	-0.1814	0.0000	-0.0301	0.1035	0.0000	-0.1687
99	0.0000	-0.0596	0.1204	0.1577	-0.0274	0.0000	-0.1407	0.1881	0.0483	-0.1346	0.1021	0.0000	-0.0176	0.1782	0.0000	0.0626
100	0.0000	-0.0596	-0.1204	0.1577	0.0273	0.0000	0.1408	0.1881	0.0482	0.1331	0.1041	0.0000	-0.0175	-0.1782	0.0000	0.0625
101	0.0000	-0.0596	-0.1204	0.1577	0.0274	0.0000	-0.1407	-0.1881	-0.0483	-0.1346	0.1021	0.0000	-0.0176	-0.1782	0.0000	-0.0626
102	0.0000	-0.0596	0.1204	0.1577	-0.0273	0.0000	0.1408	-0.1881	-0.0482	0.1331	0.1041	0.0000	-0.0175	0.1782	0.0000	-0.0625
103	0.0000	0.0420	-0.1326	0.0373	0.1584	0.0000	0.1823	0.1186	-0.0324	0.1459	0.1688	0.0000	-0.0279	-0.1422	0.0000	-0.1550
104	0.0000	0.0420	0.1326	0.0374	-0.1584	0.0000	-0.1823	0.1186	-0.0324	-0.1484	0.1667	0.0000	-0.0280	0.1422	0.0000	-0.1549
105	0.0000	0.0420	0.1326	0.0373	-0.1584	0.0000	0.1823	-0.1186	0.0324	0.1459	0.1688	0.0000	-0.0279	0.1422	0.0000	0.1550
106	0.0000	0.0420	-0.1326	0.0374	0.1584	0.0000	-0.1823	-0.1186	0.0324	-0.1484	0.1667	0.0000	-0.0280	-0.1422	0.0000	0.1549
107	0.2731	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1906	0.0000
108	0.2731	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1906	0.0000
109	0.1665	0.0000	0.0000	0.0000	0.0000	-0.2356	0.0000	0.0000	0.0000	0.0000	0.0000	0.1270	0.0000	0.0000	-0.2636	0.0000
110	0.1665	0.0000	0.0000	0.0000	0.0000	0.2356	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1271	0.0000	0.0000	-0.2636	0.0000
111	0.1665	0.0000	0.0000	0.0000	0.0000	-0.2356	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1270	0.0000	0.0000	0.2636	0.0000
112	0.1665	0.0000	0.0000	0.0000	0.0000	0.2356	0.0000	0.0000	0.0000	0.0000	0.0000	0.1271	0.0000	0.0000	0.2636	0.0000
113	0.1609	0.0000	0.0000	0.0000	0.0000	-0.2928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0559	0.0000	0.0000	-0.0999	0.0000
114	0.1610	0.0000	0.0000	0.0000	0.0000	0.2928	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0559	0.0000	0.0000	-0.0999	0.0000
115	0.1609	0.0000	0.0000	0.0000	0.0000	-0.2928	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0559	0.0000	0.0000	0.0999	0.0000
116	0.1610	0.0000	0.0000	0.0000	0.0000	0.2928	0.0000	0.0000	0.0000	0.0000	0.0000	0.0559	0.0000	0.0000	0.0999	0.0000
117	-0.0797	0.0000	0.0000	0.0000	0.0000	-0.1988	0.0000	0.0000	0.0000	0.0000	0.0000	0.2250	0.0000	0.0000	-0.1780	0.0000
118	-0.0797	0.0000	0.0000	0.0000	0.0000	0.1988	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2251	0.0000	0.0000	-0.1780	0.0000
119	-0.0797	0.0000	0.0000	0.0000	0.0000	-0.1988	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2250	0.0000	0.0000	0.1780	0.0000
120	-0.0797	0.0000	0.0000	0.0000	0.0000	0.1988	0.0000	0.0000	0.0000	0.0000	0.0000	0.2251	0.0000	0.0000	0.1780	0.0000
121	-0.1989	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0562	0.0000
122	-0.1989	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0562	0.0000
123	-0.2886	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2564	0.0000
124	-0.2886	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2564	0.0000
125	-0.2200	0.0000	0.0000	0.0000	0.0000	-0.0851	0.0000	0.0000	0.0000	0.0000	0.0000	0.1621	0.0000	0.0000	0.2516	0.0000
126	-0.2200	0.0000	0.0000	0.0000	0.0000	0.0851	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1621	0.0000	0.0000	0.2517	0.0000
127	-0.2200	0.0000	0.0000	0.0000	0.0000	-0.0851	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1621	0.0000	0.0000	-0.2516	0.0000
128	-0.2200	0.0000	0.0000	0.0000	0.0000	0.0851	0.0000	0.0000	0.0000	0.0000	0.0000	0.1621	0.0000	0.0000	-0.2517	0.0000
129	-0.1201	0.0000	0.0000	0.0000	0.0000	-0.1984	0.0000	0.0000	0.0000	0.0000	0.0000	0.2896	0.0000	0.0000	-0.0156	0.0000
130	-0.1201	0.0000	0.0000	0.0000	0.0000	0.1984	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2896	0.0000	0.0000	-0.0156	0.0000













101	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1481
102	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1513
103	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0731
104	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0747
105	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0731
106	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0747

107	0.0000	0.0000	-0.2668	-0.3312	0.0278	0.3116	0.0000	0.1360	0.0000	-0.1943	0.0000	0.0000	-0.2807	0.0738	-0.2875	0.0000	
108	0.0000	0.0000	-0.2668	0.3312	0.0278	-0.3116	0.0000	-0.1360	0.0000	-0.1943	0.0000	0.0000	0.2807	0.0738	0.2875	0.0000	
109	0.2655	0.0460	0.2645	-0.0114	-0.0197	0.0139	0.2970	0.0203	0.1604	0.2683	-0.1144	-0.2297	-0.1775	-0.1275	-0.2450	0.0000	
110	-0.2654	-0.0460	0.2645	-0.0114	-0.0197	0.0139	-0.2971	0.0203	-0.1604	0.2682	0.1144	0.2297	-0.1775	-0.1275	-0.2450	0.0000	
111	0.2655	-0.0460	0.2645	0.0114	-0.0197	-0.0139	0.2970	-0.0203	-0.1604	0.2683	-0.1144	-0.2297	0.1775	-0.1275	0.2450	0.0000	
112	-0.2654	0.0460	0.2645	0.0114	-0.0197	-0.0139	-0.2971	-0.0203	0.1604	0.2682	0.1144	-0.2297	0.1775	-0.1275	0.2450	0.0000	
113	-0.1932	0.1725	-0.1324	-0.2780	0.0003	0.2595	-0.1449	-0.1302	-0.2824	-0.0971	0.0472	0.2783	0.1694	0.0383	0.1716	0.0000	
114	0.1932	-0.1725	-0.1324	-0.2780	0.0003	0.2595	0.1449	-0.1302	0.2824	-0.0971	-0.0472	-0.2783	0.1695	0.0383	0.1716	0.0000	
115	-0.1932	-0.1725	-0.1324	0.2780	0.0003	-0.2595	-0.1449	0.1302	0.2824	-0.0971	0.0472	-0.2783	-0.1694	0.0383	-0.1716	0.0000	
116	0.1932	0.1725	-0.1324	0.2780	0.0003	-0.2595	0.1449	0.1302	-0.2824	-0.0971	-0.0472	0.2783	-0.1695	0.0383	-0.1716	0.0000	
117	0.1565	-0.2942	0.1788	-0.0175	-0.0076	0.0106	-0.2224	0.2758	0.0642	-0.1871	0.2184	0.1992	-0.0738	0.2399	0.2131	0.0000	
118	-0.1564	0.2942	0.1788	-0.0175	-0.0076	0.0106	0.2224	0.2757	-0.0643	-0.1870	-0.2184	-0.1992	-0.0738	0.2400	0.2131	0.0000	
119	0.1565	0.2942	0.1788	0.0175	-0.0076	-0.0106	-0.2224	-0.2758	-0.0642	-0.1871	0.2184	-0.1992	0.0738	0.2399	-0.2131	0.0000	
120	-0.1564	-0.2942	0.1788	0.0175	-0.0076	-0.0106	0.2224	-0.2757	0.0643	-0.1870	-0.2184	0.1992	0.0738	0.2400	-0.2131	0.0000	
121	0.0000	0.0000	-0.2859	0.2237	-0.2890	0.2110	0.0000	-0.2515	0.0000	0.0611	0.0000	0.0000	0.0000	0.1932	-0.2985	-0.2190	0.0000
122	0.0000	0.0000	-0.2859	-0.2237	-0.2890	-0.2110	0.0000	0.2515	0.0000	0.0611	0.0000	0.0000	0.0000	-0.1932	-0.2985	0.2190	0.0000
123	0.0000	0.0000	-0.0885	-0.2125	0.3260	-0.2394	0.0000	-0.2147	0.0000	0.2598	0.0000	0.0000	0.0000	-0.2855	0.2716	0.1612	0.0000
124	0.0000	0.0000	-0.0885	0.2125	0.3260	0.2394	0.0000	0.2147	0.0000	0.2598	0.0000	0.0000	0.0000	0.2855	0.2716	-0.1612	0.0000
125	0.2399	-0.2706	0.1789	-0.0051	-0.0272	0.0257	-0.2176	0.2558	-0.1821	-0.2404	-0.1730	-0.0991	0.2095	-0.1814	-0.1022	0.0000	
126	-0.2399	0.2706	0.1790	-0.0051	-0.0272	0.0258	0.2176	0.2558	0.1820	-0.2404	0.1730	0.0991	0.2094	-0.1814	-0.1022	0.0000	
127	0.2399	0.2706	0.1789	0.0051	-0.0272	-0.0257	-0.2176	-0.2558	0.1821	-0.2404	-0.1730	0.0991	-0.2095	-0.1814	0.1022	0.0000	
128	-0.2399	-0.2706	0.1790	0.0051	-0.0272	-0.0258	0.2176	-0.2558	-0.1820	-0.2404	0.1730	-0.0991	-0.2094	-0.1814	0.1022	0.0000	
129	-0.2341	0.1687	-0.1120	-0.1752	0.2849	-0.2147	0.0192	-0.1186	-0.2004	0.0192	-0.2862	-0.2054	0.1177	-0.1765	-0.1292	0.0000	
130	0.2340	-0.1687	-0.1120	-0.1752	0.2849	-0.2148	-0.0192	-0.1185	0.2004	0.0192	0.2862	0.2054	0.1177	-0.1765	-0.1292	0.0000	
131	-0.2341	-0.1687	-0.1120	0.1752	0.2849	0.2147	0.0192	0.1186	0.2004	0.0192	-0.2862	-0.2054	-0.1177	-0.1765	0.1292	0.0000	
132	0.2340	0.1687	-0.1120	0.1752	0.2849	0.2148	-0.0192	0.1185	-0.2004	0.0192	0.2862	-0.2054	-0.1177	-0.1765	0.1292	0.0000	
133	-0.0736	0.1729	-0.0751	0.1977	-0.2689	0.1900	0.2088	-0.1149	0.2591	0.1448	0.2741	0.1677	-0.1667	0.1628	0.0984	0.0000	
134	0.0736	-0.1729	-0.0751	0.1977	-0.2690	0.1900	-0.2088	-0.1149	-0.2590	0.1448	-0.2741	-0.1677	-0.1667	0.1628	0.0984	0.0000	
135	-0.0736	-0.1729	-0.0751	-0.1977	-0.2689	-0.1900	0.2088	0.1149	-0.2591	0.1448	0.2741	-0.1677	0.1667	0.1628	-0.0984	0.0000	
136	0.0736	0.1729	-0.0751	-0.1977	-0.2690	-0.1900	-0.2088	0.1149	0.2590	0.1448	-0.2741	0.1677	0.1667	0.1628	-0.0984	0.0000	

85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
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1	0.2684	-0.0562	0.0970	0.0512	0.1052	-0.0591	0.0961	0.0577	-0.2225	-0.1991	0.1470	-0.2967	0.1872	0.0822	0.0414	0.1516
2	0.2625	0.0562	-0.0969	0.0513	0.1054	0.0591	-0.0962	0.0576	0.2227	-0.1989	-0.1471	-0.2968	-0.1867	-0.0823	0.0411	-0.1519
3	-0.2684	-0.0562	-0.0970	0.0512	-0.1052	-0.0591	-0.0961	0.0577	-0.2225	0.1991	-0.1470	-0.2967	0.1872	-0.0822	-0.0414	0.1516
4	-0.2625	0.0562	0.0969	0.0513	-0.1054	0.0591	0.0962	0.0576	0.2227	0.1989	0.1471	-0.2968	-0.1867	0.0823	-0.0411	-0.1519
5	-0.0170	-0.1251	-0.2252	0.1089	-0.2298	0.2990	0.2256	-0.2591	-0.0010	-0.1438	0.0831	0.0318	0.1046	-0.1084	0.1135	-0.0684
6	-0.0168	0.1249	0.2249	0.1084	-0.2298	-0.2992	-0.2261	-0.2591	0.0009	-0.1437	-0.0832	0.0316	-0.1047	0.1080	0.1139	0.0683
7	0.0170	-0.1251	0.2252	0.1089	0.2298	0.2990	-0.2256	-0.2591	-0.0010	0.1438	-0.0831	0.0318	0.1046	0.1084	-0.1135	-0.0684
8	0.0168	0.1249	-0.2249	0.1084	0.2298	-0.2992	0.2261	-0.2591	0.0009	0.1437	0.0832	0.0316	-0.1047	-0.1080	-0.1139	0.0683
9	0.1996	-0.2261	-0.0984	0.1969	-0.0220	-0.1687	-0.1708	0.2192	0.0724	0.2355	-0.0491	0.1076	0.1096	-0.1990	0.0104	-0.1529
10	0.1956	0.2264	0.0985	0.1971	-0.0225	0.1685	0.1709	0.2190	-0.0723	0.2353	0.0493	0.1073	-0.1095	0.1988	0.0111	0.1529
11	-0.1996	-0.2261	0.0984	0.1969	0.0220	-0.1687	0.1708	0.2192	0.0724	-0.2355	0.0491	0.1076	0.1096	0.1990	-0.0104	-0.1529

