MODELLING BIOLOGICAL MACROMOLECULES IN SOLUTION: THE GENERAL TRI-AXIAL ELLIPSOID

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Appendix V FORTRAN IV computer programs

Program 1: Evaluates values of the various hydrodynamic shape functions for tri-axial ellipsoids for a user specifiable value of the axial ratios (a/b, b/c)

Program 2: Produces tables of these functions for axial ratios between 1.0 and 2.0 in steps of 0.1

Program 3: Produces a contour map of ν in the (a/b, b/c) plane for axial ratios between 1.0 and 3.0

Program 4: Produces plots of the various tri-axial functions in the (a/b, b/c) plane corresponding to the point (1.5, 1.5). Several plots allow for arbitrary errors in measurement

Program 5: Non-linear least squares iterative method for resolving a 2-term exponential birefringence decay. This program (and the following two) produces its own synthetic data

Program 6: Fourier Transform solution of the Laplace Integral Equation method

Program 7: R-constrained non-linear least squares iterative method

Function	Computer Symbol
a/b	A/B
b/c	B/C
ν	NU, S
f/f_o ($\equiv P$)	F
ζ_a/ζ_o	CA, CA/CO
ζ_b/ζ_o	CB, CB/CO
ζ_c/ζ_o	CC, CC/CO
ρ_a/ρ_o	RHOA, RHOA/RHOO
ρ_b/ρ_o	RHOB, RHOB/RHOO
ρ_c/ρ_o	RHOC, RHOC/RHOO
β	BETA
R	R
δ_a	DELTAA, DELTA(A)
δ_b	DELTAB, DELTA(B)
δ_c	DELTAC, DELTA(C)
γ_a	GAMMAA, GAMMA(A)
γ_b	GAMMAB, GAMMA(B)
γ_c	GAMMAC, GAMMA(C)
μ_a	MUA, MU(A)
μ_b	MUB, MU(B)
μ_c	MUC, MU(C)
τ_h/τ_o	TAU, TAU/TAUO
Ψ	PSI
Λ	LAMBDA
θ_+^{red}	TPLS, THETA+, Z
θ_-^{red}	TMNS, THETA-, U

Function	Computer Symbol
δ_+	DPLS, DELTA+, V
δ_-	DMNS, DELTA-, W
γ_+	GPLS, GAMMA+
γ_-	GMNS, GAMMA-
τ_1/τ_o	T1
τ_2/τ_o	T2
τ_3/τ_o	T3
τ_4/τ_o	T4
τ_5/τ_o	T5
θ_+	THPLUS
θ_-	THMNUS

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C     ****************************************************************
C        THIS PROGRAM GENERATES VALUES OF THE VARIOUS HYDRODYNAMIC
C        SHAPE FUNCTIONS FOR A USER SPECIFIABLE VALUE OF THE AXIAL
C        RATIOS A/B (=N1) & B/C (=N2)
C     ****************************************************************
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/A,C,NN
      EXTERNAL FUN
      DIMENSION ALPHA(10)
      REAL NU,M,O,P
      REAL MUA,MUB,MUC,PSI,N1,N2,RHOA,RHOB,RHOC
C ENTER AS DATA AT THE FOOT OF THE PROGRAM (A/B, B/C)
      READ(2,*)N1,N2
      NN=0
C     COMPUTE THE ELLIPTIC INTEGRALS
      DO45 K=1,10
      A=N1
      B=1.0
      C=1.0/N2
      NN=NN+1
C     SET LIMITS FOR NUMERICAL INTEGRATION (THESE LIMITS
C     BELOW HAVE BEEN PREVIOUSLY TESTED FOR CONVERGENCE)
      AA=0.0
      BB=1000000
      IF(NN.EQ.10)BB=500000000
      MAXDIV=50
      EPS=1.0E-08
      ACC=0.0
      IFAIL=0
C     CALL U.K. "NAG" LIBRARY ROUTINE FOR NUMERICAL EVALUATION
C     OF THE INTEGRALS "ALPHA" GIVEN IN THE SUBROUTINE BELOW
      CALL D01AGF(AA,BB,FUN,MAXDIV,EPS,ACC,ANS,ERROR,NOFUN,IFAIL)
      ALPHA(NN)=ANS
   45 CONTINUE
      B=1.0
C     NOW COMPUTE THE FUNCTION VALUES USING THE STORED INTEGRAL VALUES
      NU=(1.0/(A*B*C))*((4.0/15.0)*((ALPHA(7)+ALPHA(8)
     + +ALPHA(9))/(ALPHA(8)*ALPHA(9)+ALPHA(9)*ALPHA
     + (7)+ALPHA(7)*ALPHA(8)))+(1.0/5.0)*(((ALPHA(2)
     + +ALPHA(3))/(ALPHA(4)*(B*B*ALPHA(2)+C*C*ALPHA(3)
     + )))+((ALPHA(3)+ALPHA(1))/(ALPHA(5)*(C*C*ALPHA(3)
     + +A*A*ALPHA(1))))+((ALPHA(1)+ALPHA(2))/(ALPHA(6)
     + *(A*A*ALPHA(1)+B*B*ALPHA(2))))))
      M=(B*B+C*C)/(B*B*ALPHA(2)+C*C*ALPHA(3))
      O=(C*C+A*A)/(C*C*ALPHA(3)+A*A*ALPHA(1))
      P=(A*A+B*B)/(A*A*ALPHA(1)+B*B*ALPHA(2))
      TPLS=((A*B*C)/(12.0))*((((1.0/M)+(1.0/O)+(1.0/P
     + ))+(((1.0/M**2.0)+(1.0/O**2.0)+(1.0/P**2.0))-
     + ((1.0/(M*O))+(1.0/(O*P))+(1.0/(P*M
     + ))))**0.5))
      TMNS=((A*B*C)/(12.0))*((((1.0/M)+(1.0/O)+(1.0/P
     + ))-(((1.0/M**2.0)+(1.0/O**2.0)+(1.0/P**2.0))-
     + ((1.0/(M*O))+(1.0/(O*P))+(1.0/(P*M
     + ))))**0.5))
      DPLS=6.0*TPLS*NU
      DMNS=6.0*TMNS*NU
      F=2.0/(((A*B*C)**(1.0/3.0))*ALPHA(10))
      R=2.0*(1.0+(F**3.0))/NU
      BETA=(1.0/1000000.0)*(((6.0249**(1.0/3.0))*(10.0**(23.0/3.0
     +)))/((16200.0*3.141592654*3.141592654)**(1.0/3.0)))*(NU
     +**(1.0/3.0))/F
      CA=(2.0/(3.0*A*B*C))*M
      CB=(2.0/(3.0*A*B*C))*O
      CC=(2.0/(3.0*A*B*C))*P
      RHOA=2.0/((1.0/CB)+(1.0/CC))
      RHOB=2.0/((1.0/CC)+(1.0/CA))
      RHOC=2.0/((1.0/CA)+(1.0/CB))
      DELA=NU/CA
      DELB=NU/CB
      DELC=NU/CC
      TAU=3.0/((1.0/CA)+(1.0/CB)+(1.0/CC))
      PSI=F*((1.0/TAU)**(1.0/3.0))
      V=NU/TAU
      ZZ=(1.0/2.0)*(F**3.0)
      GAMMAA=ZZ*((1.0/CB)+(1.0/CC))
      GAMMAB=ZZ*((1.0/CC)+(1.0/CA))
      GAMMAC=ZZ*((1.0/CA)+(1.0/CB))
      MUA=(CA**(1.0/3.0))/F
      MUB=(CB**(1.0/3.0))/F
      MUC=(CC**(1.0/3.0))/F
      GPLS=6.0*TPLS*(F**3.0)
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      GMNS=6.0*TMNS*(F**3.0)
      X1=0.5*((1.0/RHOB)+(1.0/RHOC)-(1.0/RHOA))
      X2=0.5*((1.0/RHOC)+(1.0/RHOA)-(1.0/RHOB))
      X3=0.5*((1.0/RHOA)+(1.0/RHOB)-(1.0/RHOC))
      X4=(X1+X2+X3)/3.0
      X5=((X1**2.0)+(X2**2.0)+(X3**2.0)-(X1*X2)-(X2*X3)-(X3*X1))
     +**0.5
      T1=1.0/(X4+X1)
      T2=1.0/(X4+X2)
      T3=1.0/(X4+X3)
      T4=3.0/((6.0*X4)-(2.0*X5))
      T5=3.0/((6.0*X4)+(2.0*X5))
      WRITE(3,97)
   97 FORMAT( "    ")
      WRITE(3,98)
   98 FORMAT( "    ")
      WRITE(3,99)A,1/C
   99 FORMAT( 5X," A/B    "F7.2,"    B/C  ",F7.2)
      WRITE(3,100)NU
  100 FORMAT( 5X," NU   ",F10.5)
      WRITE(3,106)F
  106 FORMAT( 5X,"   F   ",F10.5)
      WRITE(3,101)TPLS
  101 FORMAT( 5X," THETA+   ",F15.5)
      WRITE(3,102)TMNS
  102 FORMAT( 5X," THETA-   ",F15.5)
      WRITE(3,103)DPLS
  103 FORMAT( 5X," DELTA+   ",F15.5)
      WRITE(3,104)DMNS
  104 FORMAT( 5X," DELTA-   ",F15.5)
      WRITE(3,105)R
  105 FORMAT( 5X,"    R   ",F15.5)
      WRITE(3,107)BETA
  107 FORMAT( 5X," BETA   ",F15.5)
      WRITE(3,202)
  202 FORMAT( 5X,"THE 3 ROTATIONAL FRICTIONAL RATIOS:")
      WRITE(3,108)CA
  108 FORMAT( 5X,"    CA   ",F15.5)
      WRITE(3,109)CB
  109 FORMAT( 5X,"    CB   ",F15.5)
      WRITE(3,110)CC
  110 FORMAT( 5X,"    CC   ",F15.5)
      WRITE(3,203)
  203 FORMAT( 5X,"THE 3 ROTATIONAL RELAXATION TIME RATIOS:")
      WRITE(3,111)RHOA
  111 FORMAT( 5X,"   RHOA   ",F15.5)
      WRITE(3,112)RHOB
  112 FORMAT( 5X,"   RHOB   ",F15.5)
      WRITE(3,113)RHOC
  113 FORMAT( 5X,"   RHOC   ",F15.5)
      WRITE(3,114)DELA
  114 FORMAT( 5X,"   DELTAA   ",F15.5)
      WRITE(3,115)DELB
  115 FORMAT( 5X,"   DELTAB   ",F15.5)
      WRITE(3,116)DELC
  116 FORMAT( 5X,"   DELTAC   ",F15.5)
      WRITE(3,204)
  204 FORMAT( 5X,"THE HARMONIC MEAN RELAXATION TIME RATIO:")
      WRITE(3,117)TAU
  117 FORMAT( 5X,"   TAU   ",F15.5)
      WRITE(3,118)PSI
  118 FORMAT( 5X,"   PSI   ",F15.5)
      WRITE(3,119)V
  119 FORMAT( 5X,"LAMBDA ",F15.5)
      WRITE(3,120)GAMMAA
  120 FORMAT( 5X,"GAMMAA ",F15.5)
      WRITE(3,121)GAMMAB
  121 FORMAT( 5X,"GAMMAB ",F15.5)
      WRITE(3,122)GAMMAC
  122 FORMAT( 5X,"GAMMAC ",F15.5)
      WRITE(3,123)MUA
  123 FORMAT( 5X,"   MUA   ",F15.5)
      WRITE(3,124)MUB
  124 FORMAT( 5X,"   MUB   ",F15.5)
      WRITE(3,125)MUC
  125 FORMAT( 5X,"   MUC   ",F15.5)
      WRITE(3,126)GPLS
  126 FORMAT( 5X,"GAMMA+ ",F15.5)
      WRITE(3,127)GMNS
  127 FORMAT( 5X, "GAMMA- ",F15.5)
      WRITE(3,201)
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201 FORMAT( 5X,"FLUORESCENCE ANISOTROPY RELAXATION TIME RATIOS:")
    WRITE(3,130)T1
130 FORMAT( 5X,"    T1     ",F15.5)
    WRITE(3,131)T2
131 FORMAT( 5X,"    T2     ",F15.5)
    WRITE(3,132)T3
132 FORMAT( 5X,"    T3     ",F15.5)
    WRITE(3,133)T4
133 FORMAT( 5X,"    T4     ",F15.5)
    WRITE(3,134)T5
134 FORMAT( 5X,"    T5     ",F15.5)
    STOP
    END
```

