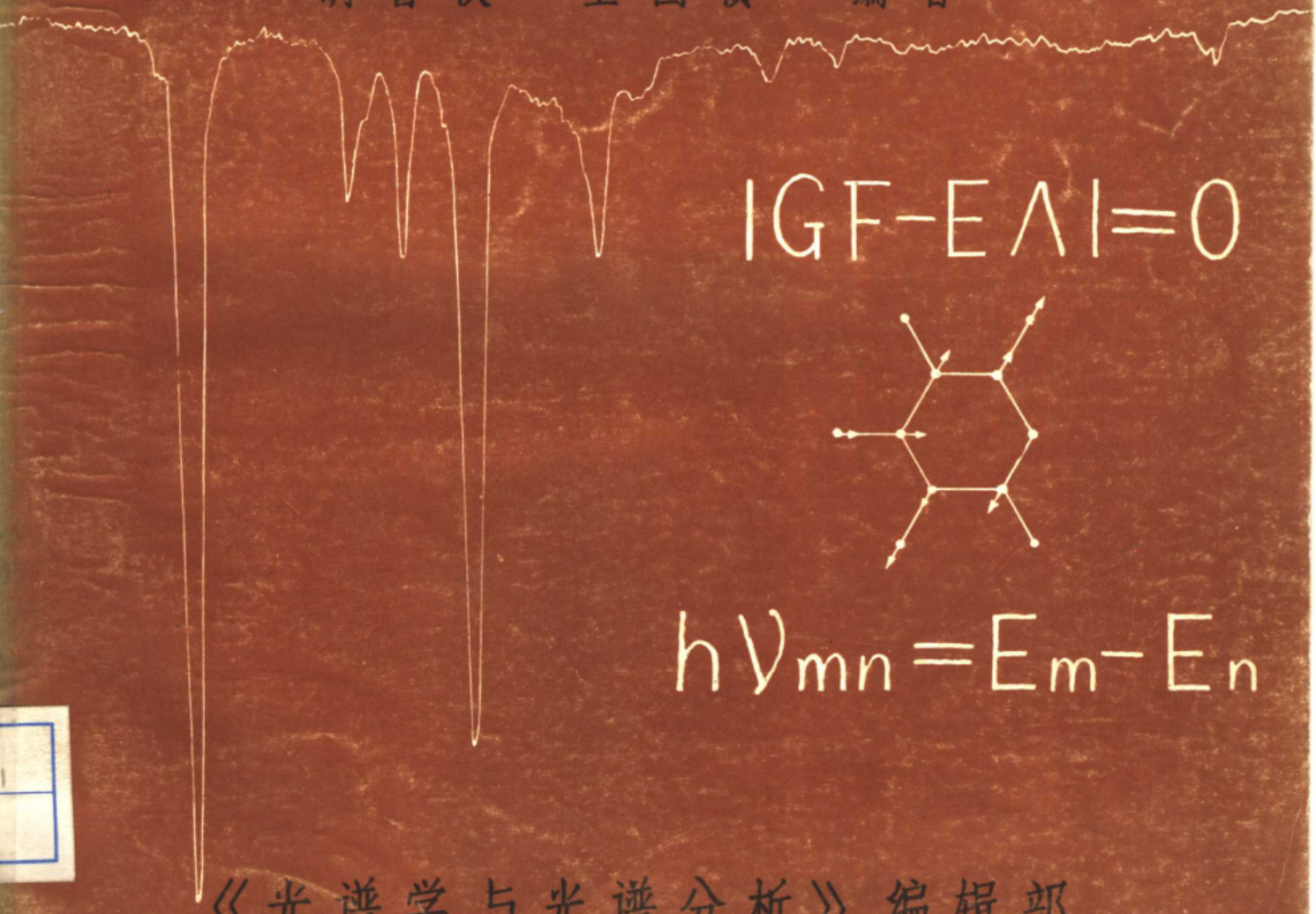
红外与拉曼光谱的计算原理和计算程序

（下 册）

胡皆汉　王国祯　编著



《光谱学与光谱分析》编辑部

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（下）

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《光谱学与光谱分析》编辑部

目　　录

第五章　振动光谱计算程序

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5.1　FELIX C-512 计算程序

5.1.1　程序 GCCC

```
.          ALLOC DVT:AD,VS:ADMAN1,FN:'XYX',AM:ANY,SZ:1
.          SEG P
.          COMPILE FORTRAN,DBL,NLG
* DEFINE FILE L0(DVT:AD, RCF : V,BFS:84)=12
* SEGMENT F%BLK,G,H
      COMMON RECORD(36),MPLAS(10),AVALU(10),Y(3,3),MAS(200),
     1          MMPA(50),MAPA(50),VALU(150),W(100),D(100,50),
     2          CRRCT(50),DELTA(100)/G/OBS(50),CPA(50),CCPA(50),
     3          DWP(50),DWD(50,50), U(50, 50), RUDWP(50),XG(3),
     4          CALC(100),VMAS(20),TI(3,3),UI(3,3),TMASX(3),
     5          AMSS(200),ASSIGN(100,3),IAN(3)
      COMMON /H/I1,I2,I3,L4,JAPA(50),KP(200),NAPA,JUD(200),
     1          IA(200,4),IP(200,3),ICOM(200,3),X(200,3),T(3,3),
     2          PARA(150)
  101 FORMAT(18A4)
  102 FORMAT(18I4)
  103 FORMAT(6F12.6)
  104 FORMAT(3I4, F12.0)
  111 FORMAT(1H1////13H0PROGRAM GCCC//5X,11HPROBLEM NO.,
     1       I4///(/9X,18A4))
  112 FORMAT(1H1/////13H PROBLEM NO. ,I4//3X,
     1          28HINTERNAL COORDINATE SET NO. ,I4/)
  113 FORMAT(13X,21HVALUE NO.       INPUT    , 5X,
     1       8HRESULT  , 5X,7HDELTA   , 4X,6HWEIGHT,5X,
     2       7HDELTA*W, 7X,10HASSIGNMENT)
  114 FORMAT(1H1/////23H CARTESIAN COORDINATE   ,/)
  115 FORMAT(1H1/// 3X,10HCYCLE NO. ,I4/
     1       /4X,30H  INPUT PARAMETER (VARIABLE)  /)
  116 FORMAT(1H0/5X,20H ADDED DATA                 /)
```

```
117   FORMAT(4X,11HPROBLEM NO.,I3// 6X,10H INTERNAL
     1          20HCOORDINATE SET NO.
     2          ,I3//23X,2HX-,12X,2HY-,12X,2HZ-,//(10H ATOM NO.
     3          ,I3,5X,3F14.6/))
118   FORMAT(1H1,////22H0CARTESIAN COORDINATE
     1          13HTRANSFORMED  /)
119   FORMAT(8H0      NO. ,I3,5X,I3,4X,5F12.6,5X,3A4)
120   FORMAT(8X, 6HLENGTH,36X, 5HANGLE/)
121   FORMAT(12X, 2(4H NO., I3, F15.6,18X)/)
122   FORMAT(12X, 4H NO.,I3, F15.6/)