12	-0.1956	0.2264	-0.0985	0.1971	0.0225	0.1685	-0.1709	0.2190	-0.0723	-0.2353	-0.0493	0.1073	-0.1095	-0.1988	-0.0111	0.1529
13	-0.1153	0.2242	0.1635	-0.2662	0.2426	-0.0176	-0.0256	0.0670	0.0810	-0.0241	0.2171	0.0381	0.2372	-0.1877	0.1153	-0.0874
14	-0.1130	-0.2242	-0.1632	-0.2660	0.2428	0.0180	0.0260	0.0674	-0.0811	-0.0238	-0.2171	0.0378	-0.2373	0.1873	0.1160	0.0874
15	0.1153	0.2242	-0.1635	-0.2662	-0.2426	-0.0176	0.0256	0.0670	0.0810	0.0241	-0.2171	0.0381	0.2372	0.1877	-0.1153	-0.0874
16	0.1130	-0.2242	0.1632	-0.2660	-0.2428	0.0180	-0.0260	0.0674	-0.0811	0.0238	0.2171	0.0378	-0.2373	-0.1873	-0.1160	0.0874
17	0.0126	0.0000	0.0000	-0.0099	0.0038	0.0000	0.0000	-0.0120	0.0000	-0.0027	0.0000	0.0197	0.0000	0.0000	0.0114	0.0000
18	-0.0126	0.0000	0.0000	-0.0099	-0.0038	0.0000	0.0000	-0.0120	0.0000	0.0027	0.0000	0.0197	0.0000	0.0000	-0.0114	0.0000
19	0.0120	0.0028	0.0113	-0.0020	0.0044	0.0001	0.0129	-0.0028	-0.0133	-0.0103	-0.0062	0.0048	-0.0098	0.0042	-0.0148	-0.0145
20	0.0117	-0.0028	-0.0113	-0.0020	0.0045	-0.0001	-0.0129	-0.0028	0.0133	-0.0103	0.0062	0.0048	0.0098	-0.0041	-0.0148	0.0145
21	-0.0120	0.0028	-0.0113	-0.0020	-0.0044	0.0001	-0.0129	-0.0028	-0.0133	0.0103	0.0062	0.0048	-0.0098	-0.0042	0.0148	-0.0145
22	-0.0117	-0.0028	0.0113	-0.0020	-0.0045	-0.0001	0.0129	-0.0028	0.0133	0.0103	-0.0062	0.0048	0.0098	0.0041	0.0148	0.0145
23	-0.0233	0.0204	-0.0026	-0.0184	-0.0058	0.0168	0.0002	-0.0212	0.0184	0.0029	-0.0087	0.0368	-0.0386	0.0047	-0.0152	-0.0226
24	-0.0228	-0.0205	0.0026	-0.0184	-0.0058	-0.0168	-0.0002	-0.0211	-0.0184	0.0029	0.0087	0.0369	0.0385	-0.0047	-0.0152	0.0227
25	0.0233	0.0204	0.0026	-0.0184	0.0058	0.0168	-0.0002	-0.0212	0.0184	-0.0029	0.0087	0.0368	-0.0386	-0.0047	0.0152	-0.0226
26	0.0228	-0.0205	-0.0026	-0.0184	0.0058	-0.0168	0.0002	-0.0211	-0.0184	-0.0029	-0.0087	0.0369	0.0385	0.0047	0.0152	0.0227
27	0.0070	-0.0100	-0.0126	0.0068	-0.0065	-0.0018	-0.0122	-0.0022	0.0161	0.0055	0.0051	0.0129	-0.0066	0.0085	0.0015	0.0125
28	0.0069	0.0100	0.0126	0.0068	-0.0066	0.0018	0.0122	-0.0022	-0.0161	0.0055	-0.0051	0.0129	0.0066	-0.0085	0.0015	-0.0125
29	-0.0070	-0.0100	0.0126	0.0068	0.0065	-0.0018	0.0122	-0.0022	0.0161	-0.0055	-0.0051	0.0129	-0.0066	-0.0085	-0.0015	0.0125
30	-0.0069	0.0100	-0.0126	0.0068	0.0066	0.0018	-0.0122	-0.0022	-0.0161	-0.0055	0.0051	0.0129	0.0066	0.0085	-0.0015	-0.0125
31	-0.0136	0.0000	0.0000	-0.0154	0.0078	0.0000	0.0000	-0.0018	0.0000	0.0011	0.0000	0.0043	0.0000	0.0000	-0.0080	0.0000
32	0.0136	0.0000	0.0000	-0.0154	-0.0078	0.0000	0.0000	-0.0018	0.0000	-0.0011	0.0000	0.0043	0.0000	0.0000	0.0080	0.0000
33	0.0019	0.0000	0.0000	0.0116	-0.0137	0.0000	0.0000	-0.0067	0.0000	-0.0003	0.0000	-0.0035	0.0000	0.0000	-0.0188	0.0000
34	-0.0019	0.0000	0.0000	0.0116	0.0137	0.0000	0.0000	-0.0067	0.0000	0.0003	0.0000	-0.0035	0.0000	0.0000	0.0188	0.0000
35	-0.0028	0.0139	0.0207	-0.0126	0.0216	-0.0250	-0.0188	0.0232	-0.0021	0.0125	-0.0105	-0.0090	-0.0197	0.0247	-0.0256	0.0189
36	-0.0027	-0.0138	-0.0207	-0.0125	0.0216	0.0250	0.0188	0.0232	0.0021	0.0125	0.0105	-0.0089	0.0197	-0.0246	-0.0257	-0.0189
37	0.0028	0.0139	-0.0207	-0.0126	-0.0216	-0.0250	0.0188	0.0232	-0.0021	-0.0125	0.0105	-0.0090	-0.0197	-0.0247	0.0256	0.0189
38	0.0027	-0.0138	0.0207	-0.0125	-0.0216	0.0250	-0.0188	0.0232	0.0021	-0.0125	-0.0105	-0.0089	0.0197	0.0246	0.0257	-0.0189
39	-0.0269	0.0224	0.0068	-0.0200	-0.0016	0.0103	0.0035	-0.0201	0.0062	-0.0080	-0.0078	0.0075	-0.0328	0.0280	-0.0033	0.0178
40	-0.0264	-0.0225	-0.0068	-0.0200	-0.0016	-0.0103	-0.0035	-0.0201	-0.0062	-0.0080	0.0078	0.0075	0.0327	-0.0280	-0.0034	-0.0178
41	0.0269	0.0224	-0.0068	-0.0200	0.0016	0.0103	-0.0035	-0.0201	0.0062	0.0080	0.0078	0.0075	-0.0328	-0.0280	0.0033	0.0178
42	0.0264	-0.0225	0.0068	-0.0200	0.0016	-0.0103	0.0035	-0.0201	-0.0062	0.0080	-0.0078	0.0075	0.0327	0.0280	0.0034	-0.0178
43	0.0030	-0.0153	-0.0146	0.0184	-0.0202	0.0049	0.0033	-0.0074	-0.0078	0.0022	-0.0273	-0.0070	-0.0435	0.0410	-0.0250	0.0258
44	0.0030	0.0153	0.0145	0.0184	-0.0202	-0.0049	-0.0034	-0.0074	0.0078	0.0021	0.0273	-0.0069	0.0435	-0.0410	-0.0251	-0.0258
45	-0.0030	-0.0153	0.0146	0.0184	0.0202	0.0049	-0.0033	-0.0074	-0.0078	-0.0022	0.0273	-0.0070	-0.0435	-0.0410	0.0250	0.0258
46	-0.0030	0.0153	-0.0145	0.0184	0.0202	-0.0049	0.0034	-0.0074	0.0078	-0.0021	-0.0273	-0.0069	0.0435	0.0410	0.0251	-0.0258
47	0.0178	0.0000	0.0000	-0.0046	0.0183	0.0000	0.0000	-0.0058	0.0000	-0.0784	0.0000	0.0024	0.0000	0.0005	-0.3222	0.0000
48	0.0178	0.0000	0.0000	0.0046	0.0183	0.0000	0.0000	0.0058	0.0000	-0.0784	0.0000	-0.0024	0.0000	0.0005	-0.3222	0.0000
49	-0.0092	-0.0461	-0.1289	-0.0007	-0.0155	-0.0022	-0.1558	-0.0012	0.2402	0.0634	0.1206	-0.1420	0.0174	0.0238	0.0496	0.1074
50	-0.0084	0.0461	0.1290	-0.0007	-0.0160	0.0022	0.1559	-0.0011	-0.2403	0.0633	-0.1206	0.1418	-0.0176	-0.0241	0.0495	-0.1073
51	-0.0092	0.0461	-0.1289	0.0007	-0.0155	0.0022	-0.1558	0.0012	-0.2402	0.0634	0.1206	-0.1420	-0.0174	0.0238	0.0496	-0.1074
52	-0.0084	-0.0461	0.1290	0.0007	-0.0160	-0.0022	0.1559	0.0011	0.2403	0.0633	-0.1206	-0.1418	0.0176	-0.0241	0.0495	0.1073
53	0.1851	-0.0151	0.0698	0.0129	0.0599	-0.0137	0.0615	0.0148	-0.0331	-0.0655	0.0629	-0.0524	0.0399	-0.0291	0.2242	0.0313
54	0.1811	0.0151	-0.0697	0.0129	0.0600	0.0136	-0.0614	0.0148	0.0332	-0.0654	-0.0629	-0.0524	-0.0398	0.0283	0.2242	-0.0314
55	0.1851	0.0151	0.0698	-0.0129	0.0599	0.0137	0.0615	-0.0148	0.0331	-0.0655	0.0629	0.0524	-0.0399	-0.0291	0.2242	-0.0313
56	0.1811	-0.0151	-0.0697	-0.0129	0.0600	-0.0136	-0.0614	-0.0148	-0.0332	-0.0654	-0.0629	0.0524	0.0398	0.0283	0.2242	0.0314
57	0.0105	-0.0595	-0.1282	0.0110	-0.0076	-0.0163	-0.1617	0.0202	0.2277	0.0705	0.1280	0.1198	0.0452	0.0098	0.0631	0.1072
58	0.0109	0.0595	0.1283	0.0110	-0.0080	0.0163	0.1618	0.0202	-0.2278	0.0704	-0.1279	0.1196	-0.0454	-0.0101	0.0630	-0.1072
59	0.0105	0.0595	-0.1282	-0.0110	-0.0076	0.0163	-0.1617	-0.0202	-0.2277	0.0705	0.1280	-0.1198	-0.0452	0.0098	0.0631	-0.1072
60	0.0109	-0.0595	0.1283	-0.0110	-0.0080	-0.0163	0.1618	-0.0202	0.2278	0.0704	-0.1279	-0.1196	0.0454	-0.0101	0.0630	0.1072





18	0.7452	1.1281	1.1427	0.9960	4.0120	-0.0120
19	0.7565	1.1212	1.1501	0.9937	4.0216	-0.0216
20	0.7565	1.1212	1.1501	0.9937	4.0216	-0.0216
21	0.7565	1.1212	1.1501	0.9937	4.0216	-0.0216
22	0.7565	1.1212	1.1501	0.9937	4.0216	-0.0216
23	0.8365	1.1440	1.0993	1.0087	4.0885	-0.0885
24	0.8365	1.1440	1.0993	1.0087	4.0885	-0.0885
25	0.8365	1.1440	1.0993	1.0087	4.0885	-0.0885
26	0.8365	1.1440	1.0993	1.0087	4.0885	-0.0885
27	0.7575	1.1217	1.1495	0.9922	4.0208	-0.0208
28	0.7575	1.1217	1.1495	0.9922	4.0208	-0.0208
29	0.7575	1.1217	1.1495	0.9922	4.0208	-0.0208
30	0.7575	1.1217	1.1495	0.9922	4.0208	-0.0208
31	0.7446	1.1376	1.1388	0.9976	4.0185	-0.0185
32	0.7446	1.1376	1.1388	0.9976	4.0185	-0.0185
33	0.7511	1.1297	1.1846	0.9772	4.0425	-0.0425
34	0.7511	1.1297	1.1846	0.9772	4.0425	-0.0425
35	0.8360	1.0990	1.1393	1.0102	4.0845	-0.0845
36	0.8360	1.0990	1.1393	1.0102	4.0845	-0.0845
37	0.8360	1.0990	1.1393	1.0102	4.0845	-0.0845
38	0.8360	1.0990	1.1393	1.0102	4.0845	-0.0845
39	0.8375	1.1438	1.0981	1.0110	4.0904	-0.0904
40	0.8375	1.1438	1.0981	1.0110	4.0904	-0.0904
41	0.8375	1.1438	1.0981	1.0110	4.0904	-0.0904
42	0.8375	1.1438	1.0981	1.0110	4.0904	-0.0904
43	0.8442	1.1425	1.1136	0.9988	4.0991	-0.0991
44	0.8442	1.1425	1.1136	0.9988	4.0991	-0.0991
45	0.8442	1.1425	1.1136	0.9988	4.0991	-0.0991
46	0.8442	1.1425	1.1136	0.9988	4.0991	-0.0991

SUM    136.0000    0.0000

PI ELECTRON CENTER OF CHARGE:    X,Y = 0.0000 , 0.0000

CHARGE CENTERED X,Y-COORDINATES FOR PI SYSTEM:

1	0.7105	0.0000
2	-0.7105	0.0000
3	-1.4271	-1.2180
4	-1.4271	1.2180
5	1.4271	-1.2180
6	1.4271	1.2180
7	-0.6997	-2.4218
8	-0.6997	2.4218
9	0.6997	-2.4218
10	0.6997	2.4218
11	-2.9143	-1.2246
12	-2.9143	1.2246
13	2.9143	-1.2246
14	2.9143	1.2246
15	-3.6178	0.0000

16	3.6178	0.0000
17	-5.0324	0.0000
18	5.0324	0.0000
19	-5.7470	-1.2100
20	-5.7470	1.2100
21	5.7470	-1.2100
22	5.7470	1.2100
23	-3.6506	-2.4290
24	-3.6505	2.4290
25	3.6506	-2.4290
26	3.6505	2.4290
27	-5.0531	-2.4263
28	-5.0530	2.4263
29	5.0531	-2.4263
30	5.0530	2.4263

SCF-CALCULATION

TERRYLENE, 15pi x 15pi\* CIS

CONFIGURATION INTERACTION:

IGCCI= 1 NB=90 NAB=90 ITRIP= 0 IDOB=-1 MCD= 1 EMAX= 20.00

OCC.ORB. NO.	VIRT.ORB. NO.	CONFIGURATION ENERGY IN EV		CONF. NO.	TRANSITION MOMENT				
		SINGLET	TRIPLET		SX	SY	SZ	OSC	
68	---->	69	2.3390	1.3282	2	-13.75565	0.00000	0.00000	1.67858
67	---->	69	3.7315	3.0256	3	0.00000	0.00033	0.00000	0.00000
66	---->	69	3.7913	3.3961	4	0.00036	0.00000	0.00000	0.00000
65	---->	69	4.1456	3.7936	5	0.00000	-1.49951	0.00000	0.03535
64	---->	69	4.5046	4.0736	6	-0.00003	0.00000	0.00000	0.00000
63	---->	69	4.5467	3.9272	7	0.00000	-7.80440	0.00000	1.05035
62	---->	69	4.9305	4.2234	8	1.13160	0.00000	0.00000	0.02395
61	---->	69	5.3965	5.0291	9	0.00000	0.58216	0.00000	0.00694
55	---->	69	6.6818	6.2025	10	0.00000	-0.00006	0.00000	0.00000
51	---->	69	6.9337	6.4371	11	-0.00002	0.00000	0.00000	0.00000
48	---->	69	7.4657	6.9910	12	-0.56669	0.00000	0.00000	0.00909
42	---->	69	7.8983	7.3113	13	0.00000	-0.00006	0.00000	0.00000
37	---->	69	8.5906	8.2822	14	0.00000	0.05924	0.00000	0.00011
33	---->	69	9.6456	9.3394	15	0.00001	0.00000	0.00000	0.00000
31	---->	69	10.1831	9.8016	16	0.00000	-0.50538	0.00000	0.00986
68	---->	70	3.6263	2.9158	17	0.00000	0.00048	0.00000	0.00000
67	---->	70	5.1716	4.3281	18	-2.84246	0.00000	0.00000	0.15848
66	---->	70	5.3687	5.0026	19	0.00000	1.82488	0.00000	0.06781
65	---->	70	5.6172	5.2995	20	-0.00011	0.00000	0.00000	0.00000
64	---->	70	5.8705	5.4114	21	0.00000	-6.44122	0.00000	0.92378
63	---->	70	5.8894	5.5823	22	-0.00022	0.00000	0.00000	0.00000



62	---->	70	6.2813	5.7634	23	0.00000	0.00049	0.00000	0.00000
61	---->	70	6.9252	6.3237	24	0.00011	0.00000	0.00000	0.00000
55	---->	70	8.1337	7.7009	25	-0.70365	0.00000	0.00000	0.01527
51	---->	70	8.3423	7.9496	26	0.00000	0.48998	0.00000	0.00760
48	---->	70	8.9012	8.3527	27	0.00000	0.00005	0.00000	0.00000
42	---->	70	9.3491	8.9557	28	0.04130	0.00000	0.00000	0.00006
37	---->	70	10.0528	9.7713	29	0.00001	0.00000	0.00000	0.00000
33	---->	70	11.0792	10.6758	30	0.00000	0.42817	0.00000	0.00770
31	---->	70	11.7135	11.4447	31	0.00000	0.00000	0.00000	0.00000
68	---->	71	3.4819	3.0862	32	0.00014	0.00000	0.00000	0.00000
67	---->	71	5.1594	4.7998	33	0.00000	-1.69552	0.00000	0.05626
66	---->	71	5.5771	4.8635	34	8.27256	0.00000	0.00000	1.44758
65	---->	71	5.8277	5.4121	35	0.00000	0.00030	0.00000	0.00000
64	---->	71	6.1270	5.8223	36	1.21198	0.00000	0.00000	0.03414
63	---->	71	6.0177	5.4871	37	0.00000	0.00034	0.00000	0.00000
62	---->	71	6.4156	5.9020	38	0.00032	0.00000	0.00000	0.00000
61	---->	71	7.1671	6.6635	39	0.00000	0.00006	0.00000	0.00000
55	---->	71	8.2585	8.0320	40	0.00000	-0.28579	0.00000	0.00256
51	---->	71	8.5917	8.0706	41	-0.40884	0.00000	0.00000	0.00545
48	---->	71	9.0547	8.8098	42	-0.00010	0.00000	0.00000	0.00000
42	---->	71	9.3831	9.0259	43	0.00000	-1.01528	0.00000	0.03668
37	---->	71	10.2982	9.8806	44	0.00000	-0.00005	0.00000	0.00000
33	---->	71	11.3348	10.9450	45	0.19988	0.00000	0.00000	0.00172
31	---->	71	11.7717	11.2670	46	0.00000	0.00001	0.00000	0.00000
68	---->	72	3.7683	3.4090	47	0.00000	-0.13094	0.00000	0.00025
67	---->	72	5.3762	5.0987	48	-0.00026	0.00000	0.00000	0.00000
66	---->	72	5.7543	5.2810	49	0.00000	-0.00043	0.00000	0.00000
65	---->	72	6.1954	5.5136	50	5.35126	0.00000	0.00000	0.67288
64	---->	72	6.4898	5.9890	51	0.00000	0.00036	0.00000	0.00000
63	---->	72	6.4489	5.5258	52	-0.82529	0.00000	0.00000	0.01666
62	---->	72	6.6322	6.2851	53	0.00000	5.88065	0.00000	0.86989
61	---->	72	7.3368	7.0242	54	-0.44838	0.00000	0.00000	0.00559
55	---->	72	8.5593	8.1245	55	-0.00004	0.00000	0.00000	0.00000
51	---->	72	8.7667	8.4466	56	0.00000	-0.00019	0.00000	0.00000
48	---->	72	9.3276	9.0487	57	0.00000	1.13147	0.00000	0.04529
42	---->	72	9.6476	9.2319	58	-0.00006	0.00000	0.00000	0.00000
37	---->	72	10.5582	10.1237	59	0.25167	0.00000	0.00000	0.00254
33	---->	72	11.5893	11.3157	60	0.00000	0.00000	0.00000	0.00000
31	---->	72	12.0349	11.6216	61	-0.01902	0.00000	0.00000	0.00002
68	---->	73	4.2855	3.8731	62	-0.00006	0.00000	0.00000	0.00000
67	---->	73	5.7667	5.3133	63	0.00000	-6.43814	0.00000	0.90658
66	---->	73	6.2416	5.9253	64	-1.16388	0.00000	0.00000	0.03207
65	---->	73	6.6366	5.9559	65	0.00000	-0.00002	0.00000	0.00000
64	---->	73	6.8051	5.7873	66	4.60496	0.00000	0.00000	0.54732
63	---->	73	6.8369	6.4623	67	0.00000	-0.00024	0.00000	0.00000
62	---->	73	7.0139	6.7549	68	-0.00023	0.00000	0.00000	0.00000
61	---->	73	7.6446	7.1985	69	0.00000	0.00011	0.00000	0.00000
55	---->	73	8.9383	8.5290	70	0.00000	-0.80694	0.00000	0.02207
51	---->	73	9.1496	8.8533	71	0.29496	0.00000	0.00000	0.00302
48	---->	73	9.6145	9.0834	72	-0.00004	0.00000	0.00000	0.00000
42	---->	73	10.1825	9.9625	73	0.00000	0.79147	0.00000	0.02419

37	---->	73	10.9256	10.5307	74	0.00000	0.00002	0.00000	0.00000
33	---->	73	11.8688	11.3818	75	-0.15745	0.00000	0.00000	0.00112
31	---->	73	12.6152	12.4036	76	0.00000	-0.00001	0.00000	0.00000
68	---->	74	4.4067	3.8182	77	0.00000	-7.87884	0.00000	1.03753
67	---->	74	5.8319	5.4879	78	-0.00018	0.00000	0.00000	0.00000
66	---->	74	6.2223	5.7300	79	0.00000	-0.00014	0.00000	0.00000
65	---->	74	6.6773	5.9323	80	0.79534	0.00000	0.00000	0.01602
64	---->	74	6.8774	6.3250	81	0.00000	-0.00029	0.00000	0.00000
63	---->	74	6.7693	5.9998	82	3.99903	0.00000	0.00000	0.41059
62	---->	74	6.9662	6.7124	83	0.00000	0.28136	0.00000	0.00209
61	---->	74	7.7479	7.4142	84	0.71260	0.00000	0.00000	0.01492
55	---->	74	8.9881	8.5376	85	-0.00004	0.00000	0.00000	0.00000
51	---->	74	9.1586	8.8606	86	0.00000	0.00007	0.00000	0.00000
48	---->	74	9.7049	9.4093	87	0.00000	-0.43707	0.00000	0.00703
42	---->	74	10.0398	9.6786	88	0.00000	0.00000	0.00000	0.00000
37	---->	74	10.9753	10.5387	89	0.06949	0.00000	0.00000	0.00020
33	---->	74	11.9764	11.6923	90	0.00000	0.00002	0.00000	0.00000
31	---->	74	12.4512	12.0812	91	0.09268	0.00000	0.00000	0.00041
68	---->	75	4.6177	3.9067	92	1.20878	0.00000	0.00000	0.02559
67	---->	75	6.0770	5.5546	93	0.00000	0.00011	0.00000	0.00000
66	---->	75	6.4125	5.8851	94	-0.00027	0.00000	0.00000	0.00000
65	---->	75	6.6837	6.3610	95	0.00000	5.83550	0.00000	0.86323
64	---->	75	6.9032	6.6584	96	-0.00018	0.00000	0.00000	0.00000
63	---->	75	6.7691	6.5132	97	0.00000	-0.64572	0.00000	0.01070
62	---->	75	7.3341	6.6796	98	-0.44218	0.00000	0.00000	0.00544
61	---->	75	7.9224	7.5425	99	0.00000	0.61846	0.00000	0.01149
55	---->	75	9.2015	8.7737	100	0.00000	0.00003	0.00000	0.00000
51	---->	75	9.4144	8.9164	101	-0.00012	0.00000	0.00000	0.00000
48	---->	75	9.9255	9.5513	102	0.03043	0.00000	0.00000	0.00003
42	---->	75	10.3128	9.8739	103	0.00000	0.00004	0.00000	0.00000
37	---->	75	11.1159	10.8050	104	0.00000	0.20856	0.00000	0.00183
33	---->	75	12.1490	11.8509	105	-0.00001	0.00000	0.00000	0.00000
31	---->	75	12.6663	12.2944	106	0.00000	-0.07700	0.00000	0.00028
68	---->	76	4.9509	4.5823	107	0.00000	-0.35776	0.00000	0.00240
67	---->	76	6.5800	5.9864	108	-0.00019	0.00000	0.00000	0.00000
66	---->	76	7.0330	6.5332	109	0.00000	0.00008	0.00000	0.00000
65	---->	76	7.2276	6.8712	110	0.35421	0.00000	0.00000	0.00344
64	---->	76	7.4041	6.9584	111	0.00000	-0.00018	0.00000	0.00000
63	---->	76	7.4766	7.1921	112	-0.77970	0.00000	0.00000	0.01724
62	---->	76	7.7859	7.4166	113	0.00000	-0.61471	0.00000	0.01116
61	---->	76	8.5053	7.8608	114	3.82925	0.00000	0.00000	0.47301
55	---->	76	9.6601	9.4180	115	0.00030	0.00000	0.00000	0.00000
51	---->	76	9.9411	9.5192	116	0.00000	-0.00018	0.00000	0.00000
48	---->	76	10.3918	10.0471	117	0.00000	1.23446	0.00000	0.06006
42	---->	76	10.9015	10.6506	118	0.00000	0.00000	0.00000	0.00000
37	---->	76	11.6687	11.3028	119	0.38451	0.00000	0.00000	0.00654
33	---->	76	12.6606	12.1777	120	0.00000	-0.00005	0.00000	0.00000
31	---->	76	13.3075	13.0034	121	0.07151	0.00000	0.00000	0.00026
68	---->	77	6.2614	5.7692	122	0.00000	-0.00011	0.00000	0.00000
67	---->	77	7.8228	7.3939	123	-0.77336	0.00000	0.00000	0.01775
66	---->	77	8.1450	7.9011	124	0.00000	0.22810	0.00000	0.00161