```
C
C
C
    REAL FUNCTION FUN(X)
    COMMON/PARAM/A,C,NN
    B=1.0
    GOTO(10,20,30,40,50,60,70,80,90,100),NN
 10 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**0.5)
    RETURN
 20 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**0.5)
    RETURN
 30 FUN=1/((A*A+X)**0.5*(B*B+X)**0.5*(C*C+X)**1.5)
    RETURN
 40 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
    RETURN
 50 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
    RETURN
 60 FUN=1/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
    RETURN
 70 FUN=X/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
    RETURN
 80 FUN=X/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
    RETURN
 90 FUN=X/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
    RETURN
100 FUN=1.0/(((A*A+X)*(B*B+X)*(C*C+X))**0.5)
    RETURN
    END
```

Program 1 Results

```
A/B       1.50    B/C       1.50
NU      2.89170
 F      1.04410
THETA+            .16261
THETA-            .11622
DELTA+           2.82127
DELTA-           2.01645
  R           1.47887
BETA            2.12334
THE 3 ROTATIONAL FRICTIONAL RATIOS:
   CA           .89762
   CB          1.39800
   CC          1.47041
THE 3 ROTATIONAL RELAXATION TIME RATIOS:
  RHOA          1.43329
  RHOB          1.11474
  RHOC          1.09327
  DELTAA          3.22152
  DELTAB          2.06846
  DELTAC          1.96660
THE HARMONIC MEAN RELAXATION TIME RATIO:
  TAU          1.19548
  PSI           .98378
LAMBDA         2.41886
GAMMAA          .79414
GAMMAB         1.02107
GAMMAC         1.04112
  MUA           .92389
  MUB          1.07092
  MUC          1.08910
GAMMA+         1.11051
GAMMA-          .79372
FLUORESCENCE ANISOTROPY RELAXATION TIME RATIOS:
   T1           1.02536
   T2           1.28883
   T3           1.31877
   T4           1.43405
   T5           1.02497
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Program 2

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C     ****************************************************************
C     THIS PROGRAM COMPUTES TABLES OF THE VISCOSITY INCREMENT NU,
C     THE TRANSLATIONAL FRICTIONAL RATIO (F/F0), THE ROTATIONAL
C     FRICTIONAL RATIOS( CA/C0, CB/C0, CC/C0 ), THE ROTATIONAL
C     RELAXATION TIME RATIOS(RHOA/RHO0, RHOB/RHO0, RHOC/RHO0), THE
C     HARMONIC MEAN RELAXATION TIME RATIO( TAU/TAU0 ), THE RIDGEWAY
C     ELECTRIC BIREFRINGENCE DECAY CONSTANTS( THETA+, THETA-), AND
C     THEIR CORRESPONDING SWELLING - INDEPENDENT FUNCTIONS:
C     R, BETA, DELTAA, DELTAB, DELTAC, GAMMAA, GAMMAB, GAMMAC,
C     MUA, MUB, MUC, PSI, DELTA+, DELTA-, GAMMA+ AND GAMMA-
C     AS FUNCTIONS OF THE AXIAL RATIOS A/B, B/C, IN THE RANGE 1.0 TO
C     2.0 IN STEPS OF 0.1, FOR A GENERAL TRIAXIAL ELLIPSOID PARTICLE
C     MODEL. ( THE SUBSCRIPT "0" REFERS TO THE CORRESPONDING COEFFICIENT
C     FOR A SPHERE OF EQUAL VOLUME )
C     ****************************************************************
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/A,C,NN
      EXTERNAL FUN
      DIMENSION ALPHA(10,11,11),NU(11,11),F(11,11),R(11,11),H(1)
     + ,BETA(11,11),CA(11,11),CB(11,11),CC(11,11),M(11,11),O(11,11)
     + ,P(11,11),TPLS(11,11),TMNS(11,11),RHOA(11,11),RHOB(11,11)
     + ,RHOC(11,11),TAU(11,11),PSI(11,11),DELA(11,11),DELB(11,11)
     + ,DELC(11,11),GAMMAA(11,11),GAMMAB(11,11),GAMMAC(11,11),MUA(11,11)
     + ,MUB(11,11),MUC(11,11),DPLS(11,11),DMNS(11,11),GPLS(11,11)
     + ,GMNS(11,11),Y(11),Z(11),ZZ(11,11)
      REAL NU,M,O,P,MUA,MUB,MUC,PSI
C     COMPUTE THE ELLIPTIC INTEGRALS
      NN=0
      DO45 K=1,10
      A=0.9
      NN=NN+1
      DO40 I=1,11
      A=A+0.1
      C=1.0/0.9
      DO30 N=1,11
      C=C/(1.0+0.1*C)
C     SET LIMITS FOR NUMERICAL INTEGRATION (THESE LIMITS
C     BELOW HAVE BEEN PREVIOUSLY TESTED FOR CONVERGENCE)
      AA=0.0
      BB=1000000
      IF(NN.EQ.10)BB=500000000
      MAXDIV=50
      EPS=1.0E-08
      ACC=0.0
      IFAIL=0
C     CALL U.K. "NAG" LIBRARY ROUTINE FOR NUMERICAL EVALUATION
C     OF THE INTEGRALS "ALPHA" GIVEN IN THE SUBROUTINE BELOW
      CALL D01AGF(AA,BB,FUN,MAXDIV,EPS,ACC,ANS,ERROR,NOFUN,IFAIL)
      ALPHA(NN,I,N)=ANS
   30 CONTINUE
   40 CONTINUE
   45 CONTINUE
      B=1.0
      A=0.9
      DO80 J=1,11
      A=A+0.1
      Y(J)=A
      C=1.0/0.9
      DO70 N=1,11
      C=C/(1.0+0.1*C)
      Z(N)=1/C
C     NOW COMPUTE THE FUNCTION VALUES USING THE STORED INTEGRAL VALUES
      NU(J,N)=(1.0/(A*B*C))*((4.0/15.0)*((ALPHA(7,J,N)+ALPHA(8,J,N)
     + +ALPHA(9,J,N))/(ALPHA(8,J,N)*ALPHA(9,J,N)+ALPHA(9,J,N)*ALPHA
     + (7,J,N)+ALPHA(7,J,N)*ALPHA(8,J,N)))+(1.0/5.0)*(((ALPHA(2,J,N)
     + +ALPHA(3,J,N))/(ALPHA(4,J,N)*(B*B*ALPHA(2,J,N)+C*C*ALPHA(3,J,N)
     + )))+((ALPHA(3,J,N)+ALPHA(1,J,N))/(ALPHA(5,J,N)*(C*C*ALPHA(3,J,N)
     + +A*A*ALPHA(1,J,N))))+((ALPHA(1,J,N)+ALPHA(2,J,N))/(ALPHA(6,J,N)
     + *(A*A*ALPHA(1,J,N)+B*B*ALPHA(2,J,N))))))
      F(J,N)=2.0/(((A*B*C)**(1.0/3.0))*ALPHA(10,J,N))
      R(J,N)=2.0*(1.0+(F(J,N)**3.0))/NU(J,N)
      BETA(J,N)=(1.0/1000000.0)*(((6.0249**(1.0/3.0))*(10.0**(23.0/3.0
     + )))/((16200.0*3.141592654*3.141592654)**(1.0/3.0)))*(NU(J,N)
     + **(1.0/3.0))/F(J,N)
      M(J,N)=(B*B+C*C)/(B*B*ALPHA(2,J,N)+C*C*ALPHA(3,J,N))
      O(J,N)=(C*C+A*A)/(C*C*ALPHA(3,J,N)+A*A*ALPHA(1,J,N))
      P(J,N)=(A*A+B*B)/(A*A*ALPHA(1,J,N)+B*B*ALPHA(2,J,N))
      TPLS(J,N)=((A*B*C)/(12.0))*((((1.0/M(J,N))+(1.0/O(J,N))+(1.0/P(J,
     + N)))+(((1.0/M(J,N)**2.0)+(1.0/O(J,N)**2.0)+(1.0/P(J,N)**2.0))-
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     + ((1.0/(M(J,N)*O(J,N)))+(1.0/(O(J,N)*P(J,N)))+(1.0/(P(J,N)*M(J,
     + N))))))**0.5))
       TMNS(J,N)=((A*B*C)/(12.0))*((((1.0/M(J,N))+(1.0/O(J,N))+(1.0/P(J,
     + N)))-(((1.0/M(J,N)**2.0)+(1.0/O(J,N)**2.0)+(1.0/P(J,N)**2.0))-
     + ((1.0/(M(J,N)*O(J,N)))+(1.0/(O(J,N)*P(J,N)))+(1.0/(P(J,N)*M(J,
     + N))))))**0.5))
       CA(J,N)=(2.0/(3.0*A*B*C))*M(J,N)
       CB(J,N)=(2.0/(3.0*A*B*C))*O(J,N)
       CC(J,N)=(2.0/(3.0*A*B*C))*P(J,N)
       RHOA(J,N)=2.0/((1.0/CB(J,N))+(1.0/CC(J,N)))
       RHOB(J,N)=2.0/((1.0/CA(J,N))+(1.0/CC(J,N)))
       RHOC(J,N)=2.0/((1.0/CA(J,N))+(1.0/CB(J,N)))
       DELA(J,N)=NU(J,N)/CA(J,N)
       DELB(J,N)=NU(J,N)/CB(J,N)
       DELC(J,N)=NU(J,N)/CC(J,N)
       TAU(J,N)=3.0/((1.0/CA(J,N))+(1.0/CB(J,N))+(1.0/CC(J,N)))
       PSI(J,N)=F(J,N)*((1.0/TAU(J,N))**(1.0/3.0))
       ZZ(J,N)=(1.0/2.0)*(F(J,N)**3.0)
       GAMMAA(J,N)=ZZ(J,N)*((1.0/CB(J,N))+(1.0/CC(J,N)))
       GAMMAB(J,N)=ZZ(J,N)*((1.0/CA(J,N))+(1.0/CC(J,N)))
       GAMMAC(J,N)=ZZ(J,N)*((1.0/CA(J,N))+(1.0/CB(J,N)))
       MUA(J,N)=(CA(J,N)**(1.0/3.0))/F(J,N)
       MUB(J,N)=(CB(J,N)**(1.0/3.0))/F(J,N)
       MUC(J,N)=(CC(J,N)**(1.0/3.0))/F(J,N)
       DPLS(J,N)=6.0*TPLS(J,N)*NU(J,N)
       DMNS(J,N)=6.0*TMNS(J,N)*NU(J,N)
       GPLS(J,N)=6.0*TPLS(J,N)*(F(J,N)**3.0)
       GMNS(J,N)=6.0*TMNS(J,N)*(F(J,N)**3.0)
   70  CONTINUE
   80  CONTINUE
C      THE PROGRAM NOW WRITES OUT THE COMPUTED VALUES IN TABLE FORM
       WRITE(3,600)
  600  FORMAT(" ")
       PRINT(3,60)
   60  FORMAT( "1    A/B     B/C     NU      F/F0      R      BETA")
       DO71 J=1,11
       DO72 N=1,11
       WRITE(3,73)Y(J),Z(N),NU(J,N),F(J,N),R(J,N),BETA(J,N)
   73  FORMAT( 2F7.1,4F8.3)
   72  CONTINUE
   71  CONTINUE
       WRITE(3,610)
  610  FORMAT(" ")
       PRINT(3,61)
   61  FORMAT( "1    A/B     B/C    CA/C0    CB/C0    CC/C0")
       DO74 J=1,11
       DO75 N=1,11
       WRITE(3,76)Y(J),Z(N),CA(J,N),CB(J,N),CC(J,N)
   76  FORMAT( 2F7.1,3F8.3)
   75  CONTINUE
   74  CONTINUE
       WRITE(3,620)
  620  FORMAT( " ")
       PRINT(3,62)
   62  FORMAT( "1    A/B     B/C RHOA/RHO0 RHOB/RHO0 RHOC/RHO0")
       DO81 J=1,11
       DO82 N=1,11
       WRITE(3,83)Y(J),Z(N),RHOA(J,N),RHOB(J,N),RHOC(J,N)
   83  FORMAT( 2F7.1,3F9.3)
   82  CONTINUE
   81  CONTINUE
       WRITE(3,630)
  630  FORMAT( " ")
       PRINT(3,63)
   63  FORMAT( "1    A/B     B/C  DELTA(A) DELTA(B) DELTA(C)")
       DO84 J=1,11
       DO85 N=1,11
       WRITE(3,86)Y(J),Z(N),DELA(J,N),DELB(J,N),DELC(J,N)
   86  FORMAT( 2F7.1,3F8.3)
   85  CONTINUE
   84  CONTINUE
       WRITE(3,640)
  640  FORMAT( " ")
       PRINT(3,64)
   64  FORMAT( "1    A/B     B/C  GAMMA(A) GAMMA(B) GAMMA(C)")
       DO91 J=1,11
       DO92 N=1,11
       WRITE(3,93)Y(J),Z(N),GAMMAA(J,N),GAMMAB(J,N),GAMMAC(J,N)
   93  FORMAT( 2F7.1,3F8.3)
   92  CONTINUE
   91  CONTINUE
```