123   FORMAT(52X, 4H NO. I3, F15.6/)
131   FORMAT(////14X, 16HEND OF SET NO.  ,I3)
132   FORMAT(//////12X,20HEND OF PROBLEM NO.  , I3)
133   FORMAT(////////10X, 10H END OF JOB)
134   FORMAT(///20X, 6HSUMD =, F20.12)
135   FORMAT(/////8X, 28HDIVERGED, SKIP TO NEXT SET  )
136   FORMAT(/////8X, 30HSOME CONTRADICTION IS IN YOUR
     1          24HLEAST SQUARE  CONDITION
     2          //8X, 20H SKIP TO NEXT SET     )
137   FORMAT(/////36H ATOM NO. IATY IS WRITTEN BUT INPUT
     1          39HDATA DO NOT SATISFY REQUIRED PRECISION
     2          //23H TO BE CALCULATED MORE
     3          14HSYMMETRICALLY  )
140   FORMAT(///5X,28HPRINCIPAL MOMENTS OF INERTIA//10X,
     1          3F18.6)
      READ(105,102) NJOB
      DO 1000 NOPROB=1,NJOB
      READ(105,101) (RECORD(I), I=1,36)
      WRITE(108,111) NOPROB,RECORD
      RAD=0.01745329252D0
      READ(105,102) NAT,NLNGS,NANGL, ICAD,NVAR,NLS,IFT,
     1        NMAS,(IAN(I),I=1,3),IATY,IATG
      IF(NVAR .EQ. 0) NVAR=1
      NLA=NLNGS+NANGL
      READ(105,103) (VALU(I),I=1, NLA)
      READ(105, 103) ((Y(J, I),I=1,3), J=1,3)
      IF(IFT .EQ. 0) GO TO 2
      READ(105,103) (VMAS(I),I=1, NMAS)
      READ(105,102) (MAS(I),I=1,NAT)
```

```
      DO 1 I=1, NAT
      J=MAS(I)
    1 AMSS(I)=VMAS(J)
    2 NATM3=NAT-3
      DO 3 I=1, NATM3
    3 READ(105, 102) (JUD(I), (IA(I,J), J=1,4), (IP(I,J), J=1,3),
     1          (ICOM(I, J), J=1, 3))
  200 DO 2000 NOVAR=1, NVAR
      DO 4 K=1, 3
      DO 4 J=1,3
      I=IAN(K)
      IF(I .EQ. 0) I=K
    4 X(I,J)=Y(K, J)
      WRITE(108,112) NOPROB,NOVAR
      DO 201 I=1, NLNGS
  201 PARA(I)=VALU(I)
      NLNGSP1=NLNGS+1
      DO 202 I=NLNGSP1, NLA
      IF(VALU(I) .EQ. -3.0) VALU(I)=109.4712206345
  202 PARA(I)=0.01745329252*VALU(I)
      READ(105, 102) NPLAS, ICOND
      IF(NPLAS .EQ. 0) GO TO 204
      READ(105, 102) (MPLAS(I), I=1, NPLAS)
      READ(105, 103) (AVALU(I), I=1, NPLAS)
      DO 203 I=1, NPLAS
      MPL=MPLAS(I)
      VALU(MPL)=AVALU(I)
      IF(VALU(MPL) .EQ. -3.0) VALU(MPL)=109.4712206345
      PARA(MPL)=VALU(MPL)
      IF(MPL .GT. NLNGS) PARA(MPL)=RAD*PARA(MPL)