65	---->	77	8.4896	8.0632	125	-0.00005	0.00000	0.00000	0.00000
64	---->	77	8.7306	8.3469	126	0.00000	-0.82913	0.00000	0.02276
63	---->	77	8.7061	8.2115	127	-0.00003	0.00000	0.00000	0.00000
62	---->	77	9.1017	8.6416	128	0.00000	0.00006	0.00000	0.00000
61	---->	77	9.6914	9.4563	129	-0.00035	0.00000	0.00000	0.00000
55	---->	77	10.9744	10.4117	130	0.96069	0.00000	0.00000	0.03841
51	---->	77	11.1809	10.8999	131	0.00000	-1.34722	0.00000	0.07697
48	---->	77	11.7100	11.3107	132	0.00000	-0.00020	0.00000	0.00000
42	---->	77	12.1312	11.6615	133	-0.11294	0.00000	0.00000	0.00059
37	---->	77	12.9283	12.6630	134	-0.00003	0.00000	0.00000	0.00000
33	---->	77	13.9591	13.7699	135	0.00000	-0.29915	0.00000	0.00474
31	---->	77	14.5130	14.2921	136	-0.00001	0.00000	0.00000	0.00000
68	---->	78	6.2634	5.7746	137	0.00015	0.00000	0.00000	0.00000
67	---->	78	7.7820	7.3985	138	0.00000	-0.39081	0.00000	0.00451
66	---->	78	8.2346	7.7099	139	-0.42381	0.00000	0.00000	0.00561
65	---->	78	8.4620	8.1515	140	0.00000	0.00012	0.00000	0.00000
64	---->	78	8.6996	8.4066	141	-0.32728	0.00000	0.00000	0.00353
63	---->	78	8.6285	8.3312	142	0.00000	-0.00005	0.00000	0.00000
62	---->	78	9.0605	8.5680	143	0.00011	0.00000	0.00000	0.00000
61	---->	78	9.7247	9.3051	144	0.00000	-0.00011	0.00000	0.00000
55	---->	78	10.9336	10.6738	145	0.00000	1.36232	0.00000	0.07696
51	---->	78	11.2094	10.6793	146	1.66408	0.00000	0.00000	0.11773
48	---->	78	11.6798	11.4333	147	0.00019	0.00000	0.00000	0.00000
42	---->	78	12.1025	11.8165	148	0.00000	-0.00337	0.00000	0.00000
37	---->	78	12.9307	12.5230	149	0.00000	0.00001	0.00000	0.00000
33	---->	78	13.9380	13.6122	150	-0.14173	0.00000	0.00000	0.00106
31	---->	78	14.4888	14.1294	151	0.00000	0.00002	0.00000	0.00000
68	---->	79	6.9866	6.5175	152	0.65970	0.00000	0.00000	0.01153
67	---->	79	8.5249	7.9730	153	0.00000	0.00005	0.00000	0.00000
66	---->	79	8.8967	8.6637	154	-0.00013	0.00000	0.00000	0.00000
65	---->	79	9.1861	8.8159	155	0.00000	-0.81083	0.00000	0.02291
64	---->	79	9.3375	8.7800	156	0.00004	0.00000	0.00000	0.00000
63	---->	79	9.4166	9.2013	157	0.00000	0.57230	0.00000	0.01170
62	---->	79	9.7659	9.3856	158	0.03391	0.00000	0.00000	0.00004
61	---->	79	10.3573	10.0078	159	0.00000	1.22848	0.00000	0.05928
55	---->	79	11.6489	11.2125	160	0.00000	0.00012	0.00000	0.00000
51	---->	79	11.8636	11.6127	161	0.00018	0.00000	0.00000	0.00000
48	---->	79	12.3685	11.7659	162	-0.73033	0.00000	0.00000	0.02502
42	---->	79	12.8791	12.5728	163	0.00000	0.00001	0.00000	0.00000
37	---->	79	13.6093	13.3937	164	0.00000	0.23921	0.00000	0.00295
33	---->	79	14.5885	14.2754	165	-0.00002	0.00000	0.00000	0.00000
31	---->	79	15.2928	15.1003	166	0.00000	-0.15385	0.00000	0.00137
68	---->	80	7.3116	6.7365	167	0.00000	-0.00004	0.00000	0.00000
67	---->	80	8.8605	8.4563	168	0.07487	0.00000	0.00000	0.00019
66	---->	80	9.1194	8.7713	169	0.00000	1.07515	0.00000	0.03998
65	---->	80	9.4738	9.1111	170	-0.00005	0.00000	0.00000	0.00000
64	---->	80	9.7806	9.5241	171	0.00000	0.70056	0.00000	0.01821
63	---->	80	9.5617	9.1505	172	0.00000	0.00000	0.00000	0.00000
62	---->	80	10.0497	9.6165	173	0.00000	0.00005	0.00000	0.00000
61	---->	80	10.7453	10.4920	174	-0.00003	0.00000	0.00000	0.00000
55	---->	80	11.9735	11.5245	175	-0.03800	0.00000	0.00000	0.00007

51	---->	80	12.1850	11.9034	176	0.00000	-0.04967	0.00000	0.00011
48	---->	80	12.7490	12.4072	177	0.00000	0.00000	0.00000	0.00000
42	---->	80	13.0509	12.5465	178	0.68828	0.00000	0.00000	0.02345
37	---->	80	13.9387	13.7200	179	0.00000	0.00000	0.00000	0.00000
33	---->	80	15.0024	14.7868	180	0.00000	0.13341	0.00000	0.00101
31	---->	80	15.4225	15.1152	181	0.00000	0.00000	0.00000	0.00000
68	---->	81	7.7907	7.4807	182	0.00000	-0.00841	0.00000	0.00000
67	---->	81	9.3649	9.0955	183	0.00004	0.00000	0.00000	0.00000
66	---->	81	9.8048	9.3843	184	0.00000	-0.00005	0.00000	0.00000
65	---->	81	10.1132	9.6946	185	-0.38673	0.00000	0.00000	0.00574
64	---->	81	10.3484	9.9732	186	0.00000	0.00000	0.00000	0.00000
63	---->	81	10.3181	9.8604	187	-0.00611	0.00000	0.00000	0.00000
62	---->	81	10.6328	10.3138	188	0.00000	-0.38435	0.00000	0.00596
61	---->	81	11.3225	10.9726	189	0.41951	0.00000	0.00000	0.00756
55	---->	81	12.5544	12.2904	190	0.00003	0.00000	0.00000	0.00000
51	---->	81	12.7984	12.3888	191	0.00000	-0.00001	0.00000	0.00000
48	---->	81	13.2999	13.0971	192	0.00000	0.21470	0.00000	0.00233
42	---->	81	13.7222	13.4917	193	-0.00001	0.00000	0.00000	0.00000
37	---->	81	14.5600	14.1329	194	0.41346	0.00000	0.00000	0.00944
33	---->	81	15.5698	15.2698	195	0.00000	-0.00002	0.00000	0.00000
31	---->	81	16.1261	15.7970	196	0.06775	0.00000	0.00000	0.00028
68	---->	82	8.7125	8.4129	197	0.00002	0.00000	0.00000	0.00000
67	---->	82	10.2471	9.8503	198	0.00000	0.56380	0.00000	0.01235
66	---->	82	10.7204	10.3407	199	-0.23183	0.00000	0.00000	0.00219
65	---->	82	10.9892	10.6422	200	0.00000	0.00003	0.00000	0.00000
64	---->	82	11.1363	10.6454	201	-0.28547	0.00000	0.00000	0.00344
63	---->	82	11.2357	11.0301	202	0.00000	0.00003	0.00000	0.00000
62	---->	82	11.5313	11.2465	203	-0.00004	0.00000	0.00000	0.00000
61	---->	82	12.1699	11.6944	204	0.00000	0.00004	0.00000	0.00000
55	---->	82	13.4409	13.2378	205	0.00000	-0.20596	0.00000	0.00216
51	---->	82	13.6679	13.3484	206	0.19367	0.00000	0.00000	0.00194
48	---->	82	14.1368	13.8165	207	0.00003	0.00000	0.00000	0.00000
42	---->	82	14.6808	14.4795	208	0.00000	0.12495	0.00000	0.00087
37	---->	82	15.4267	15.1134	209	0.00000	0.00001	0.00000	0.00000
33	---->	82	16.3935	15.9428	210	-0.14923	0.00000	0.00000	0.00138
31	---->	82	17.0851	16.8161	211	0.00000	0.00000	0.00000	0.00000
68	---->	83	9.1053	8.7327	212	0.00000	-0.65215	0.00000	0.01469
67	---->	83	10.7317	10.4578	213	-0.00002	0.00000	0.00000	0.00000
66	---->	83	11.0108	10.5226	214	0.00000	-0.00001	0.00000	0.00000
65	---->	83	11.3766	11.0314	215	0.01023	0.00000	0.00000	0.00000
64	---->	83	11.7198	11.4932	216	0.00000	-0.00002	0.00000	0.00000
63	---->	83	11.4613	11.0557	217	0.21134	0.00000	0.00000	0.00194
62	---->	83	11.9105	11.5551	218	0.00000	-0.06836	0.00000	0.00021
61	---->	83	12.6618	12.3486	219	-0.10470	0.00000	0.00000	0.00053
55	---->	83	13.8677	13.6562	220	-0.00003	0.00000	0.00000	0.00000
51	---->	83	14.0806	13.7364	221	0.00000	-0.00002	0.00000	0.00000
48	---->	83	14.6659	14.4518	222	0.00000	0.10118	0.00000	0.00057
42	---->	83	14.9240	14.6098	223	0.00000	0.00000	0.00000	0.00000
37	---->	83	15.8537	15.5397	224	-0.08694	0.00000	0.00000	0.00045
33	---->	83	16.9148	16.6281	225	0.00000	0.00000	0.00000	0.00000
31	---->	83	17.2946	16.8789	226	0.01141	0.00000	0.00000	0.00001

## SINGLET ENERGIES

0.0000	2.2353	3.2604	3.2810	3.4507	3.5086	3.5598	3.6082	3.7605	3.9566	4.3500	4.6024	4.6093	4.6275	4.8501	4.9782
5.0669	5.1652	5.2323	5.2934	5.3171	5.3350	5.3988	5.4557	5.4693	5.6148	5.6559	5.7263	5.7542	5.8377	5.9454	6.0094
6.0393	6.0868	6.1057	6.1636	6.2380	6.3039	6.3080	6.3832	6.4134	6.4403	6.5426	6.5491	6.6052	6.6450	6.7013	6.7512
6.7663	6.7853	6.8936	6.9709	7.0398	7.0997	7.1006	7.1160	7.1559	7.1676	7.1957	7.2190	7.2582	7.2727	7.3677	7.3889
7.3911	7.4808	7.5111	7.5457	7.5464	7.6297	7.7199	7.8518	7.9027	8.0423	8.1000	8.1076	8.1230	8.1669	8.2190	8.2273
8.2938	8.2961	8.3176	8.3381	8.3520	8.4252	8.4817	8.4855	8.5031	8.5449	8.5959	8.6492	8.7356	8.7564	8.7738	8.8014
8.8122	8.8194	8.8533	8.9437	8.9572	9.1197	9.1808	9.1841	9.2025	9.2151	9.2215	9.2308	9.2501	9.2846	9.2847	9.3432
9.3602	9.4081	9.5164	9.5209	9.6336	9.6805	9.6933	9.7218	9.7435	9.7965	9.8450	9.9129	9.9154	9.9635	9.9705	10.0214
10.1027	10.1525	10.1643	10.1956	10.2975	10.3403	10.3410	10.3579	10.3596	10.3798	10.3969	10.4436	10.4788	10.4832	10.6312	10.6961
10.6991	10.7038	10.7098	10.7274	10.7278	10.8027	10.8351	10.9525	10.9879	11.0322	11.0605	11.1094	11.2164	11.3271	11.3360	11.3398
11.3674	11.4228	11.4757	11.5426	11.5559	11.6614	11.6854	11.6881	11.8262	11.8265	11.9036	11.9049	11.9929	12.0129	12.0515	12.0741
12.1785	12.1997	12.2962	12.3047	12.3153	12.3845	12.5055	12.5095	12.5533	12.5622	12.5976	12.6583	12.8483	12.9232	13.0068	13.0450
13.0723	13.1113	13.1328	13.1466	13.2713	13.4788	13.5147	13.5390	13.7621	13.7776	13.8196	14.0084	14.1231	14.2392	14.2542	14.2825
14.3749	14.6118	14.6567	14.6880	14.8655	14.9474	15.2104	15.3939	15.3971	15.4679	15.9035	15.9882	16.0097	16.4330	16.5874	16.7251
17.8132	17.8971														

## SINGLET STATE EIGENVECTORS (VERTICAL)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.0000	-0.9851	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0048	0.0000	0.0202	0.0000	0.0000	0.0000
3	0.0000	0.0000	-0.0001	0.0000	-0.1795	0.0000	0.9516	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0560
4	0.0000	0.0000	0.0000	0.1718	0.0000	0.6282	0.0000	0.0000	-0.7202	0.0000	0.0000	0.1313	-0.0002	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.4436	0.0000	0.0001	0.0000	0.0000	0.1981	0.0000	0.7145	0.0000	0.0000	0.0000	-0.2136	-0.2774	0.0000
6	0.0000	0.0000	0.0000	0.0909	0.0000	-0.4586	0.0000	0.0000	-0.2602	0.0000	0.0000	0.7292	-0.0007	0.0000	0.0000	0.0000
7	0.0000	0.0000	-0.2397	0.0000	0.0000	0.0000	0.0000	0.5260	0.0000	-0.2486	0.0000	0.0000	0.0000	-0.1679	-0.4978	-0.0002
8	0.0000	-0.0321	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2049	0.0008	0.8231	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0113	0.0000	0.0000	0.0000	0.0000	0.0371	0.0000	0.1787	0.0000	0.0000	0.0000	-0.1028	0.3667	-0.0001
10	0.0000	0.0000	0.0000	0.0000	-0.0009	0.0000	-0.0477	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1618
11	0.0000	0.0000	0.0000	0.0132	0.0000	0.0261	0.0000	0.0000	-0.0412	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0125	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0184	0.0000	0.0422	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000	0.0092	0.0000	-0.0048	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0536
14	0.0000	0.0000	-0.0121	0.0000	0.0000	0.0000	0.0000	-0.0049	0.0000	-0.0651	0.0000	0.0000	0.0000	-0.0076	-0.0237	0.0000
15	0.0000	0.0000	0.0000	-0.0139	0.0000	-0.0278	0.0000	0.0000	0.0037	0.0000	0.0000	0.0198	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0049	0.0000	0.0000	0.0000	0.0000	-0.0142	0.0000	0.0076	0.0000	0.0000	0.0000	0.0106	0.0160	0.0000
17	0.0000	0.0000	-0.0001	0.0000	0.9502	0.0000	0.1931	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0552
18	0.0000	-0.1289	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2204	-0.0004	-0.4433	0.0000	0.0000	0.0000
19	0.0000	0.0000	-0.0640	0.0000	0.0000	0.0000	0.0000	-0.0147	0.0000	-0.1921	0.0000	0.0000	0.0000	0.0755	-0.4708	0.0001
20	0.0000	0.0000	0.0000	0.0361	0.0000	-0.2620	0.0000	0.0000	-0.0953	0.0000	0.0000	0.1426	-0.0001	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.1044	0.0000	0.0000	0.0000	0.0000	0.2999	0.0000	0.1358	0.0000	0.0000	0.0000	-0.0365	-0.0450	0.0000
22	0.0000	0.0000	0.0000	0.0251	0.0000	-0.1583	0.0000	0.0000	-0.0969	0.0000	0.0000	0.0362	-0.0001	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000	0.0927	0.0000	-0.1293	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0132
24	0.0000	0.0000	0.0000	-0.0286	0.0000	-0.0795	0.0000	0.0000	0.1006	0.0000	0.0000	-0.0546	0.0001	0.0000	0.0000	0.0000
25	0.0000	0.0163	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0573	-0.0001	-0.0773	0.0000	0.0000	0.0000
26	0.0000	0.0000	-0.0125	0.0000	0.0000	0.0000	0.0000	0.0035	0.0000	-0.0230	0.0000	0.0000	0.0000	-0.0315	0.0316	0.0000