```
      WRITE(3,650)
  650 FORMAT( " ")
      PRINT(3,65)
   65 FORMAT( "1    A/B     B/C     MU(A)     MU(B)     MU(C)")
      DO94 J=1,11
      DO95 N=1,11
      WRITE(3,96)Y(J),Z(N),MUA(J,N),MUB(J,N),MUC(J,N)
   96 FORMAT( 2F7.1,3F8.3)
   95 CONTINUE
   94 CONTINUE
      WRITE(3,660)
  660 FORMAT( " ")
      PRINT(3,66)
   66 FORMAT( "1    A/B     B/C   THETA+   THETA-   TAU/TAU0   PSI")
      DO101 J=1,11
      DO102 N=1,11
      WRITE(3,103)Y(J),Z(N),TPLS(J,N),TMNS(J,N),TAU(J,N),PSI(J,N)
  103 FORMAT( 2F7.1,4F8.3)
  102 CONTINUE
  101 CONTINUE
      WRITE(3,670)
  670 FORMAT( " ")
      PRINT(3,67)
   67 FORMAT( "1    A/B     B/C    DELTA+    DELTA-")
      DO104 J=1,11
      DO105 N=1,11
      WRITE(3,106)Y(J),Z(N),DPLS(J,N),DMNS(J,N)
  106 FORMAT( 2F7.1,2F8.3)
  105 CONTINUE
  104 CONTINUE
      WRITE(3,680)
  680 FORMAT( " ")
      PRINT(3,68)
   68 FORMAT( "1    A/B     B/C    GAMMA+    GAMMA-")
      DO111 J=1,11
      DO112 N=1,11
      WRITE(3,113)Y(J),Z(N),GPLS(J,N),GMNS(J,N)
  113 FORMAT( 2F7.1,2F8.3)
  112 CONTINUE
  111 CONTINUE
      WRITE(3,690)
  690 FORMAT( " ")
      DO114 J=1,11
      DO115 N=1,11
  115 CONTINUE
  114 CONTINUE
      STOP
      END