  203 CONTINUE
  204 MLA=MIN0(NLNGS, NANGL)
      MAN=MLA+NLNGS+1
      WRITE(108,120)
      DO 5 I=1, MLA
      J=I+NLNGS
    5 WRITE(108,121) I, VALU(I), J, VALU(J)
      IF(NANGL-NLNGS) 6, 8, 7
    6 MLAP1=MLA+1
```

```
      WRITE(108,122) (I,VALU(I), I=MLAP1, NLNGS)
      GO TO 8
    7 WRITE(108,123) (J,VALU(J), J=MAN, NLA)
    8 CONTINUE
      IF(NLS .EQ. 0) GO TO 213
      IF(ICOND .EQ. 1) GO TO 209
      DDD =0.0002D0
  205 READ(105,104) NATLS, NMPA, NAPA, DDDD
      NMA=NMPA+NAPA
      IF(DDDD .NE. 0.0) DDD=DDDD
      READ(105,102) (MMPA(I), I=1,NMPA)
      READ(105,102)  (JAPA(I), MAPA(I), I=1, NAPA)
      I=1
  206 KI=18*I-17
      KF=18*I
      READ(105,102) (KP(K), K=KI, KF)
      DO 207 K= KI,KF
      IF(KP(K) .LE. 0) GO TO 208
  207 CONTINUE
      I=I+1
      GO TO 206
  208 READ(105,103) (W(I), I=1, NMA)
      READ(105,101) ((ASSIGN(I,J), J=1,3),  I=1,NMA)
  209 DO 211 I=1,NMPA
      DO 210 J=1,NMA
  210 D(J,I)=0.0
      D(I,I)=1.0D0
      CRRCT(I)=0.0
  211 DELTA(I)=0.0
      DO 212 I=1,NAPA
      J=IABS(MAPA(I))
  212 OBS(I)=PARA(J)
      SUMD=0.0
   10 DO 100 NOLS=1, NLS
      WRITE(108,115) NOLS
      WRITE(108,113)
      DO 15 I=1, NMPA
      J=MMPA(I)
      PARA(J)=PARA(J)+CRRCT(I)
```

```
      CALC(J)=PARA(J)
      DELTA(I)=DELTA(I)-CRRCT(I)
      DEL=DELTA(I)
      IF(J .LE. NLNGS) GO TO 14
      CALC(J)=PARA(J)/RAD
      DEL=DELTA(I)/RAD
   14 DELW=DEL*W(I)
   15 WRITE(108,119) I, J, VALU(J), CALC(J), DEL, W(I), DELW,
     1          (ASSIGN(I,KK), KK=1,3)
      CALL CALCX(1, NATLS-3)
      WRITE (108,114)
      WRITE(108,117) NOPROB, NOVAR, (J,(X(J,I), I=1,3), J=1,NAT)
      IF(L4 .EQ. -1) GO TO 1000
      CALL CALCP(CPA)
      WRITE(108,116)
      WRITE (108,113)
      DO 17 I=1, NAPA
      J=MAPA(I)
      K=I+NMPA
      CALC(I)=CPA(I)
      IF(J .LT. 0 .AND. NOLS .EQ. 1 .AND. CPA(I)*OBS(I) .LT.  0.0)
     1          OBS(I)=-OBS(I)
      IF(J .LT. 0) J =-J
      DELTA(K)=OBS(I)-CPA(I)
      DEL=DELTA(K)
      IF(J .LE. NLNGS) GO TO 16
      CALC(I)=CPA(I)/RAD
      DEL=DELTA(K)/RAD
   16 DELW=DEL*W(K)