27	0.0000	0.0000	0.0000	0.0000	-0.0026	0.0000	-0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0448
28	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0077	0.0000	0.0164	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0152	0.0000	0.0301	0.0000	0.0000	-0.0076	0.0000	0.0000	-0.0084	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0000	0.0021	0.0000	0.0000	0.0000	0.0000	0.0147	0.0000	0.0111	0.0000	0.0000	0.0000	-0.0072	0.0003	0.0000
31	0.0000	0.0000	0.0000	-0.0028	0.0000	0.0070	0.0000	0.0000	0.0023	0.0000	0.0000	-0.0071	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000	-0.9076	0.0000	-0.1201	0.0000	0.0000	-0.3439	0.0000	0.0000	-0.0765	0.0001	0.0000	0.0000	0.0000
33	0.0000	0.0000	-0.1203	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.1733	0.0000	0.0000	0.0000	0.5364	-0.1053	0.0000
34	0.0000	-0.0460	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0353	0.0001	0.0705	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0159	0.0000	-0.0240	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.5562
36	0.0000	0.0090	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0327	-0.0001	-0.1153	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	-0.0350	0.0000	0.0721	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.3136
38	0.0000	0.0000	0.0000	-0.0534	0.0000	0.0114	0.0000	0.0000	-0.0261	0.0000	0.0000	0.0287	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	-0.0564	0.0000	-0.0270	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0073
40	0.0000	0.0000	0.0617	0.0000	0.0000	0.0000	0.0000	0.0150	0.0000	-0.0012	0.0000	0.0000	0.0000	-0.0389	-0.0111	0.0000
41	0.0000	-0.0095	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0634	0.0000	0.0336	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0252	0.0000	-0.0267	0.0000	0.0000	-0.0283	0.0000	0.0000	0.0255	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	-0.0207	0.0000	0.0000	0.0000	0.0000	0.0428	0.0000	-0.0076	0.0000	0.0000	0.0000	-0.0122	-0.0055	0.0000
44	0.0000	0.0000	0.0000	0.0000	-0.0032	0.0000	-0.0076	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0155
45	0.0000	-0.0076	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0149	0.0000	0.0005	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0073	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0069
47	0.0000	0.0000	-0.7652	0.0000	0.0000	0.0000	0.0000	-0.1452	0.0000	0.4693	0.0000	0.0000	0.0000	-0.2815	-0.0792	0.0000
48	0.0000	0.0000	0.0000	-0.1516	0.0000	0.1721	0.0000	0.0000	0.1525	0.0000	0.0000	0.0574	-0.0001	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0374	0.0000	-0.0103	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.6029
50	0.0000	-0.0511	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0065	0.0000	-0.0083	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000	0.0555	0.0000	0.0783	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0587
52	0.0000	0.0295	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0947	-0.0002	-0.1732	0.0000	0.0000	0.0000
53	0.0000	0.0000	-0.0826	0.0000	0.0000	0.0000	0.0000	0.1443	0.0000	0.0234	0.0000	0.0000	0.0000	-0.0461	-0.0699	0.0000
54	0.0000	0.0064	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0348	0.0001	0.0560	0.0000	0.0000	0.0000
55	0.0000	0.0000	0.0000	0.0066	0.0000	0.0032	0.0000	0.0000	0.0118	0.0000	0.0000	-0.0433	0.0000	0.0000	0.0000	0.0000
56	0.0000	0.0000	0.0000	0.0000	0.0236	0.0000	-0.0234	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0672
57	0.0000	0.0000	-0.0106	0.0000	0.0000	0.0000	0.0000	0.0115	0.0000	-0.0118	0.0000	0.0000	0.0000	-0.0001	-0.0042	0.0000
58	0.0000	0.0000	0.0000	0.0023	0.0000	-0.0009	0.0000	0.0000	-0.0052	0.0000	0.0000	0.0200	0.0000	0.0000	0.0000	0.0000
59	0.0000	0.0089	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	0.0059	0.0000	0.0000	0.0000
60	0.0000	0.0000	0.0000	0.0000	0.0105	0.0000	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0134
61	0.0000	-0.0023	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0064	0.0000	0.0000	0.0000
62	0.0000	0.0000	0.0000	-0.2694	0.0000	0.4410	0.0000	0.0000	0.4408	0.0000	0.0000	0.6277	-0.0007	0.0000	0.0000	0.0000
63	0.0000	0.0000	-0.1444	0.0000	0.0000	0.0000	0.0000	-0.3199	0.0000	0.0517	0.0000	0.0000	0.0000	-0.0187	0.0464	0.0000
64	0.0000	-0.0082	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0879	0.0000	-0.0139	0.0000	0.0000	0.0000
65	0.0000	0.0000	0.0000	0.0000	0.0538	0.0000	0.0875	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0374
66	0.0000	-0.0234	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0797	-0.0001	-0.1412	0.0000	0.0000	0.0000
67	0.0000	0.0000	0.0000	0.0000	0.0299	0.0000	0.0363	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0230
68	0.0000	0.0000	0.0000	0.0599	0.0000	-0.0753	0.0000	0.0000	-0.0733	0.0000	0.0000	0.0938	-0.0001	0.0000	0.0000	0.0000
69	0.0000	0.0000	0.0000	0.0000	0.0257	0.0000	-0.0168	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1338
70	0.0000	0.0000	-0.0090	0.0000	0.0000	0.0000	0.0000	-0.0109	0.0000	-0.0188	0.0000	0.0000	0.0000	0.0165	0.0270	0.0000
71	0.0000	0.0050	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0244	0.0000	0.0387	0.0000	0.0000	0.0000
72	0.0000	0.0000	0.0000	0.0069	0.0000	0.0011	0.0000	0.0000	0.0029	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000
73	0.0000	0.0000	0.0070	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0058	0.0000	0.0000	0.0000	-0.0122	-0.0088	0.0000
74	0.0000	0.0000	0.0000	0.0000	-0.0046	0.0000	-0.0111	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0048
75	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0131	0.0000	-0.0100	0.0000	0.0000	0.0000
76	0.0000	0.0000	0.0000	0.0000	-0.0080	0.0000	-0.0056	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0057
77	0.0000	0.0000	0.2175	0.0000	0.0000	0.0000	0.0001	-0.6389	0.0000	-0.0632	0.0000	0.0000	0.0000	-0.2208	-0.4736	-0.0002



129	0.0000	0.0000	0.0000	-0.0023	0.0000	0.0461	0.0000	0.0000	0.0082	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000
130	0.0000	-0.0031	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0019	0.0000	-0.0018	0.0000	0.0000	0.0000
131	0.0000	0.0000	0.0101	0.0000	0.0000	0.0000	0.0000	-0.0302	0.0000	0.0031	0.0000	0.0000	0.0000	0.0024	0.0200	0.0000
132	0.0000	0.0000	0.0000	0.0000	-0.0121	0.0000	0.0110	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
133	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0147	0.0000	-0.0114	0.0000	0.0000	0.0000
134	0.0000	0.0000	0.0000	0.0003	0.0000	-0.0011	0.0000	0.0000	0.0132	0.0000	0.0000	-0.0040	0.0000	0.0000	0.0000	0.0000
135	0.0000	0.0000	0.0038	0.0000	0.0000	0.0000	0.0000	-0.0025	0.0000	0.0017	0.0000	0.0000	0.0000	0.0079	0.0001	0.0000
136	0.0000	0.0000	0.0000	-0.0016	0.0000	-0.0011	0.0000	0.0000	-0.0014	0.0000	0.0000	0.0032	0.0000	0.0000	0.0000	0.0000
137	0.0000	0.0000	0.0000	-0.0475	0.0000	-0.0130	0.0000	0.0000	-0.0188	0.0000	0.0000	0.0173	0.0000	0.0000	0.0000	0.0000
138	0.0000	0.0000	-0.0216	0.0000	0.0000	0.0000	0.0000	0.0020	0.0000	0.0038	0.0000	0.0000	0.0000	-0.0752	0.0407	0.0000
139	0.0000	-0.0094	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0100	0.0001	0.0803	0.0000	0.0000	0.0000
140	0.0000	0.0000	0.0000	0.0000	0.0310	0.0000	-0.0150	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0482
141	0.0000	-0.0049	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0425	0.0000	0.0218	0.0000	0.0000	0.0000
142	0.0000	0.0000	0.0000	0.0000	-0.0083	0.0000	0.0121	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1481
143	0.0000	0.0000	0.0000	-0.0192	0.0000	-0.0088	0.0000	0.0000	-0.0422	0.0000	0.0000	-0.0119	0.0000	0.0000	0.0000	0.0000
144	0.0000	0.0000	0.0000	0.0000	-0.0029	0.0000	0.0338	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006
145	0.0000	0.0000	0.0099	0.0000	0.0000	0.0000	0.0000	-0.0334	0.0000	0.0012	0.0000	0.0000	0.0000	-0.0123	-0.0009	0.0000
146	0.0000	-0.0123	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0004	0.0000	0.0023	0.0000	0.0000	0.0000
147	0.0000	0.0000	0.0000	-0.0050	0.0000	0.0217	0.0000	0.0000	0.0087	0.0000	0.0000	-0.0004	0.0000	0.0000	0.0000	0.0000
148	0.0000	0.0000	-0.0209	0.0000	0.0000	0.0000	0.0000	-0.0017	0.0000	-0.0126	0.0000	0.0000	0.0000	-0.0028	-0.0003	0.0000
149	0.0000	0.0000	0.0000	0.0000	0.0089	0.0000	-0.0044	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0059
150	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0078	0.0000	-0.0019	0.0000	0.0000	0.0000
151	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0059
152	0.0000	-0.0147	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0549	0.0000	-0.0075	0.0000	0.0000	0.0000
153	0.0000	0.0000	0.0000	0.0000	0.0009	0.0000	0.0063	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0531
154	0.0000	0.0000	0.0000	-0.0029	0.0000	0.0462	0.0000	0.0000	0.0207	0.0000	0.0000	0.0117	0.0000	0.0000	0.0000	0.0000
155	0.0000	0.0000	-0.0119	0.0000	0.0000	0.0000	0.0000	0.0082	0.0000	0.0045	0.0000	0.0000	0.0000	-0.0229	0.0210	0.0000
156	0.0000	0.0000	0.0000	-0.0019	0.0000	-0.0008	0.0000	0.0000	0.0086	0.0000	0.0000	-0.0009	0.0000	0.0000	0.0000	0.0000
157	0.0000	0.0000	0.0149	0.0000	0.0000	0.0000	0.0000	-0.0077	0.0000	0.0026	0.0000	0.0000	0.0000	0.0022	0.0028	0.0000
158	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0446	0.0000	0.0234	0.0000	0.0000	0.0000
159	0.0000	0.0000	0.0194	0.0000	0.0000	0.0000	0.0000	0.0410	0.0000	0.0035	0.0000	0.0000	0.0000	-0.0015	0.0048	0.0000
160	0.0000	0.0000	0.0000	0.0000	-0.0131	0.0000	0.0064	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0008
161	0.0000	0.0000	0.0000	0.0111	0.0000	-0.0161	0.0000	0.0000	-0.0120	0.0000	0.0000	0.0064	0.0000	0.0000	0.0000	0.0000
162	0.0000	-0.0054	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025	0.0000	0.0001	0.0000	0.0000	0.0000
163	0.0000	0.0000	0.0000	0.0000	0.0103	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028
164	0.0000	0.0000	0.0024	0.0000	0.0000	0.0000	0.0000	0.0031	0.0000	0.0022	0.0000	0.0000	0.0000	0.0069	-0.0088	0.0000
165	0.0000	0.0000	0.0000	0.0061	0.0000	-0.0005	0.0000	0.0000	0.0022	0.0000	0.0000	0.0034	0.0000	0.0000	0.0000	0.0000
166	0.0000	0.0000	-0.0032	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000	0.0013	0.0000	0.0000	0.0000	0.0088	0.0021	0.0000
167	0.0000	0.0000	0.0000	0.0000	-0.0124	0.0000	0.0067	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0594
168	0.0000	-0.0014	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0194	0.0000	0.0061	0.0000	0.0000	0.0000
169	0.0000	0.0000	-0.0204	0.0000	0.0000	0.0000	0.0000	0.0467	0.0000	-0.0024	0.0000	0.0000	0.0000	-0.0111	0.0229	0.0000
170	0.0000	0.0000	0.0000	0.0026	0.0000	0.0052	0.0000	0.0000	0.0040	0.0000	0.0000	0.0182	0.0000	0.0000	0.0000	0.0000
171	0.0000	0.0000	-0.0079	0.0000	0.0000	0.0000	0.0000	0.0016	0.0000	0.0025	0.0000	0.0000	0.0000	0.0008	-0.0187	0.0000
172	0.0000	0.0000	0.0000	-0.0009	0.0000	0.0060	0.0000	0.0000	-0.0054	0.0000	0.0000	0.0023	0.0000	0.0000	0.0000	0.0000
173	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	-0.0037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0435
174	0.0000	0.0000	0.0000	-0.0100	0.0000	0.0192	0.0000	0.0000	0.0185	0.0000	0.0000	-0.0008	0.0000	0.0000	0.0000	0.0000
175	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0150	0.0000	0.0096	0.0000	0.0000	0.0000
176	0.0000	0.0000	-0.0219	0.0000	0.0000	0.0000	0.0000	-0.0033	0.0000	-0.0008	0.0000	0.0000	0.0000	-0.0011	0.0053	0.0000
177	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	-0.0099	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0034
178	0.0000	0.0089	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0004	0.0000	-0.0004	0.0000	0.0000	0.0000
179	0.0000	0.0000	0.0000	-0.0033	0.0000	0.0012	0.0000	0.0000	0.0001	0.0000	0.0000	-0.0002	0.0000	0.0000	0.0000	0.0000





2	0.0000	0.0000	0.1340	0.0000	-0.0160	0.0000	0.0653	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0369	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0832	0.0000	0.0000	0.0000	0.0000	-0.0588	0.0000	0.0000	0.0000	-0.0140	0.0000
4	0.0000	0.0000	0.0000	-0.0058	0.0000	0.0000	0.0000	0.0000	-0.0475	0.0210	0.0000	0.0000	0.0218	0.0000	0.0000	-0.0647
5	-0.1207	-0.0531	0.0000	0.0000	0.0000	0.0001	0.0000	-0.2671	0.0000	0.0000	0.0000	0.0279	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.2031	-0.0002	0.0000	0.0000	0.0000	0.2943	0.1686	0.0000	0.0000	0.0082	0.0000	0.0000	0.0405
7	0.3940	0.1860	0.0000	0.0000	0.0000	0.0001	0.0000	-0.2888	0.0000	0.0000	0.0000	0.0975	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	-0.3940	0.0003	0.2009	0.0000	-0.0705	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0584	0.0000	0.0000
9	0.2981	0.5822	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0650	0.0000	0.0000	0.0001	-0.5851	0.0000	0.0000	0.0000	0.0000
10	0.0001	0.0000	0.0000	0.0000	0.0000	0.0940	0.0000	0.0001	0.0000	0.0000	0.1321	0.0000	0.0000	0.0000	0.0150	0.0000
11	0.0000	0.0000	0.0000	-0.0465	0.0001	0.0000	0.0000	0.0000	-0.0392	0.0589	0.0000	0.0000	-0.1440	0.0000	0.0000	-0.0513
12	0.0000	0.0000	-0.0008	0.0002	0.1347	0.0000	-0.0530	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0268	0.0000	0.0000
13	0.0000	0.0000	0.0000	0.0000	0.0000	0.0859	0.0000	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000	0.0000	-0.0024	0.0000
14	-0.0314	-0.0485	0.0000	0.0000	0.0000	0.0000	0.0000	0.0056	0.0000	0.0000	0.0000	0.0175	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0000	0.0000	0.0000	-0.0081	0.0021	0.0000	0.0000	-0.0066	0.0000	0.0000	-0.0240
16	-0.0082	-0.0087	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0048	0.0000	0.0000	0.0000	0.0108	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	0.0714	0.0000	0.0000	0.0000	0.0000	-0.1034	0.0000	0.0000	0.0000	-0.0399	0.0000
18	0.0000	0.0000	-0.7783	0.0001	0.0837	0.0000	-0.1766	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.1696	0.0000	0.0000
19	-0.5571	0.0292	0.0000	0.0000	0.0000	0.0000	0.0000	0.0017	0.0000	0.0000	0.0001	-0.6062	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	-0.1739	0.0001	0.0000	0.0000	0.0000	-0.7148	0.2555	0.0000	0.0000	0.2365	0.0001	0.0000	-0.2331
21	-0.0227	0.0216	0.0000	0.0000	0.0000	-0.0002	0.0000	0.4707	0.0000	0.0000	-0.0001	-0.0485	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	-0.0561	0.0000	0.0000	0.0000	0.0000	0.1476	-0.6023	0.0000	0.0000	-0.3762	0.0000	0.0000	-0.3884
23	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0634	0.0000	-0.0001	0.0000	0.0000	-0.4306	-0.0001	0.0000	0.0000	-0.1362	0.0000
24	0.0000	0.0000	0.0000	-0.0691	0.0001	0.0000	0.0000	0.0000	-0.0519	0.1415	0.0000	0.0000	-0.2297	0.0000	0.0000	0.1473
25	0.0000	0.0000	0.0610	0.0001	0.0514	0.0000	-0.0360	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0353	0.0000	0.0000
26	-0.0066	0.0879	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0113	0.0000	0.0000	0.0000	-0.1051	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0752	0.0000	0.0000	0.0000	0.0000	-0.0218	0.0000	0.0000	0.0000	-0.0012	0.0000
28	0.0000	0.0000	0.0185	0.0001	0.0514	0.0000	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0126	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0061	0.0000	0.0000	0.0000	0.0000	0.0253	-0.0160	0.0000	0.0000	-0.0033	0.0000	0.0000	-0.0211
30	0.0148	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0127	0.0000	0.0000	0.0000	-0.0025	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0082	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0113	0.0000	0.0000	0.0092	0.0000	0.0000	0.0176
32	0.0000	0.0000	0.0000	-0.0493	0.0001	0.0000	0.0000	0.0000	0.0188	0.0022	0.0000	0.0000	0.0090	0.0000	0.0000	0.0406
33	-0.2655	0.6161	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0111	0.0000	0.0000	-0.0001	0.4003	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.1917	0.0000	-0.0814	0.0000	-0.9292	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0014	0.0000	0.0000
35	0.0002	0.0000	0.0000	0.0000	0.0000	0.2283	0.0000	0.0001	0.0000	0.0000	0.2672	0.0001	0.0000	0.0000	-0.5302	0.0000
36	0.0000	0.0000	0.1003	0.0008	0.5788	0.0000	-0.1425	0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0000	-0.1437	0.0000	0.0000
37	0.0000	-0.0001	0.0000	0.0000	0.0000	0.5686	0.0000	0.0003	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.2742	0.0000
38	0.0000	0.0000	0.0000	-0.1341	0.0002	0.0000	0.0000	0.0000	0.0034	0.1937	0.0000	0.0000	-0.4633	0.0000	0.0000	0.2222
39	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0325	0.0000	0.0000	0.0000	0.0000	-0.0284	0.0000	0.0000	0.0000	-0.0208	0.0000
40	-0.0208	-0.0483	0.0000	0.0000	0.0000	0.0000	0.0000	0.0163	0.0000	0.0000	0.0000	-0.0160	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0182	0.0000	-0.0315	0.0000	-0.0545	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0082	0.0000	0.0000
42	0.0000	0.0000	0.0000	-0.0264	0.0000	0.0000	0.0000	0.0000	-0.0073	0.0114	0.0000	0.0000	-0.0496	0.0000	0.0000	0.0420
43	0.0418	-0.0089	0.0000	0.0000	0.0000	0.0000	0.0000	0.0089	0.0000	0.0000	0.0000	0.0015	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0007	0.0000	0.0000	0.0000	0.0000	-0.0022	0.0000	0.0000	0.0000	-0.0094	0.0000
45	0.0000	0.0000	-0.0007	0.0000	0.0079	0.0000	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0123	0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	0.0000	0.0000	0.0033	0.0000
47	-0.0602	-0.0749	0.0000	0.0000	0.0000	-0.0001	0.0000	0.2065	0.0000	0.0000	0.0000	0.0086	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.8426	-0.0013	0.0000	0.0001	0.0000	-0.2555	0.0388	0.0000	0.0000	-0.1504	0.0000	0.0000	-0.1589
49	0.0002	0.0000	0.0000	0.0000	0.0000	0.0801	0.0000	0.0000	0.0000	0.0000	-0.2052	-0.0001	0.0000	0.0000	0.6699	0.0000
50	0.0000	0.0000	-0.1222	0.0001	0.0540	0.0000	0.0286	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	-0.7638	0.0000	-0.0001
51	0.0000	0.0000	0.0000	0.0000	0.0000	0.0712	0.0000	0.0001	0.0000	0.0000	0.2511	0.0000	0.0000	0.0000	-0.0718	0.0000
52	0.0000	0.0000	0.0483	0.0001	0.0291	0.0000	-0.0806	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2045	0.0000	0.0000