C
C
C
      REAL FUNCTION FUN(X)
      COMMON/PARAM/A,C,NN
      B=1.0
      GOTO(10,20,30,40,50,60,70,80,90,100),NN
   10 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**0.5)
      RETURN
   20 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   30 FUN=1/((A*A+X)**0.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   40 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   50 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   60 FUN=1/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   70 FUN=X/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   80 FUN=X/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   90 FUN=X/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
  100 FUN=1.0/(((A*A+X)*(B*B+X)*(C*C+X))**0.5)
      RETURN
      END
```

A/B	B/C	NU	F/F0	R	BETA
1.0	1.0	2.500	1.000	1.600	2.112
1.0	1.1	2.507	1.001	1.598	2.112
1.0	1.2	2.524	1.003	1.592	2.113
1.0	1.3	2.550	1.006	1.583	2.113
1.0	1.4	2.583	1.010	1.572	2.114
1.0	1.5	2.620	1.014	1.560	2.115
1.0	1.6	2.661	1.019	1.548	2.115
1.0	1.7	2.706	1.025	1.534	2.116
1.0	1.8	2.753	1.030	1.521	2.117
1.0	1.9	2.803	1.036	1.507	2.118
1.0	2.0	2.854	1.042	1.493	2.118
1.1	1.0	2.507	1.001	1.598	2.112
1.1	1.1	2.520	1.002	1.593	2.112
1.1	1.2	2.544	1.005	1.585	2.113
1.1	1.3	2.576	1.009	1.574	2.114
1.1	1.4	2.614	1.014	1.562	2.115
1.1	1.5	2.656	1.019	1.549	2.115
1.1	1.6	2.702	1.024	1.535	2.116
1.1	1.7	2.751	1.030	1.521	2.117
1.1	1.8	2.803	1.036	1.507	2.118
1.1	1.9	2.857	1.042	1.492	2.119
1.1	2.0	2.913	1.049	1.478	2.120
1.2	1.0	2.525	1.003	1.591	2.113
1.2	1.1	2.545	1.005	1.584	2.113
1.2	1.2	2.575	1.009	1.574	2.114
1.2	1.3	2.612	1.013	1.562	2.115
1.2	1.4	2.655	1.018	1.549	2.116
1.2	1.5	2.703	1.024	1.535	2.117
1.2	1.6	2.754	1.030	1.520	2.118
1.2	1.7	2.808	1.036	1.505	2.119
1.2	1.8	2.865	1.043	1.490	2.120
1.2	1.9	2.923	1.049	1.475	2.120
1.2	2.0	2.983	1.056	1.460	2.121
1.3	1.0	2.553	1.006	1.582	2.114
1.3	1.1	2.579	1.009	1.573	2.114
1.3	1.2	2.615	1.013	1.561	2.115
1.3	1.3	2.658	1.018	1.547	2.116
1.3	1.4	2.706	1.024	1.533	2.118
1.3	1.5	2.759	1.030	1.518	2.119
1.3	1.6	2.815	1.037	1.502	2.120
1.3	1.7	2.874	1.043	1.486	2.121
1.3	1.8	2.935	1.050	1.471	2.122
1.3	1.9	2.998	1.057	1.455	2.123
1.3	2.0	3.063	1.064	1.440	2.124
1.4	1.0	2.588	1.010	1.569	2.115
1.4	1.1	2.621	1.014	1.559	2.116
1.4	1.2	2.662	1.019	1.545	2.117
1.4	1.3	2.711	1.024	1.531	2.118
1.4	1.4	2.764	1.030	1.515	2.120
1.4	1.5	2.822	1.037	1.499	2.121
1.4	1.6	2.883	1.044	1.482	2.122
1.4	1.7	2.947	1.051	1.465	2.123
1.4	1.8	3.013	1.058	1.450	2.124
1.4	1.9	3.081	1.065	1.434	2.125
1.4	2.0	3.151	1.073	1.419	2.126
1.5	1.0	2.630	1.015	1.555	2.116
1.5	1.1	2.668	1.019	1.543	2.118
1.5	1.2	2.716	1.024	1.528	2.119
1.5	1.3	2.770	1.031	1.512	2.121
1.5	1.4	2.829	1.037	1.496	2.122
1.5	1.5	2.892	1.044	1.479	2.123
1.5	1.6	2.958	1.051	1.462	2.125
1.5	1.7	3.027	1.059	1.445	2.126
1.5	1.8	3.098	1.066	1.429	2.127
1.5	1.9	3.171	1.074	1.413	2.128
1.5	2.0	3.245	1.082	1.397	2.129
1.6	1.0	2.677	1.020	1.540	2.118
1.6	1.1	2.722	1.025	1.526	2.120
1.6	1.2	2.775	1.031	1.510	2.121
1.6	1.3	2.834	1.037	1.493	2.123
1.6	1.4	2.899	1.044	1.476	2.125
1.6	1.5	2.967	1.052	1.458	2.126
1.6	1.6	3.039	1.059	1.441	2.128
1.6	1.7	3.113	1.067	1.423	2.129
1.6	1.8	3.189	1.075	1.407	2.130
1.6	1.9	3.267	1.083	1.390	2.132
1.6	2.0	3.346	1.091	1.374	2.133
1.7	1.0	2.729	1.026	1.524	2.120
1.7	1.1	2.779	1.031	1.508	2.122
1.7	1.2	2.839	1.037	1.491	2.124
1.7	1.3	2.904	1.044	1.473	2.126
1.7	1.4	2.974	1.052	1.455	2.128
1.7	1.5	3.047	1.060	1.437	2.129
1.7	1.6	3.124	1.068	1.419	2.131

1.7	1.7	3.204	1.076	1.402	2.132
1.7	1.8	3.285	1.084	1.384	2.134
1.7	1.9	3.368	1.092	1.368	2.135
1.7	2.0	3.453	1.101	1.352	2.137
1.8	1.0	2.785	1.031	1.506	2.123
1.8	1.1	2.842	1.037	1.490	2.125
1.8	1.2	2.907	1.044	1.472	2.127
1.8	1.3	2.978	1.052	1.453	2.129
1.8	1.4	3.053	1.059	1.434	2.131
1.8	1.5	3.132	1.068	1.415	2.133
1.8	1.6	3.215	1.076	1.397	2.134
1.8	1.7	3.300	1.085	1.379	2.136
1.8	1.8	3.386	1.093	1.362	2.138
1.8	1.9	3.475	1.102	1.345	2.139
1.8	2.0	3.565	1.111	1.329	2.141
1.9	1.0	2.844	1.038	1.489	2.125
1.9	1.1	2.908	1.044	1.471	2.127
1.9	1.2	2.978	1.051	1.452	2.130
1.9	1.3	3.055	1.059	1.432	2.132
1.9	1.4	3.137	1.067	1.413	2.134
1.9	1.5	3.222	1.076	1.394	2.136
1.9	1.6	3.310	1.085	1.375	2.138
1.9	1.7	3.400	1.093	1.357	2.140
1.9	1.8	3.492	1.102	1.340	2.142
1.9	1.9	3.586	1.111	1.323	2.143
1.9	2.0	3.681	1.120	1.307	2.145
2.0	1.0	2.908	1.044	1.470	2.128
2.0	1.1	2.977	1.051	1.451	2.130
2.0	1.2	3.054	1.059	1.432	2.133
2.0	1.3	3.137	1.067	1.412	2.135
2.0	1.4	3.224	1.075	1.392	2.138
2.0	1.5	3.315	1.084	1.372	2.140
2.0	1.6	3.408	1.093	1.354	2.142
2.0	1.7	3.504	1.102	1.335	2.144
2.0	1.8	3.602	1.112	1.318	2.146
2.0	1.9	3.702	1.121	1.301	2.148
2.0	2.0	3.803	1.130	1.285	2.149

A/B	B/C	CA/CO	CB/CO	CC/CO
1.0	1.0	1.000	1.000	1.000
1.0	1.1	.986	.986	1.040
1.0	1.2	.983	.983	1.081
1.0	1.3	.988	.988	1.121
1.0	1.4	.998	.998	1.162
1.0	1.5	1.013	1.013	1.203
1.0	1.6	1.032	1.032	1.244
1.0	1.7	1.054	1.054	1.286
1.0	1.8	1.078	1.078	1.327
1.0	1.9	1.104	1.104	1.368
1.0	2.0	1.132	1.132	1.410
1.1	1.0	.964	1.025	1.025
1.1	1.1	.952	1.020	1.067
1.1	1.2	.950	1.026	1.110
1.1	1.3	.955	1.038	1.153
1.1	1.4	.966	1.056	1.196
1.1	1.5	.981	1.078	1.240
1.1	1.6	1.000	1.103	1.283
1.1	1.7	1.021	1.132	1.327
1.1	1.8	1.045	1.162	1.370
1.1	1.9	1.071	1.195	1.414
1.1	2.0	1.099	1.229	1.458
1.2	1.0	.934	1.058	1.058
1.2	1.1	.923	1.062	1.103
1.2	1.2	.922	1.075	1.148
1.2	1.3	.928	1.095	1.194
1.2	1.4	.939	1.120	1.240
1.2	1.5	.955	1.150	1.286
1.2	1.6	.973	1.182	1.332
1.2	1.7	.995	1.217	1.378
1.2	1.8	1.019	1.254	1.425
1.2	1.9	1.044	1.293	1.471
1.2	2.0	1.072	1.333	1.518
1.3	1.0	.909	1.097	1.097
1.3	1.1	.899	1.110	1.146
1.3	1.2	.899	1.131	1.194
1.3	1.3	.905	1.159	1.243
1.3	1.4	.917	1.191	1.292
1.3	1.5	.933	1.227	1.341
1.3	1.6	.951	1.266	1.390
1.3	1.7	.973	1.308	1.439
1.3	1.8	.997	1.351	1.488
1.3	1.9	1.022	1.397	1.538
1.3	2.0	1.049	1.443	1.587
1.4	1.0	.887	1.143	1.143
1.4	1.1	.879	1.164	1.194
1.4	1.2	.879	1.193	1.246
1.4	1.3	.886	1.228	1.298
1.4	1.4	.898	1.267	1.350
1.4	1.5	.914	1.310	1.402
1.4	1.6	.933	1.356	1.455
1.4	1.7	.954	1.404	1.507
1.4	1.8	.978	1.454	1.560
1.4	1.9	1.003	1.506	1.612
1.4	2.0	1.030	1.559	1.665
1.5	1.0	.869	1.193	1.193
1.5	1.1	.862	1.222	1.248
1.5	1.2	.862	1.259	1.304
1.5	1.3	.870	1.301	1.359
1.5	1.4	.882	1.348	1.415
1.5	1.5	.898	1.398	1.470
1.5	1.6	.917	1.451	1.526
1.5	1.7	.938	1.506	1.582
1.5	1.8	.961	1.563	1.638
1.5	1.9	.987	1.621	1.694
1.5	2.0	1.013	1.681	1.751
1.6	1.0	.853	1.248	1.248
1.6	1.1	.846	1.285	1.307
1.6	1.2	.848	1.330	1.366
1.6	1.3	.855	1.379	1.425
1.6	1.4	.868	1.433	1.485
1.6	1.5	.884	1.490	1.544
1.6	1.6	.903	1.550	1.604
1.6	1.7	.924	1.612	1.663
1.6	1.8	.947	1.676	1.723
1.6	1.9	.972	1.741	1.783
1.6	2.0	.999	1.807	1.843
1.7	1.0	.839	1.307	1.307
1.7	1.1	.833	1.352	1.370
1.7	1.2	.835	1.404	1.433
1.7	1.3	.843	1.461	1.496
1.7	1.4	.855	1.523	1.559
1.7	1.5	.871	1.587	1.623
1.7	1.6	.890	1.654	1.686

1.7	1.7	.912	1.723	1.750
1.7	1.8	.935	1.793	1.814
1.7	1.9	.960	1.865	1.877
1.7	2.0	.986	1.939	1.941
1.8	1.0	.827	1.370	1.370
1.8	1.1	.822	1.423	1.437
1.8	1.2	.824	1.483	1.504
1.8	1.3	.832	1.547	1.571
1.8	1.4	.845	1.616	1.639
1.8	1.5	.861	1.687	1.706
1.8	1.6	.880	1.762	1.774
1.8	1.7	.901	1.838	1.842
1.8	1.8	.924	1.915	1.910
1.8	1.9	.949	1.995	1.978
1.8	2.0	.975	2.075	2.046
1.9	1.0	.816	1.436	1.436
1.9	1.1	.811	1.497	1.507
1.9	1.2	.814	1.564	1.579
1.9	1.3	.822	1.637	1.650
1.9	1.4	.835	1.713	1.722
1.9	1.5	.851	1.792	1.794
1.9	1.6	.870	1.873	1.866
1.9	1.7	.892	1.957	1.938
1.9	1.8	.915	2.042	2.011
1.9	1.9	.939	2.128	2.083
1.9	2.0	.965	2.216	2.155
2.0	1.0	.807	1.505	1.505
2.0	1.1	.802	1.574	1.581
2.0	1.2	.805	1.650	1.657
2.0	1.3	.814	1.730	1.733
2.0	1.4	.826	1.813	1.810
2.0	1.5	.843	1.900	1.886
2.0	1.6	.862	1.989	1.963
2.0	1.7	.883	2.080	2.040
2.0	1.8	.906	2.172	2.116
2.0	1.9	.931	2.266	2.193
2.0	2.0	.957	2.361	2.270

A/B	B/C	RHOA/RHOO	RHOB/RHOO	RHOC/RHOO
1.0	1.0	1.000	1.000	1.000
1.0	1.1	1.013	1.013	.986
1.0	1.2	1.030	1.030	.983
1.0	1.3	1.050	1.050	.988
1.0	1.4	1.074	1.074	.998
1.0	1.5	1.100	1.100	1.013
1.0	1.6	1.128	1.128	1.032
1.0	1.7	1.158	1.158	1.054
1.0	1.8	1.189	1.189	1.078
1.0	1.9	1.222	1.222	1.104
1.0	2.0	1.256	1.256	1.132
1.1	1.0	1.025	.993	.993
1.1	1.1	1.043	1.006	.985
1.1	1.2	1.066	1.024	.986
1.1	1.3	1.092	1.045	.995
1.1	1.4	1.122	1.069	1.009
1.1	1.5	1.153	1.095	1.027
1.1	1.6	1.187	1.124	1.049
1.1	1.7	1.222	1.154	1.074
1.1	1.8	1.258	1.186	1.101
1.1	1.9	1.295	1.219	1.130
1.1	2.0	1.334	1.253	1.160
1.2	1.0	1.058	.992	.992
1.2	1.1	1.082	1.005	.988
1.2	1.2	1.111	1.023	.993
1.2	1.3	1.143	1.044	1.005
1.2	1.4	1.177	1.069	1.022
1.2	1.5	1.214	1.096	1.043
1.2	1.6	1.253	1.125	1.068
1.2	1.7	1.293	1.156	1.095
1.2	1.8	1.334	1.188	1.124
1.2	1.9	1.376	1.222	1.155
1.2	2.0	1.419	1.256	1.188
1.3	1.0	1.097	.994	.994
1.3	1.1	1.128	1.008	.994
1.3	1.2	1.162	1.026	1.002
1.3	1.3	1.199	1.048	1.017
1.3	1.4	1.239	1.072	1.036
1.3	1.5	1.281	1.100	1.060
1.3	1.6	1.325	1.130	1.086
1.3	1.7	1.370	1.161	1.116
1.3	1.8	1.417	1.194	1.147
1.3	1.9	1.464	1.228	1.180
1.3	2.0	1.512	1.263	1.215
1.4	1.0	1.143	.999	.999
1.4	1.1	1.179	1.013	1.002
1.4	1.2	1.219	1.031	1.012
1.4	1.3	1.262	1.053	1.029
1.4	1.4	1.307	1.079	1.051
1.4	1.5	1.355	1.107	1.077
1.4	1.6	1.404	1.137	1.105
1.4	1.7	1.454	1.168	1.136
1.4	1.8	1.505	1.202	1.169
1.4	1.9	1.558	1.237	1.204
1.4	2.0	1.611	1.272	1.240
1.5	1.0	1.193	1.006	1.006
1.5	1.1	1.235	1.020	1.011
1.5	1.2	1.281	1.038	1.024
1.5	1.3	1.330	1.061	1.043
1.5	1.4	1.381	1.086	1.066
1.5	1.5	1.433	1.115	1.093
1.5	1.6	1.488	1.145	1.123
1.5	1.7	1.543	1.178	1.156
1.5	1.8	1.600	1.212	1.190
1.5	1.9	1.657	1.247	1.227
1.5	2.0	1.715	1.283	1.264