   17 WRITE(108,119) I, J, VALU(J), CALC(I), DEL, W(K),
     1          DELW, (ASSIGN(K,KK), KK=1, 3)
      S=0.0
      DO 12 I=1,NMA
   12 S=S+W(I)*DELTA(I)**2
      WRITE (108,134) S
      IF (S .LT. 1.1*SUMD+1.0D-6 .OR. NOLS .EQ. 1) GO TO 13
      WRITE(108,135)
      GO TO 2000
   13 SUMD=S
```

```
      DO 19 I=1, NMPA
      K =MMPA(I)
      PARA(K) =PARA(K)+DDD
      CALL CALCX(1,NATLS-3)
      IF(L4 .EQ. -1) GO TO 1000
      CALL CALCP(CCPA)
      DO 18 J=1, NAPA
      L=NMPA+J
   18 D(L,I)=(CCPA(J)-CPA(J) )/DDD
   19 PARA(K)=PARA(K)-DDD
      DO 20 I=1, NMPA
      DWP(I)=0.0
      CRRCT(I)=0.0
      RUDWP(I)=0.0
      DO 20 J=1, NMPA
   20 DWD(I,J)=0.0
      DO 22 K=1, NMA
      DO 22 I=1, NMPA
      DO 21 J=1, NMPA
   21 DWD(I,J)=DWD(I,J)+D(K,I)*W(K)*D(K,J)
   22 DWP(I)=DWP(I) +D(K,I)*W(K)*DELTA(K)
      TRAS=0.0
      DO 23 I=1, NMPA
   23 TRAS =TRAS+DWD(I,I)
      TRAS=TRAS/FLOAT(NMPA)*1.0E-7
      CALL DJACO (DWD,U,NMPA,1,TRAS,50)
      DO 24 I=1, NMPA
      DO 24 K=1, NMPA
      IF (DWD(I,I) .GT. 1.0E-7) GO TO 24
      WRITE(108,136)
      GO TO 2000
   24 RUDWP(I) =RUDWP(I)+(1.0/DWD(I,I))*U(K,I)*DWP(K)
      DO 25 K=1, NMPA
      DO 25 I=1, NMPA
   25 CRRCT(K)=CRRCT(K)+U(K,I)*RUDWP(I)
  100 CONTINUE
  213 CALL CALCX(1,NAT-3)
      IF(L4 .EQ. -1) GO TO 1000
  214 WRITE(108,114)
```

```
      WRITE (108,117) NOPROB, NOVAR, (J,(X(J,I), I=1,3), J=1, NAT)
      IF(IFT .EQ. 0) GO TO 220
      TMAS=0.0
      DO 215 J=1,3
      TMASX(J)=0.0
      DO 215 I=1,3
  215 TI(I,J)=0.0
      DO 216 I=1, NAT
      TMAS=TMAS+AMSS(I)
      DO 216 J=1,3
  216 TMASX(J)=AMSS(I)*X(I,J)+TMASX(J)
      DO 217 J=1,3
      XG(J)=TMASX(J)/TMAS
      DO 217 I=1, NAT
  217 X(I,J)=X(I,J)-XG(J)
      DO 218 I=1,NAT
      TI(1,1)=TI(1,1) +AMSS(I)*(X(I,2)**2+X(I,3)**2)
      TI(2,2)=TI(2,2)+AMSS(I)*(X(I,1)**2+X(I,3)**2)
      TI(3,3)=TI(3,3)+AMSS(I)*(X(I,2)**2+X(I,1)**2)
      TI(1,2)=TI(1,2)-AMSS(I)*X(I,1)*X(I,2)
      TI(1,3)=TI(1,3)-AMSS(I)*X(I,1)*X(I,3)
  218 TI(2,3)=TI(2,3)-AMSS(I)*X(I,2)*X(I,3)
      TRAS=(TI(1,1)+TI(2,2)+TI(3,3))/3.0*1.0D-10
      CALL DJACO (TI,UI,3,1,TRAS,3)