53	0.1098	0.0594	0.0000	0.0000	0.0000	-0.0001	0.0000	0.2207	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000	0.0000	0.0000
54	0.0000	0.0000	-0.0370	-0.0003	-0.2339	0.0000	-0.0026	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0599	0.0000	0.0000
55	0.0000	0.0000	0.0000	-0.0348	0.0001	0.0000	0.0000	0.0000	0.0583	0.0334	0.0000	0.0000	0.0174	0.0000	0.0000	-0.0100
56	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1338	0.0000	-0.0001	0.0000	0.0000	-0.0180	0.0000	0.0000	0.0000	0.0231	0.0000
57	0.0447	0.0295	0.0000	0.0000	0.0000	0.0000	0.0000	0.0092	0.0000	0.0000	0.0000	0.0042	0.0000	0.0000	0.0000	0.0000
58	0.0000	0.0000	0.0000	-0.0379	0.0001	0.0000	0.0000	0.0000	-0.0009	0.0033	0.0000	0.0000	-0.0023	0.0000	0.0000	0.0136
59	0.0000	0.0000	0.0055	0.0000	-0.0091	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0253	0.0000	0.0000
60	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0144	0.0000	0.0000	0.0000	0.0000	0.0165	0.0000	0.0000	0.0000	-0.0096	0.0000
61	0.0000	0.0000	-0.0031	0.0000	0.0061	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0036	0.0000	0.0000
62	0.0000	0.0000	0.0000	-0.2577	0.0003	0.0000	0.0000	0.0000	-0.1342	-0.2031	0.0000	0.0000	0.0089	0.0000	0.0000	0.0386
63	-0.0355	-0.0451	0.0000	0.0000	0.0000	0.0003	0.0000	-0.5388	0.0000	0.0000	-0.0001	-0.0235	0.0000	0.0000	-0.0001	0.0000
64	0.0000	0.0000	0.0878	0.0007	0.5182	0.0000	0.0784	0.0000	-0.0001	-0.0001	0.0000	0.0000	0.0000	0.1854	0.0000	0.0000
65	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0392	0.0000	0.0000	0.0000	0.0000	0.2725	0.0000	0.0000	0.0000	-0.0543	0.0000
66	0.0000	0.0000	-0.0660	0.0000	0.0181	0.0000	-0.0481	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.3894	0.0000	0.0000
67	0.0000	0.0000	0.0000	0.0000	0.0000	0.0114	0.0000	0.0000	0.0000	0.0000	0.1857	0.0000	0.0000	0.0000	0.0550	0.0000
68	0.0000	0.0000	0.0000	-0.1891	0.0002	0.0000	0.0000	0.0000	-0.1244	-0.2225	0.0000	0.0000	0.0029	0.0000	0.0000	0.1526
69	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.2948	0.0000	-0.0002	0.0000	0.0000	0.0407	0.0000	0.0000	0.0000	-0.0964	0.0000
70	0.0191	0.0168	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0482	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000	0.0000	0.0000
71	0.0000	0.0000	-0.0209	-0.0001	-0.1045	0.0000	-0.0098	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000
72	0.0000	0.0000	0.0000	-0.0150	0.0000	0.0000	0.0000	0.0000	-0.0046	-0.0078	0.0000	0.0000	-0.0069	0.0000	0.0000	0.0189
73	0.0100	0.0078	0.0000	0.0000	0.0000	0.0000	0.0000	0.0302	0.0000	0.0000	0.0000	0.0026	0.0000	0.0000	0.0000	0.0000
74	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0098	0.0000	0.0000	0.0000	0.0000	-0.0266	0.0000	0.0000	0.0000	0.0114	0.0000
75	0.0000	0.0000	-0.0066	0.0000	-0.0115	0.0000	-0.0072	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0102	0.0000	0.0000
76	0.0000	0.0000	0.0000	0.0000	0.0000	0.0099	0.0000	0.0000	0.0000	0.0000	-0.0059	0.0000	0.0000	0.0000	-0.0053	0.0000
77	0.3143	0.2599	0.0000	0.0000	0.0000	-0.0001	0.0000	0.2550	0.0000	0.0000	0.0000	0.0781	0.0000	0.0000	0.0000	0.0000
78	0.0000	0.0000	0.0000	-0.1921	0.0004	0.0000	0.0000	0.0000	0.4048	0.4829	0.0000	0.0000	0.1482	0.0001	0.0000	-0.4539
79	0.0000	-0.0001	0.0000	0.0000	0.0000	0.5272	0.0000	0.0003	0.0000	0.0000	-0.0512	0.0000	0.0000	0.0000	-0.1259	0.0000
80	0.0000	0.0000	-0.0010	-0.0001	-0.0651	0.0000	-0.0649	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0299	0.0000	0.0000
81	0.0000	0.0000	0.0000	0.0000	0.0000	0.0028	0.0000	0.0000	0.0000	0.0000	0.2161	0.0000	0.0000	0.0000	0.0603	0.0000
82	0.0000	0.0000	-0.0596	0.0000	0.0179	0.0000	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.3274	0.0000	0.0000
83	-0.0404	-0.0280	0.0000	0.0000	0.0000	-0.0001	0.0000	0.2161	0.0000	0.0000	0.0000	0.0027	0.0000	0.0000	0.0000	0.0000
84	0.0000	0.0000	-0.0401	-0.0003	-0.2186	0.0000	-0.0296	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0167	0.0000	0.0000
85	0.0000	0.0000	0.0000	0.0586	-0.0001	0.0000	0.0000	0.0000	-0.0118	0.0073	0.0000	0.0000	-0.0209	0.0000	0.0000	0.0099
86	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0239	0.0000	0.0000	0.0000	0.0000	-0.0087	0.0000	0.0000	0.0000	-0.0215	0.0000
87	-0.0069	-0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0086	0.0000	0.0000	0.0000	0.0027	0.0000	0.0000	0.0000	0.0000
88	0.0000	0.0000	0.0000	0.0009	0.0000	0.0000	0.0000	0.0000	-0.0186	-0.0211	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0151
89	0.0000	0.0000	-0.0033	0.0000	-0.0030	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0019	0.0000	0.0000
90	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0082	0.0000	0.0000	0.0000	0.0069	0.0000
91	0.0000	0.0000	0.0092	0.0000	0.0074	0.0000	0.0072	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.0000
92	0.0000	0.0000	-0.2996	-0.0001	-0.0537	0.0000	-0.0423	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0457	0.0000	0.0000
93	0.0000	0.0000	0.0000	0.0000	0.0000	0.0645	0.0000	0.0001	0.0000	0.0000	-0.5950	-0.0001	0.0000	0.0000	-0.2735	0.0000
94	0.0000	0.0000	0.0000	-0.0586	0.0001	0.0000	0.0000	0.0000	-0.1427	0.2148	0.0000	0.0000	-0.3790	0.0000	0.0000	0.3674
95	0.0296	0.0199	0.0000	0.0000	0.0000	0.0001	0.0000	-0.2788	0.0000	0.0000	0.0000	0.0025	0.0000	0.0000	0.0000	0.0000
96	0.0000	0.0000	0.0000	0.1352	-0.0001	0.0000	0.0000	0.0000	0.2597	0.1688	0.0000	0.0000	0.0238	0.0000	0.0000	0.2224
97	-0.0293	-0.0366	0.0000	0.0000	0.0000	0.0001	0.0000	-0.1754	0.0000	0.0000	0.0000	0.0073	0.0000	0.0000	0.0000	0.0000
98	0.0000	0.0000	-0.1799	0.0000	0.0263	0.0000	-0.0845	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0719	0.0000	0.0000
99	-0.0799	0.0907	0.0000	0.0000	0.0000	0.0000	0.0000	0.0164	0.0000	0.0000	0.0000	-0.1241	0.0000	0.0000	0.0000	0.0000
100	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0420	0.0000	0.0000	0.0000	0.0000	0.0023	0.0000	0.0000	0.0000	0.0094	0.0000
101	0.0000	0.0000	0.0000	-0.0058	0.0000	0.0000	0.0000	0.0000	-0.0156	-0.0041	0.0000	0.0000	0.0014	0.0000	0.0000	-0.0047
102	0.0000	0.0000	-0.0307	0.0000	-0.0210	0.0000	-0.0058	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000
103	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0086	0.0000	0.0000	0.0000	0.0000	0.0327	0.0000	0.0000	0.0000	-0.0068	0.0000

104	0.0139	-0.0452	0.0000	0.0000	0.0000	0.0000	0.0000	0.0173	0.0000	0.0000	0.0000	0.0364	0.0000	0.0000	0.0000	0.0000
105	0.0000	0.0000	0.0000	0.0033	0.0000	0.0000	0.0000	0.0000	0.0114	0.0033	0.0000	0.0000	0.0044	0.0000	0.0000	-0.0086
106	-0.0018	0.0047	0.0000	0.0000	0.0000	0.0000	0.0000	0.0054	0.0000	0.0000	0.0000	-0.0022	0.0000	0.0000	0.0000	0.0000
107	-0.4495	0.3199	0.0000	0.0000	0.0000	0.0001	0.0000	-0.0291	0.0000	0.0000	-0.0001	0.2762	0.0000	0.0000	0.0000	0.0000
108	0.0000	0.0000	0.0000	-0.0926	0.0002	0.0000	0.0000	0.0000	-0.0533	0.2166	0.0000	0.0000	-0.4028	0.0000	0.0000	-0.0881
109	0.0000	0.0000	0.0000	0.0000	0.0000	0.0565	0.0000	0.0000	0.0000	0.0000	-0.0226	0.0000	0.0000	0.0000	-0.0156	0.0000
110	0.0000	0.0000	-0.0600	-0.0004	-0.3030	0.0000	0.0321	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0443	0.0000	0.0000
111	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.3396	0.0000	-0.0002	0.0000	0.0000	-0.0575	0.0000	0.0000	0.0000	0.0579	0.0000
112	0.0000	0.0000	-0.0278	-0.0003	-0.2020	0.0000	0.0422	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0072	0.0000	0.0000
113	-0.1154	0.1160	0.0000	0.0000	0.0000	0.0000	0.0000	0.0274	0.0000	0.0000	0.0000	0.0392	0.0000	0.0000	0.0000	0.0000
114	0.0000	0.0000	0.0428	0.0000	-0.0174	0.0000	-0.1511	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0099	0.0000	0.0000
115	0.0000	0.0000	0.0000	0.0131	0.0000	0.0000	0.0000	0.0000	0.0378	0.0166	0.0000	0.0000	-0.0433	0.0000	0.0000	0.0403
116	0.0000	0.0000	0.0000	0.0000	0.0000	0.0067	0.0000	0.0000	0.0000	0.0000	-0.0022	0.0000	0.0000	0.0000	0.0185	0.0000
117	-0.0087	0.0118	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0365	0.0000	0.0000	0.0000	-0.0019	0.0000	0.0000	0.0000	0.0000
118	0.0000	0.0000	0.0000	0.0114	0.0000	0.0000	0.0000	0.0000	0.0070	0.0155	0.0000	0.0000	0.0369	0.0000	0.0000	-0.0105
119	0.0000	0.0000	-0.0074	0.0000	0.0164	0.0000	0.0137	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0159	0.0000	0.0000
120	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0093	0.0000	0.0000	0.0000	0.0000	-0.0020	0.0000	0.0000	0.0000	-0.0021	0.0000
121	0.0000	0.0000	0.0013	0.0000	0.0049	0.0000	-0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0070	0.0000	0.0000
122	-0.0001	0.0000	0.0000	0.0000	0.0000	-0.1186	0.0000	-0.0001	0.0000	0.0000	0.2804	0.0001	0.0000	0.0000	0.2165	0.0000
123	0.0000	0.0000	0.0203	-0.0001	-0.0776	0.0000	-0.0434	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0498	0.0000	0.0000
124	0.0462	0.0212	0.0000	0.0000	0.0000	0.0000	0.0000	0.0079	0.0000	0.0000	0.0000	0.0226	0.0000	0.0000	0.0000	0.0000
125	0.0000	0.0000	0.0000	-0.0284	0.0000	0.0000	0.0000	0.0000	0.0079	-0.0628	0.0000	0.0000	-0.0318	0.0000	0.0000	-0.0051
126	0.0177	0.0155	0.0000	0.0000	0.0000	0.0000	0.0000	0.0545	0.0000	0.0000	0.0000	0.0069	0.0000	0.0000	0.0000	0.0000
127	0.0000	0.0000	0.0000	-0.0128	0.0000	0.0000	0.0000	0.0000	-0.0584	0.0207	0.0000	0.0000	0.0532	0.0000	0.0000	-0.0020
128	0.0000	0.0000	0.0000	0.0000	0.0000	0.0450	0.0000	0.0000	0.0000	0.0000	-0.0161	0.0000	0.0000	0.0000	0.0030	0.0000
129	0.0000	0.0000	0.0000	0.0340	0.0000	0.0000	0.0000	0.0000	0.0006	0.0276	0.0000	0.0000	-0.0363	0.0000	0.0000	0.0398
130	0.0000	0.0000	-0.0180	0.0000	0.0030	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0176	0.0000	0.0000
131	0.0163	-0.0248	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0267	0.0000	0.0000	0.0000	0.0297	0.0000	0.0000	0.0000	0.0000
132	0.0000	0.0000	0.0000	0.0000	0.0000	0.0083	0.0000	0.0000	0.0000	0.0000	-0.0030	0.0000	0.0000	0.0000	0.0029	0.0000
133	0.0000	0.0000	0.0022	0.0000	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000
134	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000	0.0050	0.0131	0.0000	0.0000	0.0024	0.0000	0.0000	0.0009
135	0.0004	-0.0149	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000	0.0000	0.0000	0.0104	0.0000	0.0000	0.0000	0.0000
136	0.0000	0.0000	0.0000	-0.0069	0.0000	0.0000	0.0000	0.0000	0.0055	-0.0017	0.0000	0.0000	-0.0075	0.0000	0.0000	-0.0109
137	0.0000	0.0000	0.0000	-0.0797	0.0001	0.0000	0.0000	0.0000	-0.0736	0.1496	0.0000	0.0000	-0.3794	0.0000	0.0000	-0.4913
138	-0.0598	0.1193	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0168	0.0000	0.0000	0.0000	0.0423	0.0000	0.0000	0.0000	0.0000
139	0.0000	0.0000	0.0224	0.0001	0.0394	0.0000	-0.0649	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0062	0.0000	0.0000
140	0.0000	0.0000	0.0000	0.0000	0.0000	-0.1536	0.0000	-0.0001	0.0000	0.0000	0.0345	0.0000	0.0000	0.0000	-0.0225	0.0000
141	0.0000	0.0000	-0.0218	-0.0002	-0.1205	0.0000	0.0174	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000
142	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000	-0.0065	0.0000	0.0000	0.0000	0.0218	0.0000
143	0.0000	0.0000	0.0000	-0.0149	0.0000	0.0000	0.0000	0.0000	-0.0058	-0.0198	0.0000	0.0000	0.0120	0.0000	0.0000	0.0171
144	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0139	0.0000	0.0000	0.0000	0.0000	-0.0101	0.0000	0.0000	0.0000	0.0116	0.0000
145	0.0235	-0.0376	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0313	0.0000	0.0000	0.0000	-0.0097	0.0000	0.0000	0.0000	0.0000
146	0.0000	0.0000	0.0126	0.0000	-0.0050	0.0000	-0.0470	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0111	0.0000	0.0000
147	0.0000	0.0000	0.0000	0.0080	0.0000	0.0000	0.0000	0.0000	0.0236	0.0247	0.0000	0.0000	-0.0132	0.0000	0.0000	0.0302
148	0.0000	0.0019	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0172	0.0000	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000
149	0.0000	0.0000	0.0000	0.0000	0.0000	0.0097	0.0000	0.0000	0.0000	0.0000	0.0032	0.0000	0.0000	0.0000	0.0021	0.0000
150	0.0000	0.0000	0.0007	0.0000	-0.0086	0.0000	-0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0056	0.0000	0.0000
151	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0006	0.0000	0.0000	0.0000	0.0000	0.0052	0.0000	0.0000	0.0000	0.0042	0.0000
152	0.0000	0.0000	0.0390	0.0002	0.1715	0.0000	0.0577	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0616	0.0000	0.0000
153	0.0000	0.0000	0.0000	0.0000	0.0000	0.0940	0.0000	0.0001	0.0000	0.0000	0.0121	0.0000	0.0000	0.0000	-0.0131	0.0000
154	0.0000	0.0000	0.0000	0.0158	0.0000	0.0000	0.0000	0.0000	0.0308	-0.0198	0.0000	0.0000	0.0521	0.0000	0.0000	-0.0382



206	0.0000	0.0000	-0.0017	0.0000	-0.0091	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0056	0.0000	0.0000
207	0.0000	0.0000	0.0000	-0.0026	0.0000	0.0000	0.0000	0.0000	-0.0050	0.0029	0.0000	0.0000	-0.0083	0.0000	0.0000	0.0029
208	0.0123	-0.0028	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0000	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000
209	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0029	0.0000	0.0000	0.0000	0.0000	0.0040	0.0000	0.0000	0.0000	0.0020	0.0000
210	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0014	0.0000	0.0000
211	0.0000	0.0000	0.0000	0.0000	0.0000	0.0015	0.0000	0.0000	0.0000	0.0000	0.0011	0.0000	0.0000	0.0000	-0.0011	0.0000
212	-0.0170	0.0054	0.0000	0.0000	0.0000	0.0000	0.0000	0.0108	0.0000	0.0000	0.0000	0.0084	0.0000	0.0000	0.0000	0.0000
213	0.0000	0.0000	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	-0.0183	-0.0079	0.0000	0.0000	-0.0060	0.0000	0.0000	0.0057
214	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0131	0.0000	0.0000	0.0000	0.0000	0.0015	0.0000	0.0000	0.0000	0.0033	0.0000
215	0.0000	0.0000	-0.0048	0.0000	-0.0048	0.0000	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0024	0.0000	0.0000
216	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0103	0.0000	0.0000	0.0000	0.0000	-0.0071	0.0000	0.0000	0.0000	-0.0055	0.0000
217	0.0000	0.0000	0.0082	0.0000	-0.0098	0.0000	0.0092	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0096	0.0000	0.0000
218	-0.0002	-0.0032	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0069	0.0000	0.0000	0.0000	0.0014	0.0000	0.0000	0.0000	0.0000
219	0.0000	0.0000	0.0018	0.0000	0.0047	0.0000	0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0066	0.0000	0.0000
220	0.0000	0.0000	0.0000	-0.0030	0.0000	0.0000	0.0000	0.0000	0.0114	-0.0035	0.0000	0.0000	0.0036	0.0000	0.0000	0.0098
221	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0000	0.0000	0.0000	0.0000	-0.0027	0.0000	0.0000	0.0000	0.0014	0.0000
222	-0.0003	-0.0104	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0050	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000	0.0000	0.0000
223	0.0000	0.0000	0.0000	0.0032	0.0000	0.0000	0.0000	0.0000	0.0002	0.0049	0.0000	0.0000	0.0024	0.0000	0.0000	0.0014
224	0.0000	0.0000	-0.0004	0.0000	0.0034	0.0000	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000
225	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0014	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	-0.0012	0.0000
226	0.0000	0.0000	0.0036	0.0000	-0.0009	0.0000	-0.0046	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0006	0.0000	0.0000