1.6	1.0	1.248	1.014	1.014
1.6	1.1	1.296	1.028	1.021
1.6	1.2	1.348	1.046	1.035
1.6	1.3	1.402	1.069	1.056
1.6	1.4	1.458	1.095	1.081
1.6	1.5	1.517	1.124	1.109
1.6	1.6	1.576	1.155	1.141
1.6	1.7	1.637	1.188	1.175
1.6	1.8	1.699	1.223	1.210
1.6	1.9	1.762	1.258	1.248
1.6	2.0	1.825	1.295	1.287
1.7	1.0	1.307	1.022	1.022
1.7	1.1	1.361	1.036	1.031
1.7	1.2	1.418	1.055	1.047
1.7	1.3	1.479	1.078	1.069
1.7	1.4	1.541	1.105	1.095
1.7	1.5	1.605	1.134	1.125
1.7	1.6	1.670	1.165	1.158

1.7	1.7	1.736	1.199	1.192
1.7	1.8	1.803	1.234	1.229
1.7	1.9	1.871	1.270	1.268
1.7	2.0	1.940	1.308	1.307
1.8	1.0	1.370	1.032	1.032
1.8	1.1	1.430	1.045	1.042
1.8	1.2	1.493	1.065	1.059
1.8	1.3	1.559	1.088	1.082
1.8	1.4	1.627	1.115	1.109
1.8	1.5	1.697	1.144	1.140
1.8	1.6	1.768	1.176	1.173
1.8	1.7	1.840	1.210	1.209
1.8	1.8	1.913	1.246	1.247
1.8	1.9	1.986	1.283	1.286
1.8	2.0	2.060	1.321	1.327
1.9	1.0	1.436	1.041	1.041
1.9	1.1	1.502	1.055	1.052
1.9	1.2	1.572	1.074	1.071
1.9	1.3	1.644	1.098	1.095
1.9	1.4	1.718	1.125	1.123
1.9	1.5	1.793	1.155	1.154
1.9	1.6	1.870	1.187	1.188
1.9	1.7	1.948	1.221	1.225
1.9	1.8	2.026	1.257	1.263
1.9	1.9	2.105	1.295	1.303
1.9	2.0	2.185	1.334	1.345
2.0	1.0	1.505	1.050	1.050
2.0	1.1	1.577	1.064	1.063
2.0	1.2	1.653	1.084	1.082
2.0	1.3	1.731	1.107	1.107
2.0	1.4	1.812	1.135	1.135
2.0	1.5	1.893	1.165	1.168
2.0	1.6	1.976	1.198	1.203
2.0	1.7	2.059	1.233	1.240
2.0	1.8	2.144	1.269	1.279
2.0	1.9	2.229	1.307	1.320
2.0	2.0	2.314	1.346	1.362

A/B	B/C	DELTA(A)	DELTA(B)	DELTA(C)
1.0	1.0	2.500	2.500	2.500
1.0	1.1	2.541	2.541	2.410
1.0	1.2	2.568	2.568	2.336
1.0	1.3	2.582	2.582	2.274
1.0	1.4	2.588	2.588	2.222
1.0	1.5	2.586	2.586	2.178
1.0	1.6	2.579	2.579	2.139
1.0	1.7	2.568	2.568	2.105
1.0	1.8	2.555	2.555	2.075
1.0	1.9	2.539	2.539	2.048
1.0	2.0	2.522	2.522	2.024
1.1	1.0	2.601	2.446	2.446
1.1	1.1	2.648	2.470	2.362
1.1	1.2	2.679	2.481	2.292
1.1	1.3	2.697	2.482	2.234
1.1	1.4	2.706	2.475	2.185
1.1	1.5	2.707	2.464	2.143
1.1	1.6	2.702	2.449	2.106
1.1	1.7	2.694	2.431	2.074
1.1	1.8	2.682	2.412	2.046
1.1	1.9	2.667	2.392	2.020
1.1	2.0	2.651	2.371	1.998
1.2	1.0	2.704	2.387	2.387
1.2	1.1	2.757	2.397	2.308
1.2	1.2	2.793	2.395	2.242
1.2	1.3	2.815	2.385	2.188
1.2	1.4	2.827	2.370	2.141
1.2	1.5	2.831	2.351	2.102
1.2	1.6	2.829	2.330	2.067
1.2	1.7	2.822	2.308	2.037
1.2	1.8	2.812	2.285	2.010
1.2	1.9	2.799	2.261	1.987
1.2	2.0	2.784	2.238	1.966
1.3	1.0	2.809	2.326	2.326
1.3	1.1	2.868	2.323	2.251
1.3	1.2	2.909	2.311	2.190
1.3	1.3	2.936	2.293	2.139
1.3	1.4	2.951	2.272	2.095
1.3	1.5	2.958	2.248	2.058
1.3	1.6	2.959	2.223	2.025
1.3	1.7	2.954	2.197	1.997
1.3	1.8	2.945	2.172	1.972
1.3	1.9	2.934	2.147	1.950
1.3	2.0	2.920	2.122	1.930
1.4	1.0	2.916	2.264	2.264
1.4	1.1	2.981	2.252	2.194
1.4	1.2	3.028	2.232	2.136
1.4	1.3	3.059	2.208	2.088
1.4	1.4	3.078	2.181	2.047
1.4	1.5	3.088	2.154	2.012
1.4	1.6	3.091	2.126	1.982
1.4	1.7	3.089	2.099	1.955
1.4	1.8	3.082	2.072	1.932
1.4	1.9	3.072	2.046	1.911
1.4	2.0	3.060	2.021	1.892
1.5	1.0	3.026	2.203	2.203
1.5	1.1	3.097	2.183	2.137
1.5	1.2	3.149	2.157	2.083
1.5	1.3	3.185	2.128	2.038
1.5	1.4	3.208	2.098	2.000
1.5	1.5	3.222	2.068	1.967
1.5	1.6	3.227	2.039	1.938
1.5	1.7	3.227	2.010	1.913
1.5	1.8	3.222	1.983	1.891
1.5	1.9	3.214	1.956	1.871
1.5	2.0	3.204	1.931	1.854
1.6	1.0	3.137	2.144	2.144
1.6	1.1	3.215	2.117	2.082
1.6	1.2	3.273	2.087	2.031
1.6	1.3	3.313	2.055	1.989
1.6	1.4	3.341	2.023	1.953
1.6	1.5	3.358	1.991	1.922
1.6	1.6	3.366	1.960	1.895
1.6	1.7	3.369	1.931	1.871
1.6	1.8	3.366	1.903	1.851
1.6	1.9	3.360	1.877	1.832
1.6	2.0	3.351	1.852	1.816
1.7	1.0	3.251	2.087	2.087
1.7	1.1	3.336	2.055	2.029
1.7	1.2	3.399	2.021	1.981
1.7	1.3	3.445	1.987	1.941
1.7	1.4	3.476	1.953	1.907
1.7	1.5	3.497	1.920	1.878
1.7	1.6	3.509	1.889	1.853

1.7	1.7	3.514	1.860	1.831
1.7	1.8	3.513	1.832	1.811
1.7	1.9	3.509	1.806	1.794
1.7	2.0	3.501	1.781	1.779
1.8	1.0	3.366	2.033	2.033
1.8	1.1	3.459	1.997	1.978
1.8	1.2	3.528	1.960	1.933
1.8	1.3	3.579	1.924	1.895
1.8	1.4	3.615	1.889	1.863
1.8	1.5	3.639	1.856	1.836
1.8	1.6	3.654	1.825	1.812
1.8	1.7	3.662	1.796	1.792
1.8	1.8	3.664	1.768	1.773
1.8	1.9	3.661	1.742	1.757
1.8	2.0	3.655	1.718	1.743
1.9	1.0	3.484	1.981	1.981
1.9	1.1	3.584	1.942	1.929
1.9	1.2	3.660	1.904	1.887
1.9	1.3	3.716	1.867	1.851
1.9	1.4	3.757	1.831	1.821
1.9	1.5	3.785	1.798	1.796
1.9	1.6	3.803	1.767	1.773
1.9	1.7	3.813	1.738	1.754
1.9	1.8	3.818	1.710	1.737
1.9	1.9	3.817	1.685	1.722
1.9	2.0	3.813	1.662	1.708
2.0	1.0	3.604	1.932	1.932
2.0	1.1	3.712	1.891	1.883
2.0	1.2	3.794	1.851	1.843
2.0	1.3	3.856	1.814	1.810
2.0	1.4	3.901	1.778	1.781
2.0	1.5	3.933	1.745	1.757
2.0	1.6	3.955	1.714	1.736
2.0	1.7	3.968	1.685	1.718
2.0	1.8	3.975	1.658	1.702
2.0	1.9	3.977	1.634	1.688
2.0	2.0	3.975	1.611	1.675

A/B	B/C	GAMMA(A)	GAMMA(B)	GAMMA(C)
1.0	1.0	1.000	1.000	1.000
1.0	1.1	.990	.990	1.016
1.0	1.2	.980	.980	1.026
1.0	1.3	.970	.970	1.031
1.0	1.4	.959	.959	1.032
1.0	1.5	.949	.949	1.031
1.0	1.6	.939	.939	1.027
1.0	1.7	.929	.929	1.021
1.0	1.8	.919	.919	1.015
1.0	1.9	.910	.910	1.008
1.0	2.0	.901	.901	1.000
1.1	1.0	.978	1.009	1.009
1.1	1.1	.966	1.001	1.023
1.1	1.2	.953	.993	1.030
1.1	1.3	.941	.984	1.033
1.1	1.4	.929	.974	1.032
1.1	1.5	.917	.965	1.029
1.1	1.6	.905	.956	1.024
1.1	1.7	.894	.947	1.017
1.1	1.8	.884	.937	1.010
1.1	1.9	.874	.929	1.002
1.1	2.0	.864	.920	.994
1.2	1.0	.954	1.017	1.017
1.2	1.1	.939	1.011	1.029
1.2	1.2	.925	1.004	1.034
1.2	1.3	.911	.996	1.036
1.2	1.4	.897	.988	1.034
1.2	1.5	.885	.980	1.029
1.2	1.6	.872	.971	1.023
1.2	1.7	.861	.963	1.016
1.2	1.8	.850	.954	1.008
1.2	1.9	.840	.946	1.000
1.2	2.0	.830	.938	.991
1.3	1.0	.928	1.025	1.025
1.3	1.1	.912	1.020	1.035
1.3	1.2	.896	1.015	1.039
1.3	1.3	.881	1.008	1.039
1.3	1.4	.867	1.001	1.036
1.3	1.5	.853	.994	1.031
1.3	1.6	.840	.986	1.025
1.3	1.7	.829	.978	1.018
1.3	1.8	.817	.970	1.009
1.3	1.9	.807	.962	1.001
1.3	2.0	.797	.954	.992
1.4	1.0	.902	1.032	1.032
1.4	1.1	.884	1.029	1.041
1.4	1.2	.867	1.025	1.044
1.4	1.3	.851	1.020	1.044
1.4	1.4	.837	1.014	1.041
1.4	1.5	.823	1.007	1.035
1.4	1.6	.810	1.000	1.029
1.4	1.7	.798	.993	1.021
1.4	1.8	.787	.986	1.013
1.4	1.9	.777	.978	1.005
1.4	2.0	.767	.971	.996
1.5	1.0	.876	1.039	1.039
1.5	1.1	.857	1.038	1.047
1.5	1.2	.839	1.036	1.050
1.5	1.3	.823	1.032	1.050
1.5	1.4	.808	1.027	1.046
1.5	1.5	.794	1.021	1.041
1.5	1.6	.781	1.015	1.035
1.5	1.7	.769	1.008	1.027
1.5	1.8	.758	1.001	1.019
1.5	1.9	.748	.994	1.011
1.5	2.0	.739	.987	1.002
1.6	1.0	.850	1.047	1.047
1.6	1.1	.831	1.048	1.055
1.6	1.2	.813	1.047	1.058
1.6	1.3	.796	1.044	1.057
1.6	1.4	.781	1.040	1.054
1.6	1.5	.767	1.035	1.048
1.6	1.6	.754	1.029	1.042
1.6	1.7	.742	1.023	1.035
1.6	1.8	.731	1.017	1.027
1.6	1.9	.721	1.010	1.019
1.6	2.0	.712	1.003	1.010
1.7	1.0	.825	1.055	1.055
1.7	1.1	.805	1.058	1.063
1.7	1.2	.787	1.058	1.066
1.7	1.3	.770	1.056	1.065
1.7	1.4	.755	1.053	1.062
1.7	1.5	.741	1.049	1.057
1.7	1.6	.729	1.044	1.051

1.7	1.7	.717	1.038	1.044
1.7	1.8	.706	1.032	1.036
1.7	1.9	.697	1.026	1.029
1.7	2.0	.688	1.020	1.020
1.8	1.0	.801	1.064	1.064
1.8	1.1	.781	1.068	1.072
1.8	1.2	.763	1.070	1.075
1.8	1.3	.746	1.069	1.075
1.8	1.4	.731	1.067	1.072
1.8	1.5	.717	1.064	1.068
1.8	1.6	.705	1.059	1.062
1.8	1.7	.693	1.054	1.055
1.8	1.8	.683	1.049	1.048
1.8	1.9	.674	1.043	1.040
1.8	2.0	.665	1.037	1.032
1.9	1.0	.778	1.073	1.073
1.9	1.1	.758	1.079	1.081
1.9	1.2	.739	1.082	1.085
1.9	1.3	.723	1.082	1.085
1.9	1.4	.708	1.081	1.083
1.9	1.5	.695	1.079	1.079
1.9	1.6	.682	1.075	1.074
1.9	1.7	.671	1.070	1.067
1.9	1.8	.661	1.065	1.060
1.9	1.9	.652	1.060	1.053
1.9	2.0	.643	1.054	1.045
2.0	1.0	.756	1.083	1.083
2.0	1.1	.736	1.090	1.092
2.0	1.2	.717	1.095	1.096
2.0	1.3	.701	1.096	1.097
2.0	1.4	.687	1.096	1.095
2.0	1.5	.673	1.094	1.092
2.0	1.6	.661	1.091	1.087
2.0	1.7	.651	1.087	1.081
2.0	1.8	.641	1.083	1.074
2.0	1.9	.632	1.078	1.067
2.0	2.0	.624	1.072	1.060

A/B	B/C	MU(A)	MU(B)	MU(C)
1.0	1.0	1.000	1.000	1.000
1.0	1.1	.995	.995	1.012
1.0	1.2	.991	.991	1.023
1.0	1.3	.990	.990	1.033
1.0	1.4	.989	.989	1.041
1.0	1.5	.990	.990	1.048
1.0	1.6	.991	.991	1.055
1.0	1.7	.993	.993	1.061
1.0	1.8	.995	.995	1.067
1.0	1.9	.998	.998	1.072
1.0	2.0	1.000	1.000	1.076
1.1	1.0	.987	1.007	1.007
1.1	1.1	.981	1.004	1.019
1.1	1.2	.978	1.003	1.030
1.1	1.3	.976	1.003	1.039
1.1	1.4	.975	1.005	1.047
1.1	1.5	.975	1.007	1.055
1.1	1.6	.976	1.009	1.061
1.1	1.7	.978	1.012	1.067
1.1	1.8	.980	1.015	1.072
1.1	1.9	.982	1.018	1.077
1.1	2.0	.984	1.022	1.081
1.2	1.0	.975	1.016	1.016
1.2	1.1	.969	1.015	1.028
1.2	1.2	.965	1.015	1.038
1.2	1.3	.963	1.017	1.047
1.2	1.4	.962	1.020	1.055
1.2	1.5	.962	1.023	1.062
1.2	1.6	.962	1.027	1.068
1.2	1.7	.963	1.030	1.074
1.2	1.8	.965	1.034	1.079
1.2	1.9	.967	1.038	1.084
1.2	2.0	.969	1.042	1.088
1.3	1.0	.963	1.025	1.025
1.3	1.1	.956	1.026	1.037
1.3	1.2	.952	1.028	1.047
1.3	1.3	.950	1.031	1.056
1.3	1.4	.949	1.035	1.063
1.3	1.5	.948	1.039	1.070
1.3	1.6	.949	1.044	1.077
1.3	1.7	.950	1.048	1.082
1.3	1.8	.951	1.053	1.087
1.3	1.9	.953	1.057	1.092
1.3	2.0	.955	1.062	1.096
1.4	1.0	.951	1.035	1.035
1.4	1.1	.945	1.037	1.046
1.4	1.2	.940	1.041	1.056
1.4	1.3	.938	1.045	1.065
1.4	1.4	.936	1.050	1.073
1.4	1.5	.936	1.055	1.080
1.4	1.6	.936	1.060	1.086
1.4	1.7	.937	1.066	1.091
1.4	1.8	.938	1.071	1.096
1.4	1.9	.939	1.076	1.101
1.4	2.0	.941	1.081	1.105
1.5	1.0	.940	1.045	1.045
1.5	1.1	.934	1.049	1.056
1.5	1.2	.929	1.054	1.066
1.5	1.3	.926	1.059	1.075
1.5	1.4	.925	1.065	1.082
1.5	1.5	.924	1.071	1.089
1.5	1.6	.924	1.077	1.095
1.5	1.7	.924	1.082	1.101
1.5	1.8	.925	1.088	1.105
1.5	1.9	.927	1.094	1.110
1.5	2.0	.928	1.099	1.114
1.6	1.0	.930	1.056	1.056
1.6	1.1	.923	1.061	1.067
1.6	1.2	.918	1.067	1.076
1.6	1.3	.915	1.073	1.085
1.6	1.4	.913	1.080	1.092
1.6	1.5	.912	1.086	1.099
1.6	1.6	.912	1.092	1.105
1.6	1.7	.913	1.099	1.110