      WRITE(108,140) (TI(I,I), I=1, 3)
      TI1=DABS(TI(2,2)-TI(3,3))
      IF(TI1 .GT. 1.0 D-4) GO TO 232
      DO 231 I=1, 3
      UUI=UI(I,3)
      UI(I,3)=UI(I,1)
  231 UI(I,1)=UUI
      GO TO 234
  232 TI2=DABS( TI(1,1)-TI(3,3))
      IF(TI2 .GT. 1.0D-4) GO TO 234
      DO 233 I=1,3
      UUI =UI(I, 3)
      UI(I, 3)=UI(I, 2)
  233 UI(I, 2)=UUI
  234 DO 235 I=1, NAT
```

```
      DO 219 J=1, 3
219   XG(J)=UI(1,J)*X(I,1)+UI(2,J)*X(I,2)+UI(3,J)*X(I,3)
      DO 235 J=1, 3
235   X(I,J)=XG(J)
      IF(IATY .EQ. 0) GO TO 239
      TI3=DABS(TI(1,1)-TI(2,2))
      IF(TI1.GT. 1.0D-4.AND. TI2.GT. 1.0D-4.AND. TI3.GT. 1.0D-4)
     1          WRITE (108, 137)
      R=DSQRT(X(IATY ,1)**2+X(IATY, 2)**2)
      COSY=X(IATY, 2)/R
      SINY=DSIN(TETA1(COSY, 1))
      DO 237 I=1, NAT
      XG(1)=COSY*X(I, 1)+SINY*X(I, 2)
      X(I,2)=-SINY*X(I, 1)+COSY*X(I, 2)
237   X(I, 1)=XG(1)
239   IF(IATG .EQ. 0) GO TO 241
      DO 240 J=1, 3
      XG(J)=X(IATG,J)
      DO 240 I=1, NAT
240   X(I,J)=X(I, J)-XG(J)
241   WRITE(108, 118)
      WRITE(108,117) NOPROB, NOVAR, (J, (X(J, I), I=1,3), J=1,NAT)
220   CONTINUE
      IF(ICAD .EQ. 0) GO TO 221
      WRITE(108,102) NOPROB, NOVAR
      REAL XY(200,3)
      DO 243 J=1,NAT
      DO 242 I=1, 3
242   XY(J, I)=X(J, I)
243   CONTINUE
      WRITE(12,103) ((XY(J,I),I=1, 3), J=1, NAT)
      WRITE(108,103) ((X(J,I), I=1, 3), J=1, NAT)
221   CONTINUE
      WRITE(108,131) NOVAR
2000  CONTINUE
      WRITE(108,132) NOPROB
1000  CONTINUE
      WRITE(108,133)
```

```
      REWIND 12
      STOP
      END

.           SEG Q
.           COMPILE FORTRAN, DBL, NLG
* SEGMENT H
      SUBROUTINE CALCX(NIA, NFA)
      COMMON/H/I1,I2,I3,L4,JAPA(50), KP(200),NAPA,JUD(200),
     1            IA(200,4), IP(200,3), ICOM(200,3),
     2            X(200,3), T(3,3), PARA(150)
      DIMENSION TX(3), TY(3), TZ(3), TXY(3)
C     TETA TO R1
      TETA2(R1, R2, R3)=TETA1 ((R2**2+R3**2-R1**2)/
     1       (2.0*R2*R3), 1)
      DO 100 I=NIA, NFA
      K1=IP(I,1)
      K1=IABS(IP(I,1))
      K2=IABS(IP(I,2))
      K3=IABS(IP(I,3))
      P1=PARA(K1)