NO	EV	KK	NM	SX	SY	SZ	OSC	LOGEPS
2	2.235347	18.0303	554.6	12.905086	0.000000	0.000000	1.411963	4.885149
3	3.260431	26.2986	380.2	0.000000	-0.190183	0.000000	0.000447	1.385900
4	3.281005	26.4646	377.9	-0.000227	0.000000	0.000000	0.000000	0.000000
5	3.450697	27.8333	359.3	0.000000	0.000242	0.000000	0.000000	0.000000
6	3.508650	28.3008	353.3	0.000168	0.000000	0.000000	0.000000	0.000000
7	3.559844	28.7137	348.3	0.000000	0.000124	0.000000	0.000000	0.000000
8	3.608246	29.1041	343.6	0.000000	0.687434	0.000000	0.006467	2.546040
9	3.760464	30.3319	329.7	-0.000368	0.000000	0.000000	0.000000	0.000000
10	3.956572	31.9137	313.3	0.000000	0.115298	0.000000	0.000199	1.035248
11	4.350044	35.0875	285.0	-1.397312	0.000000	0.000000	0.032213	3.243363
12	4.602449	37.1234	269.4	0.001972	0.000000	0.000000	0.000000	0.000000
13	4.609270	37.1784	269.0	1.649448	0.000000	0.000000	0.047563	3.412592
14	4.627519	37.3256	267.9	0.000000	2.858394	0.000000	0.143400	3.891875
15	4.850141	39.1212	255.6	0.000000	6.495366	0.000000	0.776101	4.625244
16	4.978248	40.1545	249.0	0.000000	0.002246	0.000000	0.000000	0.000000
17	5.066889	40.8695	244.7	0.000000	-4.268190	0.000000	0.350095	4.279511
18	5.165179	41.6623	240.0	0.000000	-3.521452	0.000000	0.242932	4.120811
19	5.232287	42.2036	236.9	0.114761	0.000000	0.000000	0.000261	1.152563
20	5.293397	42.6965	234.2	0.000533	0.000000	0.000000	0.000000	0.000000
21	5.317146	42.8881	233.2	-0.090147	0.000000	0.000000	0.000164	0.949861
22	5.335031	43.0324	232.4	0.000000	-0.000354	0.000000	0.000000	0.000000
23	5.398795	43.5467	229.6	-9.008882	0.000000	0.000000	1.661863	4.955921
24	5.455740	44.0060	227.2	0.000000	0.866102	0.000000	0.015522	2.926274
25	5.469284	44.1152	226.7	-0.000408	0.000000	0.000000	0.000000	0.000000
26	5.614828	45.2892	220.8	0.000330	0.000000	0.000000	0.000000	0.000000
27	5.655886	45.6204	219.2	0.000000	0.001572	0.000000	0.000000	0.000000
28	5.726297	46.1883	216.5	0.000000	-3.338644	0.000000	0.242086	4.119296

29	5.754189	46.4133	215.5	0.000743	0.000000	0.000000	0.000000	0.000000
30	5.837714	47.0870	212.4	-8.433341	0.000000	0.000000	1.574703	4.932524
31	5.945375	47.9554	208.5	0.000000	0.000058	0.000000	0.000000	0.000000
32	6.009444	48.4722	206.3	-0.000501	0.000000	0.000000	0.000000	0.000000
33	6.039252	48.7126	205.3	0.000000	9.986385	0.000000	2.284317	5.094082
34	6.086810	49.0962	203.7	0.000000	0.000116	0.000000	0.000000	0.000000
35	6.105724	49.2488	203.1	-0.000342	0.000000	0.000000	0.000000	0.000000
36	6.163595	49.7156	201.1	0.000000	0.000732	0.000000	0.000000	0.000000
37	6.237980	50.3155	198.7	1.659044	0.000000	0.000000	0.065120	3.549042
38	6.303860	50.8469	196.7	-1.333208	0.000000	0.000000	0.042497	3.363684
39	6.308032	50.8806	196.5	0.000000	-0.445280	0.000000	0.004744	2.411442
40	6.383179	51.4867	194.2	0.000000	-0.000665	0.000000	0.000000	0.000000
41	6.413415	51.7306	193.3	0.000000	0.000319	0.000000	0.000000	0.000000
42	6.440284	51.9473	192.5	-0.000125	0.000000	0.000000	0.000000	0.000000
43	6.542551	52.7722	189.5	0.000000	-0.000831	0.000000	0.000000	0.000000
44	6.549070	52.8248	189.3	-0.762681	0.000000	0.000000	0.014448	2.895148
45	6.605248	53.2779	187.7	0.000000	-0.000014	0.000000	0.000000	0.000000
46	6.644961	53.5983	186.6	0.377366	0.000000	0.000000	0.003589	2.290301
47	6.701260	54.0524	185.0	0.000000	-0.002870	0.000000	0.000000	0.000000
48	6.751245	54.4555	183.6	-1.569186	0.000000	0.000000	0.063051	3.535015
49	6.766260	54.5767	183.2	0.000000	-9.464715	0.000000	2.298901	5.096846
50	6.785277	54.7300	182.7	0.000390	0.000000	0.000000	0.000000	0.000000
51	6.893572	55.6036	179.8	0.000583	0.000000	0.000000	0.000000	0.000000
52	6.970865	56.2270	177.9	0.000000	-0.000323	0.000000	0.000000	0.000000
53	7.039825	56.7832	176.1	0.000000	0.000109	0.000000	0.000000	0.000000
54	7.099700	57.2662	174.6	-3.052719	0.000000	0.000000	0.250940	4.134896
55	7.100606	57.2735	174.6	-0.036137	0.000000	0.000000	0.000035	0.281472
56	7.116011	57.3977	174.2	0.000000	0.327049	0.000000	0.002887	2.195744
57	7.155915	57.7196	173.3	2.302949	0.000000	0.000000	0.143943	3.893516
58	7.167629	57.8141	173.0	0.000000	0.123042	0.000000	0.000412	1.349765
59	7.195746	58.0409	172.3	0.000809	0.000000	0.000000	0.000000	0.000000
60	7.219040	58.2288	171.7	0.000000	-0.000223	0.000000	0.000000	0.000000
61	7.258200	58.5446	170.8	0.000000	1.149827	0.000000	0.036396	3.296376
62	7.272729	58.6618	170.5	0.000195	0.000000	0.000000	0.000000	0.000000
63	7.367689	59.4278	168.3	-0.750991	0.000000	0.000000	0.015760	2.932883
64	7.388883	59.5987	167.8	-0.432733	0.000000	0.000000	0.005248	2.455301
65	7.391055	59.6162	167.7	0.000000	-0.000083	0.000000	0.000000	0.000000
66	7.480824	60.3403	165.7	1.255958	0.000000	0.000000	0.044757	3.386182
67	7.511051	60.5841	165.1	0.000000	0.290461	0.000000	0.002403	2.116158
68	7.545693	60.8636	164.3	-0.247285	0.000000	0.000000	0.001750	1.978377
69	7.546351	60.8689	164.3	0.000000	-0.000021	0.000000	0.000000	0.000000
70	7.629663	61.5409	162.5	0.000000	-0.026140	0.000000	0.000020	0.031403
71	7.719871	62.2685	160.6	0.000000	0.000116	0.000000	0.000000	0.000000
72	7.851820	63.3328	157.9	0.975976	0.000000	0.000000	0.028366	3.188131
73	7.902748	63.7436	156.9	-1.299863	0.000000	0.000000	0.050644	3.439856
74	8.042264	64.8689	154.2	0.000000	0.000017	0.000000	0.000000	0.000000
75	8.100029	65.3348	153.1	1.944949	0.000000	0.000000	0.116214	3.800585
76	8.107600	65.3959	152.9	0.000000	0.066570	0.000000	0.000136	0.869727
77	8.122982	65.5200	152.6	-0.001401	0.000000	0.000000	0.000000	0.000000
78	8.166943	65.8746	151.8	0.000000	0.314799	0.000000	0.003070	2.222407
79	8.219023	66.2946	150.8	0.003038	0.000000	0.000000	0.000000	0.000000

80	8.227281	66.3612	150.7	1.279534	0.000000	0.000000	0.051088	3.443642
81	8.293752	66.8974	149.5	0.000139	0.000000	0.000000	0.000000	0.000000
82	8.296121	66.9165	149.4	0.000000	-0.650398	0.000000	0.013310	2.859516
83	8.317640	67.0901	149.1	0.000000	-0.000086	0.000000	0.000000	0.000000
84	8.338111	67.2552	148.7	0.000000	0.068498	0.000000	0.000148	0.906700
85	8.352039	67.3675	148.4	0.000081	0.000000	0.000000	0.000000	0.000000
86	8.425161	67.9573	147.2	-0.988521	0.000000	0.000000	0.031225	3.229832
87	8.481688	68.4133	146.2	0.000000	0.000558	0.000000	0.000000	0.000000
88	8.485520	68.4442	146.1	0.000000	0.075066	0.000000	0.000181	0.993844
89	8.503076	68.5858	145.8	0.000039	0.000000	0.000000	0.000000	0.000000
90	8.544861	68.9228	145.1	0.000000	1.161432	0.000000	0.043717	3.375975
91	8.595910	69.3346	144.2	0.000000	1.183733	0.000000	0.045683	3.395082
92	8.649224	69.7646	143.3	0.000130	0.000000	0.000000	0.000000	0.000000
93	8.735595	70.4613	141.9	-0.000343	0.000000	0.000000	0.000000	0.000000
94	8.756429	70.6294	141.6	0.000000	-0.000071	0.000000	0.000000	0.000000
95	8.773752	70.7691	141.3	-0.072402	0.000000	0.000000	0.000174	0.976969
96	8.801373	70.9919	140.9	0.000000	-0.000071	0.000000	0.000000	0.000000
97	8.812224	71.0794	140.7	-0.153341	0.000000	0.000000	0.000786	1.630685
98	8.819428	71.1375	140.6	0.000000	0.309296	0.000000	0.003200	2.240471
99	8.853283	71.4106	140.0	0.000000	0.000450	0.000000	0.000000	0.000000
100	8.943712	72.1400	138.6	-1.198030	0.000000	0.000000	0.048687	3.422736
101	8.957211	72.2489	138.4	0.000000	0.621016	0.000000	0.013102	2.852661
102	9.119747	73.5599	135.9	-0.000041	0.000000	0.000000	0.000000	0.000000
103	9.180779	74.0522	135.0	0.000214	0.000000	0.000000	0.000000	0.000000
104	9.184146	74.0793	135.0	0.000000	0.000146	0.000000	0.000000	0.000000
105	9.202536	74.2277	134.7	-0.152704	0.000000	0.000000	0.000814	1.645891
106	9.215148	74.3294	134.5	0.000000	0.040375	0.000000	0.000057	0.491015
107	9.221514	74.3807	134.4	0.000000	-0.000201	0.000000	0.000000	0.000000
108	9.230837	74.4559	134.3	-0.000001	0.000000	0.000000	0.000000	0.000000
109	9.250065	74.6110	134.0	0.176578	0.000000	0.000000	0.001094	1.774302
110	9.284576	74.8894	133.5	0.000000	0.048998	0.000000	0.000085	0.662408
111	9.284737	74.8907	133.5	0.000000	1.478561	0.000000	0.076985	3.621730
112	9.343202	75.3623	132.7	0.000000	-0.293165	0.000000	0.003046	2.219004
113	9.360179	75.4992	132.5	0.000000	0.000140	0.000000	0.000000	0.000000
114	9.408050	75.8853	131.8	0.000024	0.000000	0.000000	0.000000	0.000000
115	9.516368	76.7590	130.3	0.000000	2.200145	0.000000	0.174715	3.977656
116	9.520925	76.7958	130.2	-0.000089	0.000000	0.000000	0.000000	0.000000
117	9.633583	77.7045	128.7	-0.000059	0.000000	0.000000	0.000000	0.000000
118	9.680508	78.0830	128.1	-0.000003	0.000000	0.000000	0.000000	0.000000
119	9.693329	78.1864	127.9	0.000000	0.540470	0.000000	0.010739	2.766298
120	9.721817	78.4162	127.5	-0.000021	0.000000	0.000000	0.000000	0.000000
121	9.743537	78.5914	127.2	0.000000	0.000064	0.000000	0.000000	0.000000
122	9.796543	79.0189	126.6	0.433685	0.000000	0.000000	0.006988	2.579703
123	9.845015	79.4099	125.9	-0.000149	0.000000	0.000000	0.000000	0.000000
124	9.912920	79.9576	125.1	0.036551	0.000000	0.000000	0.000050	0.436286
125	9.915361	79.9773	125.0	0.000000	0.000004	0.000000	0.000000	0.000000
126	9.963548	80.3660	124.4	-0.000321	0.000000	0.000000	0.000000	0.000000
127	9.970476	80.4219	124.3	0.000000	-1.056558	0.000000	0.042214	3.360784
128	10.021421	80.8328	123.7	-0.021636	0.000000	0.000000	0.000018	0.000000
129	10.102739	81.4887	122.7	0.000000	-1.711803	0.000000	0.112280	3.785629
130	10.152493	81.8900	122.1	0.000000	0.000328	0.000000	0.000000	0.000000



131	10.164262	81.9849	122.0	-0.247116	0.000000	0.000000	0.002354	2.107161
132	10.195647	82.2381	121.6	0.000000	0.000127	0.000000	0.000000	0.000000
133	10.297491	83.0596	120.4	1.421330	0.000000	0.000000	0.078900	3.632404
134	10.340300	83.4049	119.9	0.000276	0.000000	0.000000	0.000000	0.000000
135	10.340967	83.4102	119.9	0.000000	0.203681	0.000000	0.001627	1.946742
136	10.357887	83.5467	119.7	0.000000	0.469681	0.000000	0.008666	2.673159
137	10.359647	83.5609	119.7	0.000199	0.000000	0.000000	0.000000	0.000000
138	10.379784	83.7233	119.4	-0.413762	0.000000	0.000000	0.006740	2.563972
139	10.396868	83.8611	119.2	0.000000	-0.000187	0.000000	0.000000	0.000000
140	10.443581	84.2379	118.7	0.000397	0.000000	0.000000	0.000000	0.000000
141	10.478807	84.5221	118.3	0.000000	0.001356	0.000000	0.000000	0.000000
142	10.483236	84.5578	118.3	0.000000	0.652763	0.000000	0.016942	2.964289
143	10.631223	85.7514	116.6	0.000000	0.000097	0.000000	0.000000	0.000000
144	10.696074	86.2745	115.9	0.000000	0.215826	0.000000	0.001890	2.011714
145	10.699090	86.2989	115.9	0.000652	0.000000	0.000000	0.000000	0.000000
146	10.703782	86.3367	115.8	0.255075	0.000000	0.000000	0.002641	2.157154
147	10.709754	86.3849	115.8	1.136653	0.000000	0.000000	0.052480	3.455317
148	10.727430	86.5274	115.6	-0.000748	0.000000	0.000000	0.000000	0.000000
149	10.727761	86.5301	115.6	0.000000	-0.000049	0.000000	0.000000	0.000000
150	10.802728	87.1348	114.8	0.000000	-0.308948	0.000000	0.003911	2.327586
151	10.835109	87.3960	114.4	-0.000253	0.000000	0.000000	0.000000	0.000000
152	10.952472	88.3426	113.2	0.000000	0.186328	0.000000	0.001442	1.894350
153	10.987910	88.6285	112.8	-0.222737	0.000000	0.000000	0.002068	2.050781
154	11.032176	88.9855	112.4	0.000000	0.000027	0.000000	0.000000	0.000000
155	11.060516	89.2141	112.1	0.078116	0.000000	0.000000	0.000256	1.143535
156	11.109407	89.6085	111.6	0.000000	-0.121245	0.000000	0.000619	1.527301
157	11.216391	90.4714	110.5	0.000000	0.000006	0.000000	0.000000	0.000000
158	11.327129	91.3646	109.5	0.305248	0.000000	0.000000	0.004003	2.337707
159	11.336005	91.4362	109.4	0.000000	-0.314139	0.000000	0.004243	2.362985
160	11.339795	91.4668	109.3	0.007449	0.000000	0.000000	0.000002	0.000000
161	11.367380	91.6893	109.1	0.000000	0.000074	0.000000	0.000000	0.000000
162	11.422828	92.1365	108.5	0.000000	-0.000026	0.000000	0.000000	0.000000
163	11.475731	92.5632	108.0	-0.000014	0.000000	0.000000	0.000000	0.000000
164	11.542594	93.1026	107.4	0.000000	0.285583	0.000000	0.003570	2.288051
165	11.555887	93.2098	107.3	-0.162464	0.000000	0.000000	0.001157	1.798599
166	11.661383	94.0607	106.3	-0.084981	0.000000	0.000000	0.000319	1.239677
167	11.685401	94.2544	106.1	0.000000	-0.000002	0.000000	0.000000	0.000000
168	11.688108	94.2763	106.1	-0.000049	0.000000	0.000000	0.000000	0.000000
169	11.826195	95.3901	104.8	-0.031113	0.000000	0.000000	0.000043	0.373001
170	11.826474	95.3923	104.8	0.000000	0.114261	0.000000	0.000586	1.502935
171	11.903609	96.0145	104.2	0.000028	0.000000	0.000000	0.000000	0.000000
172	11.904911	96.0250	104.1	0.000000	-0.000007	0.000000	0.000000	0.000000
173	11.992924	96.7349	103.4	0.051442	0.000000	0.000000	0.000120	0.815848
174	12.012890	96.8960	103.2	-0.093450	0.000000	0.000000	0.000398	1.335086
175	12.051520	97.2076	102.9	0.000000	-0.000024	0.000000	0.000000	0.000000
176	12.074133	97.3900	102.7	0.000064	0.000000	0.000000	0.000000	0.000000
177	12.178468	98.2315	101.8	0.000000	0.000049	0.000000	0.000000	0.000000
178	12.199731	98.4030	101.6	0.000000	-0.028235	0.000000	0.000037	0.302200
179	12.296210	99.1812	100.8	0.000000	-0.005651	0.000000	0.000001	0.000000
180	12.304670	99.2495	100.8	-0.009755	0.000000	0.000000	0.000004	0.000000
181	12.315318	99.3354	100.7	0.000000	0.000002	0.000000	0.000000	0.000000