1.6	1.8	.913	1.105	1.115
1.6	1.9	.915	1.111	1.119
1.6	2.0	.916	1.116	1.123
1.7	1.0	.920	1.066	1.066
1.7	1.1	.913	1.073	1.077
1.7	1.2	.908	1.080	1.087
1.7	1.3	.905	1.087	1.095
1.7	1.4	.903	1.094	1.103
1.7	1.5	.901	1.101	1.109
1.7	1.6	.901	1.108	1.115

1.7	1.7	.901	1.114	1.120
1.7	1.8	.902	1.121	1.125
1.7	1.9	.903	1.127	1.129
1.7	2.0	.904	1.133	1.133
1.8	1.0	.910	1.077	1.077
1.8	1.1	.903	1.084	1.088
1.8	1.2	.898	1.092	1.097
1.8	1.3	.894	1.100	1.105
1.8	1.4	.892	1.108	1.113
1.8	1.5	.891	1.115	1.119
1.8	1.6	.890	1.122	1.125
1.8	1.7	.891	1.129	1.130
1.8	1.8	.891	1.136	1.135
1.8	1.9	.892	1.142	1.139
1.8	2.0	.893	1.149	1.143
1.9	1.0	.901	1.087	1.087
1.9	1.1	.893	1.096	1.098
1.9	1.2	.888	1.104	1.108
1.9	1.3	.885	1.113	1.116
1.9	1.4	.882	1.121	1.123
1.9	1.5	.881	1.129	1.129
1.9	1.6	.880	1.137	1.135
1.9	1.7	.880	1.144	1.140
1.9	1.8	.881	1.151	1.145
1.9	1.9	.881	1.157	1.149
1.9	2.0	.882	1.164	1.153
2.0	1.0	.892	1.098	1.098
2.0	1.1	.884	1.107	1.109
2.0	1.2	.879	1.116	1.118
2.0	1.3	.875	1.125	1.126
2.0	1.4	.873	1.134	1.133
2.0	1.5	.871	1.142	1.140
2.0	1.6	.870	1.150	1.145
2.0	1.7	.870	1.158	1.150
2.0	1.8	.870	1.165	1.155
2.0	1.9	.871	1.172	1.159
2.0	2.0	.872	1.178	1.163

A/B	B/C	THETA+	THETA-	TAU/TAU0	PSI
1.0	1.0	.167	.167	1.000	1.000
1.0	1.1	.169	.163	1.004	1.000
1.0	1.2	.170	.159	1.014	.998
1.0	1.3	.169	.155	1.029	.997
1.0	1.4	.167	.151	1.047	.995
1.0	1.5	.165	.147	1.069	.992
1.0	1.6	.162	.143	1.094	.989
1.0	1.7	.158	.139	1.121	.986
1.0	1.8	.155	.135	1.150	.983
1.0	1.9	.151	.132	1.180	.980
1.0	2.0	.147	.128	1.211	.977
1.1	1.0	.170	.163	1.004	1.000
1.1	1.1	.170	.159	1.011	.999
1.1	1.2	.170	.155	1.024	.997
1.1	1.3	.169	.151	1.042	.995
1.1	1.4	.166	.147	1.064	.993
1.1	1.5	.163	.143	1.089	.990
1.1	1.6	.160	.139	1.117	.987
1.1	1.7	.156	.134	1.147	.984
1.1	1.8	.152	.131	1.178	.981
1.1	1.9	.149	.127	1.211	.978
1.1	2.0	.145	.123	1.245	.975
1.2	1.0	.172	.158	1.013	.999
1.2	1.1	.172	.154	1.023	.998
1.2	1.2	.171	.150	1.040	.996
1.2	1.3	.169	.145	1.061	.994
1.2	1.4	.166	.141	1.085	.991
1.2	1.5	.163	.137	1.113	.988
1.2	1.6	.159	.132	1.143	.985
1.2	1.7	.155	.128	1.175	.982
1.2	1.8	.152	.124	1.209	.979
1.2	1.9	.148	.120	1.244	.976
1.2	2.0	.144	.117	1.281	.972
1.3	1.0	.173	.152	1.026	.998
1.3	1.1	.173	.148	1.040	.996
1.3	1.2	.172	.143	1.059	.994
1.3	1.3	.169	.139	1.082	.992
1.3	1.4	.166	.134	1.109	.989
1.3	1.5	.163	.130	1.139	.986
1.3	1.6	.159	.125	1.172	.983
1.3	1.7	.155	.121	1.206	.980
1.3	1.8	.151	.117	1.242	.977
1.3	1.9	.147	.114	1.279	.974
1.3	2.0	.143	.110	1.318	.971
1.4	1.0	.174	.146	1.043	.996
1.4	1.1	.174	.141	1.059	.995
1.4	1.2	.172	.137	1.080	.993
1.4	1.3	.170	.132	1.106	.991
1.4	1.4	.166	.127	1.135	.988
1.4	1.5	.163	.123	1.167	.985
1.4	1.6	.159	.119	1.201	.982
1.4	1.7	.155	.114	1.238	.979
1.4	1.8	.151	.111	1.276	.976
1.4	1.9	.147	.107	1.315	.972
1.4	2.0	.143	.103	1.356	.969
1.5	1.0	.174	.140	1.061	.995
1.5	1.1	.174	.135	1.079	.994
1.5	1.2	.172	.130	1.103	.992
1.5	1.3	.170	.125	1.130	.989
1.5	1.4	.166	.121	1.161	.987
1.5	1.5	.163	.116	1.195	.984
1.5	1.6	.159	.112	1.232	.981
1.5	1.7	.155	.108	1.270	.978
1.5	1.8	.150	.104	1.310	.975
1.5	1.9	.146	.101	1.351	.972
1.5	2.0	.142	.097	1.393	.969
1.6	1.0	.175	.134	1.081	.994
1.6	1.1	.174	.129	1.101	.993
1.6	1.2	.172	.124	1.126	.991
1.6	1.3	.170	.119	1.156	.988
1.6	1.4	.166	.114	1.189	.986
1.6	1.5	.162	.110	1.224	.983
1.6	1.6	.158	.106	1.262	.980
1.6	1.7	.154	.102	1.302	.977
1.6	1.8	.150	.098	1.344	.974
1.6	1.9	.146	.095	1.386	.971
1.6	2.0	.142	.091	1.430	.969
1.7	1.0	.175	.127	1.102	.993
1.7	1.1	.174	.122	1.124	.992
1.7	1.2	.172	.117	1.151	.990
1.7	1.3	.169	.113	1.182	.988
1.7	1.4	.166	.108	1.216	.985
1.7	1.5	.162	.104	1.253	.983
1.7	1.6	.158	.100	1.293	.980

1.7	1.7	.154	.096	1.334	.977
1.7	1.8	.150	.092	1.377	.974
1.7	1.9	.145	.089	1.422	.972
1.7	2.0	.141	.086	1.467	.969
1.8	1.0	.175	.122	1.124	.992
1.8	1.1	.174	.117	1.147	.991
1.8	1.2	.172	.112	1.175	.990
1.8	1.3	.169	.107	1.207	.988
1.8	1.4	.166	.102	1.243	.985
1.8	1.5	.162	.098	1.282	.983
1.8	1.6	.158	.094	1.323	.980
1.8	1.7	.154	.091	1.366	.978
1.8	1.8	.149	.087	1.410	.975
1.8	1.9	.145	.084	1.456	.972
1.8	2.0	.141	.081	1.503	.970
1.9	1.0	.175	.116	1.146	.992
1.9	1.1	.174	.111	1.170	.991
1.9	1.2	.172	.106	1.199	.989
1.9	1.3	.169	.101	1.233	.988
1.9	1.4	.165	.097	1.270	.986
1.9	1.5	.162	.093	1.310	.983
1.9	1.6	.157	.089	1.352	.981
1.9	1.7	.153	.086	1.396	.978
1.9	1.8	.149	.082	1.442	.976
1.9	1.9	.145	.079	1.489	.973
1.9	2.0	.141	.076	1.538	.971
2.0	1.0	.175	.111	1.168	.991
2.0	1.1	.174	.106	1.193	.991
2.0	1.2	.172	.101	1.224	.990
2.0	1.3	.169	.096	1.258	.988
2.0	1.4	.165	.092	1.296	.986
2.0	1.5	.161	.088	1.337	.984
2.0	1.6	.157	.084	1.381	.982
2.0	1.7	.153	.081	1.426	.979
2.0	1.8	.149	.078	1.473	.977
2.0	1.9	.144	.075	1.522	.975
2.0	2.0	.140	.072	1.571	.972

A/B	B/C	DELTA+	DELTA-
1.0	1.0	2.500	2.500
1.0	1.1	2.541	2.454
1.0	1.2	2.568	2.413
1.0	1.3	2.582	2.377
1.0	1.4	2.588	2.344
1.0	1.5	2.586	2.314
1.0	1.6	2.579	2.286
1.0	1.7	2.568	2.259
1.0	1.8	2.555	2.235
1.0	1.9	2.539	2.212
1.0	2.0	2.522	2.190
1.1	1.0	2.549	2.446
1.1	1.1	2.577	2.410
1.1	1.2	2.596	2.372
1.1	1.3	2.605	2.337
1.1	1.4	2.606	2.305
1.1	1.5	2.601	2.274
1.1	1.6	2.592	2.246
1.1	1.7	2.579	2.220
1.1	1.8	2.564	2.195
1.1	1.9	2.547	2.172
1.1	2.0	2.529	2.151
1.2	1.0	2.599	2.387
1.2	1.1	2.624	2.350
1.2	1.2	2.641	2.313
1.2	1.3	2.648	2.277
1.2	1.4	2.648	2.245
1.2	1.5	2.642	2.214
1.2	1.6	2.632	2.185
1.2	1.7	2.619	2.159
1.2	1.8	2.604	2.134
1.2	1.9	2.587	2.111
1.2	2.0	2.570	2.089
1.3	1.0	2.648	2.326
1.3	1.1	2.675	2.286
1.3	1.2	2.692	2.248
1.3	1.3	2.700	2.212
1.3	1.4	2.700	2.178
1.3	1.5	2.695	2.147
1.3	1.6	2.686	2.118
1.3	1.7	2.674	2.091
1.3	1.8	2.660	2.066
1.3	1.9	2.644	2.043
1.3	2.0	2.627	2.021
1.4	1.0	2.699	2.264
1.4	1.1	2.729	2.222
1.4	1.2	2.748	2.183
1.4	1.3	2.757	2.146
1.4	1.4	2.759	2.112
1.4	1.5	2.756	2.081
1.4	1.6	2.748	2.051
1.4	1.7	2.737	2.024
1.4	1.8	2.724	1.999
1.4	1.9	2.710	1.976
1.4	2.0	2.694	1.954
1.5	1.0	2.752	2.203
1.5	1.1	2.785	2.160
1.5	1.2	2.807	2.119
1.5	1.3	2.818	2.082
1.5	1.4	2.823	2.048
1.5	1.5	2.821	2.016
1.5	1.6	2.815	1.987
1.5	1.7	2.806	1.961
1.5	1.8	2.795	1.936
1.5	1.9	2.781	1.913
1.5	2.0	2.767	1.892
1.6	1.0	2.806	2.144
1.6	1.1	2.844	2.100
1.6	1.2	2.868	2.059
1.6	1.3	2.883	2.021
1.6	1.4	2.890	1.987
1.6	1.5	2.891	1.956
1.6	1.6	2.887	1.927
1.6	1.7	2.880	1.901
1.6	1.8	2.870	1.877
1.6	1.9	2.858	1.854
1.6	2.0	2.845	1.834
1.7	1.0	2.863	2.087
1.7	1.1	2.905	2.042
1.7	1.2	2.933	2.001
1.7	1.3	2.951	1.964
1.7	1.4	2.961	1.930
1.7	1.5	2.965	1.899
1.7	1.6	2.963	1.871

1.7	1.7	2.958	1.845
1.7	1.8	2.949	1.822
1.7	1.9	2.939	1.800
1.7	2.0	2.927	1.780
1.8	1.0	2.922	2.033
1.8	1.1	2.968	1.987
1.8	1.2	3.001	1.946
1.8	1.3	3.023	1.910
1.8	1.4	3.036	1.876
1.8	1.5	3.042	1.846
1.8	1.6	3.042	1.819
1.8	1.7	3.039	1.794
1.8	1.8	3.033	1.771
1.8	1.9	3.024	1.750
1.8	2.0	3.014	1.730
1.9	1.0	2.983	1.981
1.9	1.1	3.035	1.936
1.9	1.2	3.071	1.895
1.9	1.3	3.097	1.859
1.9	1.4	3.113	1.826
1.9	1.5	3.122	1.797
1.9	1.6	3.125	1.770
1.9	1.7	3.124	1.746
1.9	1.8	3.120	1.724
1.9	1.9	3.113	1.703
1.9	2.0	3.104	1.685
2.0	1.0	3.047	1.932
2.0	1.1	3.103	1.887
2.0	1.2	3.145	1.847
2.0	1.3	3.174	1.812
2.0	1.4	3.194	1.780
2.0	1.5	3.206	1.751
2.0	1.6	3.212	1.725
2.0	1.7	3.213	1.702
2.0	1.8	3.210	1.680
2.0	1.9	3.205	1.661
2.0	2.0	3.198	1.643

A/B	B/C	GAMMA+	GAMMA-
1.0	1.0	1.000	1.000
1.0	1.1	1.016	.981
1.0	1.2	1.026	.965
1.0	1.3	1.031	.949
1.0	1.4	1.032	.935
1.0	1.5	1.031	.922
1.0	1.6	1.027	.910
1.0	1.7	1.021	.898
1.0	1.8	1.015	.888
1.0	1.9	1.008	.878
1.0	2.0	1.000	.868
1.1	1.0	1.020	.978
1.1	1.1	1.030	.963
1.1	1.2	1.037	.947
1.1	1.3	1.039	.932
1.1	1.4	1.039	.918
1.1	1.5	1.035	.905
1.1	1.6	1.030	.893
1.1	1.7	1.024	.881
1.1	1.8	1.017	.871
1.1	1.9	1.009	.861
1.1	2.0	1.001	.851
1.2	1.0	1.038	.954
1.2	1.1	1.048	.938
1.2	1.2	1.053	.922
1.2	1.3	1.055	.907
1.2	1.4	1.053	.893
1.2	1.5	1.050	.880
1.2	1.6	1.044	.867
1.2	1.7	1.038	.855
1.2	1.8	1.030	.844
1.2	1.9	1.023	.834
1.2	2.0	1.015	.825
1.3	1.0	1.057	.928
1.3	1.1	1.066	.911
1.3	1.2	1.072	.895
1.3	1.3	1.073	.879
1.3	1.4	1.072	.865
1.3	1.5	1.068	.851
1.3	1.6	1.063	.838
1.3	1.7	1.057	.826
1.3	1.8	1.049	.815
1.3	1.9	1.042	.805
1.3	2.0	1.034	.795
1.4	1.0	1.075	.902
1.4	1.1	1.085	.884
1.4	1.2	1.091	.867
1.4	1.3	1.093	.851
1.4	1.4	1.092	.836
1.4	1.5	1.089	.822
1.4	1.6	1.084	.809
1.4	1.7	1.078	.797
1.4	1.8	1.071	.786
1.4	1.9	1.064	.776
1.4	2.0	1.056	.766
1.5	1.0	1.094	.876
1.5	1.1	1.105	.857
1.5	1.2	1.111	.839
1.5	1.3	1.114	.823
1.5	1.4	1.113	.808
1.5	1.5	1.111	.794
1.5	1.6	1.106	.781
1.5	1.7	1.101	.769
1.5	1.8	1.094	.758
1.5	1.9	1.087	.748
1.5	2.0	1.080	.738
1.6	1.0	1.113	.850
1.6	1.1	1.125	.831
1.6	1.2	1.132	.812
1.6	1.3	1.135	.796
1.6	1.4	1.136	.781
1.6	1.5	1.133	.767
1.6	1.6	1.130	.754
1.6	1.7	1.125	.742
1.6	1.8	1.119	.731
1.6	1.9	1.112	.721
1.6	2.0	1.105	.712
1.7	1.0	1.132	.825
1.7	1.1	1.145	.805
1.7	1.2	1.154	.787
1.7	1.3	1.158	.770
1.7	1.4	1.159	.755
1.7	1.5	1.157	.741
1.7	1.6	1.154	.729

1.7	1.7	1.149	.717
1.7	1.8	1.144	.706
1.7	1.9	1.138	.697
1.7	2.0	1.131	.688
1.8	1.0	1.151	.801
1.8	1.1	1.166	.781
1.8	1.2	1.176	.762
1.8	1.3	1.181	.746
1.8	1.4	1.182	.731
1.8	1.5	1.182	.717
1.8	1.6	1.179	.705
1.8	1.7	1.175	.693
1.8	1.8	1.170	.683
1.8	1.9	1.164	.674
1.8	2.0	1.158	.665
1.9	1.0	1.172	.778
1.9	1.1	1.188	.758
1.9	1.2	1.198	.739
1.9	1.3	1.204	.723
1.9	1.4	1.207	.708
1.9	1.5	1.207	.695
1.9	1.6	1.205	.682
1.9	1.7	1.201	.671
1.9	1.8	1.197	.661
1.9	1.9	1.191	.652
1.9	2.0	1.185	.643
2.0	1.0	1.192	.756
2.0	1.1	1.210	.736
2.0	1.2	1.221	.717
2.0	1.3	1.229	.701
2.0	1.4	1.232	.687
2.0	1.5	1.233	.673
2.0	1.6	1.231	.661
2.0	1.7	1.229	.651
2.0	1.8	1.224	.641
2.0	1.9	1.219	.632
2.0	2.0	1.214	.624

Program 3