      P2=PARA(K2)
      P3=PARA(K3)
      IF(IP(I,1) .LT. 0) P1=-P1
      IF(IP(I,2) .LT. 0) P2=-P2
      IF(IP(I,3) .LT. 0) P3=-P3
      I1=IA(I,1)
      I2=IA(I,2)
      I3=IA(I,3)
      DO 1 J=1, 3
      T(J,1)=(X(I3,J)-X(I2, J))/DSQRT(AD2(I2,I3))
      TX(J)=T(J,1)
    1 TXY(J)=(X(I1,J)-X(I2,J))
      CALL VPN(TX, TXY, TZ)
      CALL VPN(TZ, TX, TY)
      DO 2 J=1, 3
      T(J, 3)=TZ(J)
    2 T(J,2)=TY(J)
      L4=IA(I,4)
```

```
      JJ=JUD(I)
      GO TO (91,92, 93,94,95,96),JJ
C
   91 CALL CASE1(P1, P2, P3)
      GO TO 100
   92 CALL CASE2(P1, P2, P3, ICOM(I,1))
      GO TO 100
   93 AB2=TETA2(P2, P1, DSQRT(AD2(I1, I3)))
      IF(AB2 .EQ.-10.0) GO TO 9
      CALL CASE2(P1, P3, AB2, ICOM(I,1))
      GO TO 100
   94 AB1=TETA2(P2, P3, DSQRT(AD2(I2, I3)))
      AB2=TETA2(P1, P3, DSQRT(AD2 (I1, I3)))
      IF(AB1 .EQ.-10.0 .OR. AB2 .EQ.-10.0) GO TO 9
      CALL CASE2(P3, AB1, AB2, ICOM(I,1))
      GO TO 100
   95 TO=0.0
      IF(ICOM(I,2) .LT. 0) TO=3.1415926535898
      IF(P3 .EQ. 0.0) GO TO 4
    3 COSTO=DSQRT(1.0-(DSIN(P3)/DSIN(P2))**2)
      TO=TETA1(DSIGN(COSTO, FLOAT(ICOM(I, 2))), ICOM(I, 1))
    4 CALL CASE1(P1, P2, TO)
      GO TO 100
   96 I5=ICOM(I,1)
      A=(P1**2+AD2(I3,I5)-P2**2)/(2.0*P1*DSQRT(AD2(I3, I5)))
      C235=TETA3(I2, I3, I5)
      D=TOR(I1, I2, I3, I5)
      B=DCOS(C235)
      C=DSIN(C235)*DCOS(D)*DCOS(P3)+DSIN(C235)*DSIN(D)
     1          *DSIN(P3)
      COSAB=(A*B+DSIGN(C*DSQRT(C**2+B**2-A**2),
     1          FLOAT(ICOM(I, 2))))/(B**2+C**2)
      AB=TETA1(COSAB, 1)
      IF(AB .EQ. -10.0) GO TO 9
      CALL CASE1(P1, AB, P3)
  100 CONTINUE
  101 FORMAT(////10X,34HTHERE ARE CONTRADICTIONS IN INPUT,
     1          11HDATA,  CASE I4, 3X, 8HATOM NO. I4//10X,
     2          24HJUMP TO NEXT PROBLEM      )
```

```
      GO TO 10
    9 WRITE(108, 101) JJ, L4
      L4=-1
   10 RETURN
      END

* SEGMENT H
      SUBROUTINE CASE1(R, AB, TO)
      COMMON/H/I1, I2, I3, L4, JAPA(50),KP(200),NAPA, JUD(200),
     1         IA(200,4), IP(200, 3),ICOM(200, 3),X(200,3),
     2         T(3, 3),PARA(150)
      DIMENSION XL(3)