182	12.384479	99.8932	100.1	0.016695	0.000000	0.000000	0.000013	0.000000
183	12.505513	100.8695	99.1	0.000209	0.000000	0.000000	0.000000	0.000000
184	12.509504	100.9017	99.1	-0.069693	0.000000	0.000000	0.000230	1.097901
185	12.553294	101.2549	98.8	0.000141	0.000000	0.000000	0.000000	0.000000
186	12.562243	101.3271	98.7	0.237339	0.000000	0.000000	0.002684	2.164089
187	12.597563	101.6119	98.4	0.000000	0.000017	0.000000	0.000000	0.000000
188	12.658339	102.1022	97.9	0.000000	0.000029	0.000000	0.000000	0.000000
189	12.848314	103.6345	96.5	0.000000	0.101858	0.000000	0.000506	1.439121
190	12.923207	104.2386	95.9	0.000000	0.016115	0.000000	0.000013	0.000000
191	13.006820	104.9130	95.3	0.000000	-0.000008	0.000000	0.000000	0.000000
192	13.045028	105.2212	95.0	-0.000006	0.000000	0.000000	0.000000	0.000000
193	13.072338	105.4415	94.8	-0.000055	0.000000	0.000000	0.000000	0.000000
194	13.111257	105.7554	94.6	0.075367	0.000000	0.000000	0.000282	1.186289
195	13.132845	105.9295	94.4	0.000000	0.000003	0.000000	0.000000	0.000000
196	13.146588	106.0404	94.3	-0.046690	0.000000	0.000000	0.000109	0.771545
197	13.271336	107.0466	93.4	0.000000	0.000005	0.000000	0.000000	0.000000
198	13.478837	108.7203	92.0	0.000000	-0.000012	0.000000	0.000000	0.000000
199	13.514743	109.0099	91.7	0.000000	-0.021352	0.000000	0.000023	0.103954
200	13.538953	109.2052	91.6	-0.035569	0.000000	0.000000	0.000065	0.548004
201	13.762112	111.0052	90.1	0.000030	0.000000	0.000000	0.000000	0.000000
202	13.777640	111.1304	90.0	0.000000	0.035843	0.000000	0.000067	0.562269
203	13.819594	111.4688	89.7	0.145291	0.000000	0.000000	0.001106	1.779256
204	14.008372	112.9915	88.5	0.000000	-0.000009	0.000000	0.000000	0.000000
205	14.123069	113.9167	87.8	-0.000002	0.000000	0.000000	0.000000	0.000000
206	14.239188	114.8533	87.1	0.060165	0.000000	0.000000	0.000195	1.026460
207	14.254166	114.9741	87.0	0.000025	0.000000	0.000000	0.000000	0.000000
208	14.282465	115.2024	86.8	0.000000	-0.164254	0.000000	0.001461	1.900115
209	14.374931	115.9482	86.2	0.000000	-0.036133	0.000000	0.000071	0.587690
210	14.611765	117.8585	84.8	0.000000	-0.000013	0.000000	0.000000	0.000000
211	14.656697	118.2209	84.6	-0.000041	0.000000	0.000000	0.000000	0.000000
212	14.687983	118.4733	84.4	-0.139267	0.000000	0.000000	0.001080	1.768942
213	14.865485	119.9050	83.4	-0.000003	0.000000	0.000000	0.000000	0.000000
214	14.947387	120.5656	82.9	0.000000	-0.008816	0.000000	0.000004	0.000000
215	15.210431	122.6873	81.5	0.000000	-0.000002	0.000000	0.000000	0.000000
216	15.393915	124.1673	80.5	0.000000	0.021185	0.000000	0.000026	0.153705
217	15.397056	124.1927	80.5	0.119750	0.000000	0.000000	0.000837	1.658272
218	15.467913	124.7642	80.2	-0.000030	0.000000	0.000000	0.000000	0.000000
219	15.903522	128.2778	78.0	0.000000	-0.049418	0.000000	0.000147	0.903553
220	15.988159	128.9605	77.5	-0.000001	0.000000	0.000000	0.000000	0.000000
221	16.009698	129.1342	77.4	0.000000	-0.000003	0.000000	0.000000	0.000000
222	16.432987	132.5485	75.4	0.020484	0.000000	0.000000	0.000026	0.152825
223	16.587411	133.7941	74.7	0.069355	0.000000	0.000000	0.000303	1.216216
224	16.725133	134.9049	74.1	0.000000	-0.000004	0.000000	0.000000	0.000000
225	17.813176	143.6811	69.6	0.000000	0.000000	0.000000	0.000000	0.000000
226	17.897138	144.3583	69.3	-0.024627	0.000000	0.000000	0.000041	0.349903

TERRYLENE, 15pi x 15pi\* CIS



39.000	:	-----Y	:	:	256.
38.500	:		:	:	260.
38.000	:		:	:	263.
37.500	:	-----Y	:	:	267.
37.000	:	X-----X	:	:	270.
36.500	:		:	:	274.
36.000	:		:	:	278.
35.500	:		:	:	282.
35.000	:	-----X	:	:	286.
34.500	:		:	:	290.
34.000	:		:	:	294.
33.500	:		:	:	299.
33.000	:		:	:	303.
32.500	:		:	:	308.
32.000	:		:	:	313.
31.500	:		:	:	317.
31.000	:		:	:	323.
30.500	:	X	:	:	328.
30.000	:		:	:	333.
29.500	:		:	:	339.
29.000	:	-----Y	:	:	345.
28.500	:	Y	:	:	351.
28.000	:	Y	:	:	357.
27.500	:		:	:	364.
27.000	:		:	:	370.
26.500	:	X-----Y	:	:	377.
26.000	:		:	:	385.
25.500	:		:	:	392.
25.000	:		:	:	400.
24.500	:		:	:	408.
24.000	:		:	:	417.
23.500	:		:	:	426.
23.000	:		:	:	435.
22.500	:		:	:	444.
22.000	:		:	:	455.
21.500	:		:	:	465.
21.000	:		:	:	476.
20.500	:		:	:	488.
20.000	:		:	:	500.
19.500	:		:	:	513.
19.000	:		:	:	526.
18.500	:		:	:	541.
18.000	:	-----X	:	:	556.
17.500	:		:	:	571.
17.000	:		:	:	588.
16.500	:		:	:	606.
16.000	:		:	:	625.
15.500	:		:	:	645.
15.000	:		:	:	667.
14.500	:		:	:	690.
14.000	:		:	:	714.



3	0.0460	0.2645	-0.0114	-0.0197	0.0139	0.2970	0.0203	0.1604	0.2683	-0.1144	-0.2297	-0.1775	-0.1275	-0.2450
4	-0.0460	0.2645	-0.0114	-0.0197	0.0139	-0.2971	0.0203	-0.1604	0.2682	0.1144	0.2297	-0.1775	-0.1275	-0.2450
5	-0.0460	0.2645	0.0114	-0.0197	-0.0139	0.2970	-0.0203	-0.1604	0.2683	-0.1144	0.2297	0.1775	-0.1275	0.2450
6	0.0460	0.2645	0.0114	-0.0197	-0.0139	-0.2971	-0.0203	0.1604	0.2682	0.1144	-0.2297	0.1775	-0.1275	0.2450
7	0.1725	-0.1324	-0.2780	0.0003	0.2595	-0.1449	-0.1302	-0.2824	-0.0971	0.0472	0.2783	0.1694	0.0383	0.1716
8	-0.1725	-0.1324	-0.2780	0.0003	0.2595	0.1449	-0.1302	0.2824	-0.0971	-0.0472	-0.2783	0.1694	0.0383	0.1716
9	-0.1725	-0.1324	0.2780	0.0003	-0.2595	-0.1449	0.1302	0.2824	-0.0971	0.0472	-0.2783	-0.1694	0.0383	-0.1716
10	0.1725	-0.1324	0.2780	0.0003	-0.2595	0.1449	0.1302	-0.2824	-0.0971	-0.0472	0.2783	-0.1694	0.0383	-0.1716
11	-0.2942	0.1788	-0.0175	-0.0076	0.0106	-0.2224	0.2758	0.0642	-0.1871	0.2184	0.1992	-0.0738	0.2399	0.2131
12	0.2942	0.1788	-0.0175	-0.0076	0.0106	0.2224	0.2757	-0.0643	-0.1870	-0.2184	-0.1992	-0.0738	0.2400	0.2131
13	0.2942	0.1788	0.0175	-0.0076	-0.0106	-0.2224	-0.2758	-0.0642	-0.1871	0.2184	-0.1992	0.0738	0.2399	-0.2131
14	-0.2942	0.1788	0.0175	-0.0076	-0.0106	0.2224	-0.2757	0.0643	-0.1870	-0.2184	0.1992	0.0738	0.2400	-0.2131
15	0.0000	-0.2859	0.2237	-0.2890	0.2110	0.0000	-0.2515	0.0000	0.0611	0.0000	0.0000	0.1932	-0.2985	-0.2190
16	0.0000	-0.2859	-0.2237	-0.2890	-0.2110	0.0000	0.2515	0.0000	0.0611	0.0000	0.0000	-0.1932	-0.2985	0.2190
17	0.0000	-0.0885	-0.2125	0.3260	-0.2394	0.0000	-0.2147	0.0000	0.2598	0.0000	0.0000	-0.2855	0.2716	0.1612
18	0.0000	-0.0885	0.2125	0.3260	0.2394	0.0000	0.2147	0.0000	0.2598	0.0000	0.0000	0.2855	0.2716	-0.1612
19	-0.2706	0.1789	-0.0051	-0.0272	0.0257	-0.2176	0.2558	-0.1821	-0.2404	-0.1730	-0.0991	0.2095	-0.1814	-0.1022
20	0.2706	0.1790	-0.0051	-0.0272	0.0258	0.2176	0.2558	0.1820	-0.2404	0.1730	0.0991	0.2094	-0.1814	-0.1022
21	0.2706	0.1789	0.0051	-0.0272	-0.0257	-0.2176	-0.2558	0.1821	-0.2404	-0.1730	0.0991	-0.2095	-0.1814	0.1022
22	-0.2706	0.1790	0.0051	-0.0272	-0.0258	0.2176	-0.2558	-0.1820	-0.2404	0.1730	-0.0991	-0.2094	-0.1814	0.1022
23	0.1687	-0.1120	-0.1752	0.2849	-0.2147	0.0192	-0.1186	-0.2004	0.0192	-0.2862	-0.2054	0.1177	-0.1765	-0.1292
24	-0.1687	-0.1120	-0.1752	0.2849	-0.2148	-0.0192	-0.1185	0.2004	0.0192	0.2862	0.2054	0.1177	-0.1765	-0.1292
25	-0.1687	-0.1120	0.1752	0.2849	0.2147	0.0192	0.1186	0.2004	0.0192	-0.2862	0.2054	-0.1177	-0.1765	0.1292
26	0.1687	-0.1120	0.1752	0.2849	0.2148	-0.0192	0.1185	-0.2004	0.0192	0.2862	-0.2054	-0.1177	-0.1765	0.1292
27	0.1729	-0.0751	0.1977	-0.2689	0.1900	0.2088	-0.1149	0.2591	0.1448	0.2741	0.1677	-0.1667	0.1628	0.0984
28	-0.1729	-0.0751	0.1977	-0.2690	0.1900	-0.2088	-0.1149	-0.2590	0.1448	-0.2741	-0.1677	-0.1667	0.1628	0.0984
29	-0.1729	-0.0751	-0.1977	-0.2689	-0.1900	0.2088	0.1149	-0.2591	0.1448	0.2741	-0.1677	0.1667	0.1628	-0.0984
30	0.1729	-0.0751	-0.1977	-0.2690	-0.1900	-0.2088	0.1149	0.2590	0.1448	-0.2741	0.1677	0.1667	0.1628	-0.0984

OCCUPATION NUMBERS

1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	

PI TYPE BETA MATRIX FOR MAGNETIC DIPOLE INTEGRALS

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	-4.1022															
2	-2.4477	-4.1022														
3	0.3103	-2.4595	-4.2179													
4	0.3103	-2.4596	0.2899	-4.2179												
5	-2.4595	0.3103	-0.1341	-0.0162	-4.2179											
6	-2.4596	0.3103	-0.0162	-0.1341	0.2899	-4.2179										
7	-0.1385	0.2959	-2.4253	-0.0091	0.3187	0.0180	-4.6543									
8	-0.1385	0.2959	-0.0091	-2.4256	0.0180	0.3187	-0.0030	-4.6542								
9	0.2959	-0.1385	0.3187	0.0180	-2.4253	-0.0091	-2.4088	-0.0026	-4.6543							
10	0.2959	-0.1385	0.0180	0.3187	-0.0091	-2.4256	-0.0026	-2.4089	-0.0030	-4.6542						































2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000
4	0.0024	-0.0003	0.0000	-0.1020
5	0.0000	0.0000	0.0000	0.0000
6	0.0027	-0.0005	0.0000	0.0228
7	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000
9	-0.0021	-0.0026	0.0000	0.0783
10	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000
12	-0.0003	-0.0008	0.0000	0.0076
13	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000	0.0000
20	-0.0031	0.0010	0.0000	-0.0248
21	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000
25	0.0008	-0.0011	0.0000	0.0326
26	0.0016	-0.0021	0.0000	0.0315
27	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000
29	0.0001	-0.0002	0.0000	0.0032
30	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000
32	-0.0029	-0.0054	0.0000	-0.0048
33	0.0000	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000
35	-0.0010	0.0100	0.0000	0.0444
36	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000
42	-0.0026	0.0006	0.0000	-0.0478
43	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000
50	0.0002	-0.0006	0.0000	0.0047
51	-0.0003	-0.0006	0.0000	-0.0141
52	0.0000	0.0000	0.0000	0.0000

53	0.0000	0.0000	0.0000	0.0000
54	0.0000	0.0000	0.0000	0.0000
55	-0.0006	-0.0016	0.0000	0.0039
56	0.0000	0.0000	0.0000	0.0000
57	0.0000	0.0000	0.0000	0.0000
58	0.0000	0.0000	0.0000	0.0000
59	0.0038	0.0111	0.0000	-0.0449
60	0.0000	0.0000	0.0000	0.0000
61	0.0000	0.0000	0.0000	0.0000
62	0.0004	-0.0030	0.0000	0.0051
63	0.0000	0.0000	0.0000	0.0000
64	0.0000	0.0000	0.0000	0.0000
65	0.0000	0.0000	0.0000	0.0000
66	0.0000	0.0000	0.0000	0.0000
67	0.0000	0.0000	0.0000	0.0000
68	0.0000	0.0000	0.0000	0.0000
69	0.0000	0.0000	0.0000	0.0000
70	0.0000	0.0000	0.0000	0.0000
71	0.0000	0.0000	0.0000	0.0000
72	0.0000	0.0000	0.0000	0.0000
73	0.0000	0.0000	0.0000	0.0000
74	0.0000	0.0000	0.0000	0.0000
75	0.0000	0.0000	0.0000	0.0000
76	0.0000	0.0000	0.0000	0.0000
77	0.0001	0.0004	0.0000	-0.0003
78	0.0000	0.0000	0.0000	0.0000
79	0.0001	-0.0001	0.0000	-0.0001
80	0.0000	0.0000	0.0000	0.0000
81	-0.0001	0.0001	0.0000	-0.0001
82	0.0000	0.0000	0.0000	0.0000
83	0.0000	0.0000	0.0000	0.0000
84	0.0000	0.0000	0.0000	0.0000
85	-0.0001	0.0005	0.0000	-0.0010
86	0.0000	0.0000	0.0000	0.0000
87	0.0000	0.0000	0.0000	0.0000
88	0.0000	0.0000	0.0000	0.0000
89	-0.0008	0.0010	0.0000	-0.0021
90	0.0000	0.0000	0.0000	0.0000
91	0.0000	0.0000	0.0000	0.0000
92	-0.0002	-0.0003	0.0000	0.0026
93	0.0000	0.0000	0.0000	0.0000
94	0.0000	0.0000	0.0000	0.0000
95	0.0000	0.0000	0.0000	0.0000
96	0.0000	0.0000	0.0000	0.0000
97	0.0000	0.0000	0.0000	0.0000
98	0.0000	0.0000	0.0000	0.0000
99	0.0000	0.0000	0.0000	0.0000
100	0.0000	0.0000	0.0000	0.0000

CONTRIBUTIONS TO MCD B-TERMS B(F) DUE TO MIXING OF I'TH STATE WITH F'TH STATE





99	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
100	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0258	-0.0685	0.0000

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	-0.3043	-0.2643	0.0000	0.0000	0.0000	0.0000	0.0000	0.3117	0.0000	0.0000	0.0000	0.1897	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0003	0.0000	0.0000	0.0000	-0.0194	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0010	0.0000	-0.0016	0.0000	0.0233	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2760	0.0000	0.0000
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
11	-0.0574	0.3687	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0305	0.0000	0.0000	0.0000	-0.0771	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	-1.9406	-0.2257	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2110	0.0000	0.0000	0.0000	0.2609	0.0000	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0191	0.0000	-0.0007	0.0000	-1.8583	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.6349	0.0000	0.0000
15	0.0000	0.0000	-0.0480	0.0000	0.1910	0.0000	7.6744	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9629	0.0000	0.0000
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.1171	0.0000	-0.1718	0.0000	-12.9187	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-2.2060	0.0000	0.0000
18	0.0000	0.0000	-0.4035	0.0000	-0.1544	0.0000	6.0494	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.3395	0.0000	0.0000
19	-0.1171	0.4035	0.0000	0.0000	0.0000	0.0000	0.0000	0.0314	0.0000	0.0000	0.0000	0.0141	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	0.1718	0.1544	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0289	0.0000	0.0000	0.0000	-0.1255	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23	12.9187	-6.0494	0.0000	0.0000	0.0000	0.0000	0.0000	3.1250	0.0000	0.0000	0.0000	-3.3691	0.0000	0.0000	0.0000	0.0000
24	0.0000	0.0000	-0.0314	0.0000	0.0289	0.0000	-3.1250	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6962	0.0000	0.0000
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	-0.0141	0.0000	0.1255	0.0000	3.3691	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-3.1143	0.0000	0.0000
29	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30	2.2060	-1.3395	0.0000	0.0000	0.0000	0.0000	0.0000	-0.6962	0.0000	0.0000	0.0000	3.1143	0.0000	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	0.0000	0.0000	0.0046	0.0000	0.2701	0.0000	-0.3742	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	8.5760	0.0000	0.0000
34	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	-0.2820	0.1164	0.0000	0.0000	0.0000	0.0000	0.0000	-0.2411	0.0000	0.0000	0.0000	-0.1900	0.0000	0.0000	0.0000	0.0000
38	-0.1968	0.0579	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0971	0.0000	0.0000	0.0000	-0.0269	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	-0.0014	0.0000	0.0034	0.0000	0.0076	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-1.1349	0.0000	0.0000
40	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	-0.0638	-0.0638	0.0000	0.0000	0.0000	0.0000	0.0000	0.0236	0.0000	0.0000	0.0000	0.0115	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
46	0.0088	-0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0055	0.0000	0.0000	0.0000	-0.0068	0.0000	0.0000	0.0000	0.0000