```
C
C     ****************************************************************
C      THIS PROGRAM PRODUCES A CONTOUR MAP OF THE VISCOSITY
C      INCREMENT OVER THE AXIAL RANGE A/B, B/C 1.0 TO 3.0, IN
C      STEPS OF 0.5 OF THE FUNCTION FROM NU=2.5 TO NU=7.0
C     ****************************************************************
C
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/A,C,NN
      EXTERNAL FUN
      DIMENSION ALPHA(10,21,21),NU(21,21),H(10)
      REAL NU
      NN=0
C     COMPUTE THE ELLIPTIC INTEGRALS
      DO45 K=1,10
      A=0.9
      NN=NN+1
      DO40 I=1,21
      A=A+0.1
      C=1.0/0.9
      DO30 N=1,21
      C=C/(1.0+0.1*C)
C     SET LIMITS FOR NUMERICAL INTEGRATION (THESE LIMITS
C     BELOW HAVE BEEN PREVIOUSLY TESTED FOR CONVERGENCE)
      AA=0.0
      BB=1000000
      IF(NN.EQ.10)BB=500000000
      MAXDIV=50
      EPS=1.0E-08
      ACC=0.0
      IFAIL=0
C     CALL U.K. "NAG" LIBRARY ROUTINE FOR NUMERICAL EVALUATION
C     OF THE INTEGRALS "ALPHA" GIVEN IN THE SUBROUTINE BELOW
      CALL D01AGF(AA,BB,FUN,MAXDIV,EPS,ACC,ANS,ERROR,NOFUN,IFAIL)
      ALPHA(NN,I,N)=ANS
   30 CONTINUE
   40 CONTINUE
   45 CONTINUE
      B=1.0
      A=0.9
      DO80 J=1,21
      A=A+0.1
      C=1.0/0.9
      DO70 N=1,21
      C=C/(1.0+0.1*C)
C     NOW COMPUTE THE FUNCTION VALUES USING THE STORED INTEGRAL VALUES
      NU(J,N)=(1.0/(A*B*C))*((4.0/15.0)*((ALPHA(7,J,N)+ALPHA(8,J,N)
     + +ALPHA(9,J,N))/(ALPHA(8,J,N)*ALPHA(9,J,N)+ALPHA(9,J,N)*ALPHA
     + (7,J,N)+ALPHA(7,J,N)*ALPHA(8,J,N)))+(1.0/5.0)*(((ALPHA(2,J,N)
     + +ALPHA(3,J,N))/(ALPHA(4,J,N)*(B*B*ALPHA(2,J,N)+C*C*ALPHA(3,J,N)
     + )))+((ALPHA(3,J,N)+ALPHA(1,J,N))/(ALPHA(5,J,N)*(C*C*ALPHA(3,J,N)
     + +A*A*ALPHA(1,J,N))))+((ALPHA(1,J,N)+ALPHA(2,J,N))/(ALPHA(6,J,N)
     + *(A*A*ALPHA(1,J,N)+B*B*ALPHA(2,J,N))))))
   70 CONTINUE
   80 CONTINUE
C
C     CALL CONTOUR PLOTTING ROUTINE
C
      CALL PAPER(1)
      H(1)=2.5
      H(2)=3.0
      H(3)=3.5
      H(4)=4.0
      H(5)=4.5
      H(6)=5.0
      H(7)=5.5
      H(8)=6.0
      H(9)=6.5
      H(10)=7.0
      CALL MAP(1.0,3.0,1.0,3.0)
      CALL SCALES
      CALL BORDER
      CALL CONTRL(NU,1,21,21,1,21,21,H,1,10)
      CALL GRENO
      STOP
      END
```