      XL(1)=-R*DCOS(AB)
      XL(2)=R*DSIN(AB)*DCOS(TO)
      XL(3)=R*DSIN(AB)*DSIN(TO)
      DO 1 J=1, 3
    1 X(L4,J)=X(I3,J)+T(J,1)*XL(1)+T(J,2)*XL(2)+T(J,3)*XL(3)
      RETURN
      END

* SEGMENT H
      SUBROUTINE CASE2(R, AB1, AB2, NP)
      COMMON/H/I1, I2, I3, L4, JAPA(50),KP(200),NAPA, JUD(200),
     1         IA(200,4),IP(200, 3),ICOM(200, 3),
     2         X(200, 3), T(3, 3), PARA(150)
      C132=TETA3(I1, I3, I2)
      COSTO=(DCOS(AB2)-DCOS(C132)*DCOS(AB1))/(DSIN(C132)
     1         *DSIN(AB1))
      TO=TETA1(COSTO, NP)
      IF(TO .EQ. -10.0) GO TO 9
      CALL CASE1(R, AB1, TO)
      GO TO 10
  101 FORMAT(////10X, 28HTHERE ARE CONTRADICTIONS IN
     1         21HINPUT DATA,  CASE   2, 3X, 8HATOM NO.
     2         I4//10X,24HJUMP TO NEXT PROBLEM        )
    9 WRITE(108,101) L4
      L4=-1
   10 RETURN
      END
```

```
* SEGMENT H
      SUBROUTINE CALCP(CP)
      COMMON/H/I1, I2, I3, L4, JAPA(50), KP(200), NAPA, JUD(200),
     1          IA(200,4),IP(200, 3), ICOM(200, 3),
     2          X(200, 3), T(3, 3 ), PARA(150)
      DIMENSION CP(50), A1(3), A2(3), A4(3), A5(3), B1(3), B2(3)
      K=1
      DO 100 I=1, NAPA
      JP=JAPA(I)
      NA1=KP(K)
      NA2=KP(K+1)
      NA3=KP(K+2)
      NA4=KP(K+3)
      GO TO (11, 12, 13, 14, 15, 16, 17) JP
   11 IXYZ=KP(K+1)
      IATOM =KP(K)
      CP(I)=X(IATOM, IXYZ)
      K=K+2
      GO TO 100
   12 CP(I)=DSQRT(AD2(NA1, NA2))
      K=K+2
      GO TO 100
   13 CP(I)=TETA3(NA1, NA2, NA3))
      K=K+3
      GO TO 100
   14 CP(I)=TOR(NA1, NA2, NA3, NA4)
      K=K+4
      GO TO 100
C     OUT OF PLANE
   15 DO 1 J=1,3
      A1(J) =X(NA1, J)-X(NA3, J)
      A2(J)=X(NA2, J)-X(NA3, J)
    1 A4(J)=X(NA4, J)-X(NA3, J)
      CALL VPN(A1, A2, B1, )
      CP(I)=3.14159265359/2.0-TETA1(SPN(A4, B1), 1)
      K=K+4
      GO TO 100
C     TETA BETWEEN PLANES
```

```
   16   NA5=KP(K+4)
        NA6=KP(K+5)
        DO 2 J=1, 3
        A1(J)=X(NA1, J)-X(NA3, J)
        A2(J)=X(NA2, J)-X(NA3, J)
        A4(J)=X(NA4, J)-X(NA6, J)
    2   A5(J)=X(NA5, J)-X(NA6, J)
        CALL VPN(A1, A2, B1)
        CALL VPN(A4, A5, B2)