97	0.0141	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
98	0.0000	0.0000	0.0000	0.0000	-0.0012	-0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0005	0.0000	0.0001	0.0000	-0.0014
99	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
100	0.0263	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64
1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	-0.0493	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033	0.0000	-0.0001	0.0000	0.0000	-0.0159	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0022	0.0000	0.0000	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	0.0001
4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0122	0.0000	0.0000	-0.0035	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0064	-0.0009
9	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0001	0.0000
11	-0.2043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0057	0.0000	-0.0002	0.0000	0.0000	0.0336	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
13	0.0319	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0039	0.0000	0.0002	0.0000	0.0000	-0.0749	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0180	0.0000	0.0000	0.0535	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0061	0.0056
15	0.0000	0.0000	0.0000	0.0000	0.0000	0.1495	0.0000	0.0000	0.2672	0.0000	0.0000	0.0000	0.0000	0.0000	0.0799	0.0153
16	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0082	0.0000	0.0000	-0.0947	0.0000	0.0000	0.0000	0.0000	0.0000	0.0027	0.0139
18	0.0000	0.0000	0.0000	0.0000	0.0000	0.0252	0.0000	0.0000	-0.1504	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0253	0.0064
19	-0.0020	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0000	0.0000	0.0000	0.0000	-0.0013	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
21	-0.0728	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0000	0.0000	0.0000	0.0000	0.0036	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
23	0.1910	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0042	0.0000	-0.0001	0.0000	0.0000	-0.0521	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0535	0.0000	0.0000	-0.0131	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0098	0.0028
25	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000	0.0000	0.0000	0.1366	0.0000	0.0000	0.0313	0.0000	0.0000	0.0000	0.0000	0.0000	0.1175	-0.0135
29	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
30	-1.3490	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0691	0.0000	-0.0016	0.0000	0.0000	0.1530	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
33	0.0000	0.0000	0.0000	0.0000	0.0000	1.1295	0.0002	0.0000	-0.4439	0.0000	0.0000	0.0000	0.0000	0.0000	0.4498	-0.0022
34	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
37	0.8192	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0003	0.0000	0.0001	0.0000	0.0000	0.0127	0.0000	0.0000	0.0000
38	0.0376	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0071	0.0000	-0.0001	0.0000	0.0000	0.0088	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0738	0.0000	0.0000	-0.0290	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0249	-0.0073
40	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
44	-1.5561	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0107	0.0000	-0.0003	0.0000	0.0000	0.0727	0.0000	0.0000	0.0000













94	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
95	0.0000	0.0007	0.0000	0.0002	0.0000	0.0000	0.0000	-0.0023	0.0000	0.0006	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
96	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
97	0.0000	-0.0039	0.0000	-0.0001	0.0000	0.0000	0.0000	0.0072	0.0000	-0.0166	-0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
98	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0037	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0035	0.0000
99	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
100	0.0000	0.0215	0.0000	-0.0322	0.0000	0.0000	0.0000	0.0269	0.0000	0.0472	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000

97      98      99      100

1	0.0000	0.0000	0.0000	0.0000
2	0.0000	-0.0002	0.0000	0.0000
3	0.0000	0.0000	0.0000	-0.0001
4	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000	0.0000
8	-0.0001	0.0000	0.0000	0.0003
9	0.0000	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000	0.0000
13	0.0000	-0.0004	0.0000	0.0000
14	0.0014	0.0000	0.0000	-0.0258
15	0.0020	0.0000	0.0000	0.0685
16	0.0000	0.0000	0.0000	0.0000
17	0.0026	0.0000	0.0000	-0.0593
18	0.0002	0.0000	0.0000	0.0129
19	0.0000	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000	0.0000
23	0.0000	-0.0005	0.0000	0.0000
24	0.0013	0.0000	0.0000	-0.0007
25	0.0000	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000	0.0000
28	-0.0021	0.0000	0.0000	0.0221
29	0.0000	0.0000	0.0000	0.0000
30	0.0000	0.0051	0.0000	0.0000
31	0.0000	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000	0.0000
33	-0.0141	0.0000	0.0000	-0.0263
34	0.0000	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000	0.0000
37	0.0000	0.0012	0.0000	0.0000
38	0.0000	0.0011	0.0000	0.0000
39	-0.0004	0.0000	0.0000	0.0004
40	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000

42	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0005	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000
46	0.0000	-0.0001	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0014	0.0000	0.0000
49	0.0017	0.0000	0.0000	-0.0123
50	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000
53	0.0000	0.0000	0.0000	0.0000
54	0.0000	-0.0027	0.0000	0.0000
55	0.0000	0.0000	0.0000	0.0000
56	0.0004	0.0000	0.0000	0.0011
57	0.0000	-0.0016	0.0000	0.0000
58	0.0000	0.0000	0.0000	0.0001
59	0.0000	0.0000	0.0000	0.0000
60	0.0000	0.0000	0.0000	0.0000
61	0.0016	0.0000	0.0000	-0.0002
62	0.0000	0.0000	0.0000	0.0000
63	0.0000	-0.0020	0.0000	0.0000
64	0.0000	-0.0005	0.0000	0.0000
65	0.0000	0.0000	0.0000	0.0000
66	0.0000	-0.0020	0.0000	0.0000
67	-0.0007	0.0000	0.0000	-0.0140
68	0.0000	-0.0001	0.0000	0.0000
69	0.0000	0.0000	0.0000	0.0000
70	0.0012	0.0000	0.0000	-0.0003
71	0.0000	0.0000	0.0000	0.0000
72	0.0000	-0.0002	0.0000	0.0000
73	0.0000	-0.0008	0.0000	0.0000
74	0.0000	0.0000	0.0000	0.0000
75	0.0000	-0.0007	0.0000	0.0000
76	0.0018	0.0000	0.0000	0.0062
77	0.0000	0.0000	0.0000	0.0000
78	-0.0032	0.0000	0.0000	0.0089
79	0.0000	0.0000	0.0000	0.0000
80	0.0000	0.0082	0.0000	0.0000
81	0.0000	0.0000	0.0000	0.0000
82	0.0039	0.0000	0.0000	-0.0215
83	0.0000	0.0000	0.0000	0.0000
84	0.0001	0.0000	0.0000	0.0322
85	0.0000	0.0000	0.0000	0.0000
86	0.0000	-0.0037	0.0000	0.0000
87	0.0000	0.0000	0.0000	0.0000
88	-0.0072	0.0000	0.0000	-0.0269
89	0.0000	0.0000	0.0000	0.0000
90	0.0166	0.0000	0.0000	-0.0472
91	0.0001	0.0000	0.0000	-0.0002
92	0.0000	0.0000	0.0000	0.0000

93	0.0000	0.0000	0.0000	0.0000
94	0.0000	0.0000	0.0000	0.0000
95	0.0000	-0.0035	0.0000	0.0000
96	0.0000	0.0000	0.0000	0.0000
97	0.0000	0.0078	0.0000	0.0000
98	-0.0078	0.0000	0.0000	0.0457
99	0.0000	0.0000	0.0000	0.0000
100	0.0000	-0.0457	0.0000	0.0000

WAVENUMBERS IN KK = 1000CM-1,  
MCD B-TERMS IN (BOHR-MAGNETON DEBYE\*\*2)/KK,  
ELECTRIC TRANSITION MOMENTS IN DEBYES  
TRANSITION MOMENT ANGLES IN DEG  
OSCILLATOR STRENGTHS OSC

F	W	BG	+	BF	=	B	M(X)	M(Y)	PHI (X-->Y)	OSC
2	18.030	-0.563372	1.439657	0.876286	-12.948827	0.000000	0.000000	0.000000	1.421551	
3	26.298	-0.003387	-0.110414	-0.113801	0.000000	0.163429	90.000000	0.000330		
4	26.464	0.000000	0.000000	0.000000	0.000218	0.000000	0.000000	0.000000		
5	27.833	0.000000	0.000000	0.000000	0.000000	-0.000229	90.000000	0.000000		
6	28.300	0.000000	0.000000	0.000000	-0.000170	0.000000	0.000000	0.000000		
7	28.713	0.000000	0.000000	0.000000	0.000000	-0.000137	90.000000	0.000000		
8	29.103	0.442816	-1.688218	-1.245401	0.000000	-0.722669	90.000000	0.007147		
9	30.331	0.000000	0.000000	0.000000	0.000341	0.000000	0.000000	0.000000		
10	31.913	0.000663	-0.001670	-0.001007	0.000000	-0.020157	90.000000	0.000006		
11	35.087	0.170993	1.029028	1.200021	1.465678	0.000000	0.000000	0.035443		
12	37.122	0.000000	0.000003	0.000002	-0.002215	0.000000	0.000000	0.000000		
13	37.177	-0.151339	4.468392	4.317053	-1.893582	0.000000	0.000000	0.062684		
14	37.325	1.279312	-7.345405	-6.066094	0.000000	-2.651184	90.000000	0.123363		
15	39.120	-1.280548	-2.238188	-3.518735	0.000000	-6.625143	90.000000	0.807423		
16	40.154	0.000000	0.000001	0.000001	0.000000	-0.002291	90.000000	0.000000		
17	40.869	1.930684	12.595148	14.525832	0.000000	4.588373	90.000000	0.404590		
18	41.661	-1.990269	-6.740607	-8.730876	0.000000	3.274749	90.000000	0.210086		
19	42.203	0.007567	-0.352532	-0.344965	0.055705	0.000000	0.000000	0.000062		
20	42.695	0.000000	0.000000	-0.000001	-0.000226	0.000000	0.000000	0.000000		
21	42.887	0.166784	0.358380	0.525164	0.252339	0.000000	0.000000	0.001284		
22	43.031	0.000000	-0.000001	-0.000001	0.000000	0.000373	90.000000	0.000000		
23	43.546	0.543106	-1.369196	-0.826090	8.428799	0.000000	0.000000	1.454738		
24	44.005	-0.609029	2.275593	1.666564	0.000000	-0.954013	90.000000	0.018833		
25	44.114	0.000000	0.000000	0.000000	0.000331	0.000000	0.000000	0.000000		
26	45.288	0.000000	0.000000	0.000000	-0.000362	0.000000	0.000000	0.000000		
27	45.619	0.000000	0.000001	0.000001	0.000000	-0.001545	90.000000	0.000000		
28	46.187	0.868075	-0.380016	0.488059	0.000000	3.174812	90.000000	0.218910		
29	46.412	0.000000	-0.000001	-0.000001	-0.000755	0.000000	0.000000	0.000000		
30	47.086	0.063428	6.228560	6.291988	8.502776	0.000000	0.000000	1.600740		
31	47.954	0.000000	0.000000	0.000000	0.000000	-0.000095	90.000000	0.000000		
32	48.471	0.000000	-0.000001	-0.000001	0.000401	0.000000	0.000000	0.000000		
33	48.711	-0.058940	-5.901639	-5.960579	0.000000	-9.959509	90.000000	2.272038		
34	49.095	0.000000	0.000000	0.000000	0.000000	-0.000141	90.000000	0.000000		

35	49.248	0.000000	0.000000	0.000000	0.000436	0.000000	0.000000	0.000000
36	49.714	0.000000	0.000000	0.000000	0.000000	-0.000786	90.000000	0.000000
37	50.314	-0.242259	-3.171599	-3.413858	-2.262285	0.000000	0.000000	0.121086
38	50.846	-0.122509	-4.158076	-4.280586	0.887132	0.000000	0.000000	0.018817
39	50.879	-0.210331	4.328060	4.117729	0.000000	0.569866	90.000000	0.007770
40	51.485	0.000000	0.000000	0.000000	0.000000	0.000575	90.000000	0.000000
41	51.729	0.000000	0.000000	0.000000	0.000000	-0.000274	90.000000	0.000000
42	51.946	0.000000	0.000000	0.000000	0.000080	0.000000	0.000000	0.000000
43	52.771	0.000000	0.000000	0.000000	0.000000	0.000820	90.000000	0.000000
44	52.823	-0.093896	2.151917	2.058022	0.801814	0.000000	0.000000	0.015969
45	53.277	0.000000	0.000000	0.000000	0.000000	0.000017	90.000000	0.000000
46	53.597	-0.011160	-0.460553	-0.471714	0.134093	0.000000	0.000000	0.000453
47	54.051	0.000000	-0.000001	0.000000	0.000000	0.002841	90.000000	0.000000
48	54.454	0.431055	-15.867365	-15.436310	0.849012	0.000000	0.000000	0.018457
49	54.575	-0.116069	12.714189	12.598120	0.000000	9.295986	90.000000	2.217666
50	54.729	0.000000	0.000001	0.000001	-0.000135	0.000000	-0.000001	0.000000
51	55.602	0.000000	0.000000	0.000000	-0.000292	0.000000	0.000000	0.000000
52	56.226	0.000000	0.000000	0.000000	0.000000	0.000298	90.000000	0.000000
53	56.782	0.000000	0.000000	0.000000	0.000000	-0.000175	90.000000	0.000000
54	57.265	-0.535468	-0.326449	-0.861917	2.126929	0.000000	0.000000	0.121816
55	57.272	-0.000075	-0.000055	-0.000129	0.025113	0.000000	0.000000	0.000017
56	57.396	0.007917	0.385710	0.393627	0.000000	-0.131897	90.000000	0.000470
57	57.718	-0.437156	2.271243	1.834087	-2.133828	0.000000	0.000000	0.123578
58	57.813	0.000548	0.027992	0.028540	0.000000	-0.008691	90.000000	0.000002
59	58.039	0.000000	0.000000	0.000000	-0.000620	0.000000	0.000000	0.000000
60	58.227	0.000000	0.000000	0.000000	0.000000	0.000226	90.000000	0.000000
61	58.543	-0.065943	-0.500696	-0.566639	0.000000	-1.050191	90.000000	0.030361
62	58.660	0.000000	0.000000	0.000000	-0.000231	0.000000	0.000000	0.000000
63	59.426	-0.113117	-0.281828	-0.394944	1.160548	0.000000	0.000000	0.037637
64	59.597	0.009884	-0.099575	-0.089690	0.207421	0.000000	0.000000	0.001206
65	59.615	0.000000	0.000000	0.000000	0.000000	0.000096	90.000000	0.000000
66	60.339	-0.312074	0.203715	-0.108358	-0.881563	0.000000	0.000000	0.022050
67	60.583	-0.065438	0.234359	0.168921	0.000000	-0.365099	90.000000	0.003797
68	60.862	0.000182	-0.007194	-0.007012	0.192360	0.000000	0.000000	0.001059
69	60.867	0.000000	0.000000	0.000000	0.000000	0.000031	90.000000	0.000000
70	61.539	0.023875	0.069675	0.093550	0.000000	-0.312007	90.000000	0.002817
71	62.267	0.000000	0.000000	0.000000	0.000000	-0.000155	90.000000	0.000000
72	63.331	0.004342	0.000781	0.005123	-0.072220	0.000000	0.000000	0.000155
73	63.742	-0.284197	0.189991	-0.094205	0.790355	0.000000	0.000000	0.018723
74	64.867	0.000000	0.000000	0.000000	0.000000	0.000089	90.000000	0.000000
75	65.333	-0.007680	0.003221	-0.004459	0.166150	0.000000	0.000000	0.000848
76	65.394	-0.003850	0.023525	0.019675	0.000000	0.512199	90.000000	0.008067
77	65.518	0.000000	0.000000	0.000000	0.000010	0.000000	0.000000	0.000000
78	65.873	-0.133038	-0.062128	-0.195166	0.000000	-0.556636	90.000000	0.009598
79	66.293	-0.000001	0.000001	0.000000	-0.001869	0.000000	0.000000	0.000000
80	66.360	-0.214611	0.281815	0.067204	-0.895104	0.000000	0.000000	0.025001
81	66.896	0.000000	0.000000	0.000000	-0.000059	0.000000	0.000000	0.000000
82	66.915	0.056496	-0.372904	-0.316408	0.000000	0.598894	90.000000	0.011286
83	67.088	0.000000	0.000000	0.000000	0.000000	-0.000009	0.000000	0.000000
84	67.254	-0.035666	0.261546	0.225880	0.000000	-0.189208	90.000000	0.001132
85	67.366	0.000000	0.000000	0.000000	0.000063	0.000000	0.000000	0.000000



51.500	:Y	:	:	:	:	:	194.
51.000	:+++++	Y-----	X	:	:	:	196.
50.500	:-----		X	:	:	:	198.
50.000	:	:	:	:	:	:	200.
49.500	:Y	:	:	:	:	:	202.
49.000	:X	:	:	:	:	:	204.
48.500	:X-----					Y	206.
48.000	:Y	:	:	:	:	:	208.
47.500	:	:	:	:	:	:	211.
47.000	:+++++					X	213.
46.500	:X	:	:	:	:	:	215.
46.000	:+++++					Y	217.
45.500	:Y	:	:	:	:	:	220.
45.000	:	:	:	:	:	:	222.
44.500	:	:	:	:	:	:	225.
44.000	:X+++++		Y	:	:	:	227.
43.500	:-----					X:	230.
43.000	:Y	:	:	:	:	:	233.
42.500	:X	:	:	:	:	:	235.
42.000	:--X	:	:	:	:	:	238.
41.500	:-----					Y	241.
41.000	:+++++					Y	244.
40.500	:	:	:	:	:	:	247.
40.000	:Y	:	:	:	:	:	250.
39.500	:	:	:	:	:	:	253.
39.000	:-----					Y	256.
38.500	:	:	:	:	:	:	260.
38.000	:	:	:	:	:	:	263.
37.500	:-----					Y	267.
37.000	:X+++++					X	270.
36.500	:	:	:	:	:	:	274.
36.000	:	:	:	:	:	:	278.
35.500	:	:	:	:	:	:	282.
35.000	:+++++					X	286.
34.500	:	:	:	:	:	:	290.
34.000	:	:	:	:	:	:	294.
33.500	:	:	:	:	:	:	299.
33.000	:	:	:	:	:	:	303.
32.500	:	:	:	:	:	:	308.
32.000	:	:	:	:	:	:	313.
31.500	:	:	:	:	:	:	317.
31.000	:	:	:	:	:	:	323.
30.500	:X	:	:	:	:	:	328.
30.000	:	:	:	:	:	:	333.
29.500	:	:	:	:	:	:	339.
29.000	:-----					Y	345.
28.500	:Y	:	:	:	:	:	351.
28.000	:Y	:	:	:	:	:	357.
27.500	:	:	:	:	:	:	364.
27.000	:	:	:	:	:	:	370.
26.500	:X-----					Y	377.

26.000	:	:	:	:	:	:	385.
25.500	:	:	:	:	:	:	392.
25.000	:	:	:	:	:	:	400.
24.500	:	:	:	:	:	:	408.
24.000	:	:	:	:	:	:	417.
23.500	:	:	:	:	:	:	426.
23.000	:	:	:	:	:	:	435.
22.500	:	:	:	:	:	:	444.
22.000	:	:	:	:	:	:	455.
21.500	:	:	:	:	:	:	465.
21.000	:	:	:	:	:	:	476.
20.500	:	:	:	:	:	:	488.
20.000	:	:	:	:	:	:	500.
19.500	:	:	:	:	:	:	513.
19.000	:	:	:	:	:	:	526.
18.500	:	:	:	:	:	:	541.
18.000	:	+++++	+++++	+++++	+++++	+++++	556.
17.500	:	:	:	:	:	:	571.
17.000	:	:	:	:	:	:	588.
16.500	:	:	:	:	:	:	606.
16.000	:	:	:	:	:	:	625.
15.500	:	:	:	:	:	:	645.
15.000	:	:	:	:	:	:	667.
14.500	:	:	:	:	:	:	690.
14.000	:	:	:	:	:	:	714.
13.500	:	:	:	:	:	:	741.

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KK : . . . . . 1.0 : . . . . . 1.5 : . . . . . 2.0 : . . . . . 2.5 : . . . . . 3.0 : . . . . . 3.5 : . . . . . 4.0 : . . . . . 4.5 : . . . . . 5.0 : . . . . . 5.5 : . . . . . 6.0 : NM

L O G E P S I L O N