        CP(I)=TETA1(SPN(B1, B2), 1)
        K=K+6
        GO TO 100
C       TETA BETWEEN LINES
   17   DO 3 J=1, 3
        A2(J)=X(NA2, J)-X(NA1, J)
    3   A4(J)=X(NA4, J)-X(NA3, J)
        CP(I)=TETA1(SPN(A2, A4), 1)
        K=K+4
  100   CONTINUE
        RETURN
        END
* SEGMENT H
        DOUBLE PRECISION FUNCTION AD2(NB1, NB2)
C       SQUARE DISTANCE BETWEEN ATOM NB1, NB2
        COMMON/H/I1, I2, I3, L4, JAPA(50), KP(200), NAPA,
       1         JUD(200), IA(200, 4), IP(200, 3),
       2         ICOM(200, 3), X(200, 3), T(3, 3), PARA(150)
        AD2=0.0
        DO 1 I=1, 3
    1   AD2=AD2+(X(NB1, I)-X(NB2, I))**2
        RETURN
        END
        DOUBLE PRECISION FUNCTION TETA1(COSTE, J)
C       ARCCOSINE
        TETA1=-10.0
        SINTE=0.0
        IF(DABS(COSTE) .GT. (1.0+1.0E-5)) GO TO 2
        IF(DABS(COSTE) .GE. 1.0) GO TO 1
        SINTE=DSQRT(1.0-COSTE**2)
```

```
      IF(J .LT. 0) SINTE=-SINTE
    1 TETA1=DATAN2(SINTE, COSTE)
    2 RETURN
      END
      DOUBLE PRECISION FUNCTION TETA3(NA1, NA2, NA3)
C     TETA TO NA2
      R2=AD2(NA1, NA3)
      R1=AD2(NA2, NA3)
      R3=AD2(NA1, NA2)
      COSTE=(R1+R3-R2)/(2.0*DSQRT(R1)*DSQRT(R3))
      TETA3=TETA1(COSTE, 1)
      RETURN
      END

* SEGMENT H
      DOUBLE PRECISION FUNCTION TOR(NA1, NA2, NA3, NA4)
      COMMON/H/I1, I2, I3, L4, JAPA(50), KP(200), NAPA, JUD(200),
     1         IA(200, 4), IP(200, 3),
     2         ICOM(200, 3),X(200, 3), T(3,3 ), PARA(150)
      DIMENSION A1(3), A2(3), A3(3), A4(3), B1(3), B2(3)
      DO 1 I=1, 3
      A1(I)=X(NA3, I)-X(NA2, I)
      A2(I)=X(NA1, I)-X(NA2, I)
      A3(I)=-A1(I)
    1 A4(I)=X(NA4, I)-X(NA3, I)
      CALL VPN(A1, A2, B1)
      CALL VPN(A4, A3, B2)
      N=DSIGN(1.0, SPN(B1, A4))
      TOR=TETA1(SPN(B1, B2), N)
      RETURN
      END
      DOUBLE PRECISION FUNCTION SPN(A1, A2)
C     SCALAR PRODUCT NORMALIZED
      DIMENSION A1(3), A2(3)
      SRDI1=DSQRT(A1(1)**2+A1(2)**2+A1(3)**2)
      SRDI2=DSQRT(A2(1)**2+A2(2)**2+A2(3)**2)
      SPN=(A1(1)*A2(1)+A1(2)*A2(2)+A1(3)*A2(3))/(SRDI1*SRDI2)
      RETURN
      END
```