```
C
C
C
      REAL FUNCTION FUN(X)
      COMMON/PARAM/A,C,NN
      B=1.0
      GOTO(10,20,30,40,50,60,70,80,90,100),NN
   10 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**0.5)
      RETURN
   20 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   30 FUN=1/((A*A+X)**0.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   40 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   50 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   60 FUN=1/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   70 FUN=X/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   80 FUN=X/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   90 FUN=X/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
  100 FUN=1.0/(((A*A+X)*(B*B+X)*(C*C+X))**0.5)
      RETURN
      END
```

Program 4

```
C
C     ***********************************************************
C      THIS PROGRAM GIVES PLOTS OF THE LINE SOLUTIONS OF THE
C      VARIOUS TRIAXIAL SHAPE FUNCTIONS ( AS TABULATED IN THE
C      PREVIOUS PROGRAM) FOR AXIAL RATIOS A/B = B/C = 1.5, IN
C      ORDER TO DETERMINE THE BEST COMBINATION FOR PRODUCING
C      A UNIQUE SOLUTION.
C     ***********************************************************
C
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/A,C,NN
      EXTERNAL FUN
      DIMENSION ALPHA(10,21,21),NU(21,21),F(21,21),R(21,21),H(1)
     + ,BETA(21,21),CA(21,21),CB(21,21),CC(21,21),M(21,21),O(21,21)
     + ,P(21,21),TPLS(21,21),TMNS(21,21),RHOA(21,21),RHOB(21,21)
     + ,RHOC(21,21),TAU(21,21),PSI(21,21),DELA(21,21),DELB(21,21)
     + ,DELC(21,21),GAMMAA(21,21),GAMMAB(21,21),GAMMAC(21,21),MUA(21,21)
     + ,MUB(21,21),MUC(21,21),DPLS(21,21),DMNS(21,21),GPLS(21,21)
     + ,GMNS(21,21),V(21,21)
     + ,X1(21,21),X2(21,21),X3(21,21),X4(21,21),X5(21,21)
     + ,T1(21,21),T2(21,21),T3(21,21),T4(21,21),T5(21,21)
      REAL NU,M,O,P,MUA,MUB,MUC,PSI
C     COMPUTE THE ELLIPTIC INTEGRALS
      NN=0
      DO45 K=1,10
      A=0.95
      NN=NN+1
      DO40 I=1,21
      A=A+0.05
      C=1.0/0.95
      DO30 N=1,21
      C=C/(1.0+0.05*C)
C     SET LIMITS FOR NUMERICAL INTEGRATION (THESE LIMITS
C     BELOW HAVE BEEN PREVIOUSLY TESTED FOR CONVERGENCE)
      AA=0.0
      BB=1000000
      IF(NN.EQ.10)BB=500000000
      MAXDIV=50
      EPS=1.0E-08
      ACC=0.0
      IFAIL=0
C     CALL U.K. "NAG" LIBRARY ROUTINE FOR NUMERICAL EVALUATION
C     OF THE INTEGRALS "ALPHA" GIVEN IN THE SUBROUTINE BELOW
      CALL D01AGF(AA,BB,FUN,MAXDIV,EPS,ACC,ANS,ERROR,NOFUN,IFAIL)
      ALPHA(NN,I,N)=ANS
   30 CONTINUE
   40 CONTINUE
   45 CONTINUE
      B=1.0
      A=0.95
      DO80 J=1,21
      A=A+0.05
      C=1.0/0.95
      DO70 N=1,21
      C=C/(1.0+0.05*C)
C     NOW COMPUTE THE FUNCTION VALUES USING THE STORED INTEGRAL VALUES
      NU(J,N)=(1.0/(A*B*C))*((4.0/15.0)*((ALPHA(7,J,N)+ALPHA(8,J,N)
     + +ALPHA(9,J,N))/(ALPHA(8,J,N)*ALPHA(9,J,N)+ALPHA(9,J,N)*ALPHA
     + (7,J,N)+ALPHA(7,J,N)*ALPHA(8,J,N)))+(1.0/5.0)*(((ALPHA(2,J,N)
     + +ALPHA(3,J,N))/(ALPHA(4,J,N)*(B*B*ALPHA(2,J,N)+C*C*ALPHA(3,J,N)
     + )))+((ALPHA(3,J,N)+ALPHA(1,J,N))/(ALPHA(5,J,N)*(C*C*ALPHA(3,J,N)
     + +A*A*ALPHA(1,J,N))))+((ALPHA(1,J,N)+ALPHA(2,J,N))/(ALPHA(6,J,N)
     + *(A*A*ALPHA(1,J,N)+B*B*ALPHA(2,J,N))))))
      F(J,N)=2.0/(((A*B*C)**(1.0/3.0))*ALPHA(10,J,N))
      R(J,N)=2.0*(1.0+(F(J,N)**3.0))/NU(J,N)
      BETA(J,N)=(1.0/1000000.0)*(((6.0249**(1.0/3.0))*(10.0**(23.0/3.0
     + )))/((16200.0*3.141592654*3.141592654)**(1.0/3.0)))*(NU(J,N)
     + **(1.0/3.0))/F(J,N)
      M(J,N)=(B*B+C*C)/(B*B*ALPHA(2,J,N)+C*C*ALPHA(3,J,N))
      O(J,N)=(C*C+A*A)/(C*C*ALPHA(3,J,N)+A*A*ALPHA(1,J,N))
      P(J,N)=(A*A+B*B)/(A*A*ALPHA(1,J,N)+B*B*ALPHA(2,J,N))
      TPLS(J,N)=((A*B*C)/(12.0))*((((1.0/M(J,N))+(1.0/O(J,N))+(1.0/P(J,
     + N)))+(((1.0/M(J,N)**2.0)+(1.0/O(J,N)**2.0)+(1.0/P(J,N)**2.0))-
     + ((1.0/(M(J,N)*O(J,N)))+(1.0/(O(J,N)*P(J,N)))+(1.0/(P(J,N)*M(J,
     + N)))))**0.5))
      TMNS(J,N)=((A*B*C)/(12.0))*((((1.0/M(J,N))+(1.0/O(J,N))+(1.0/P(J,
     + N)))-(((1.0/M(J,N)**2.0)+(1.0/O(J,N)**2.0)+(1.0/P(J,N)**2.0))-
     + ((1.0/(M(J,N)*O(J,N)))+(1.0/(O(J,N)*P(J,N)))+(1.0/(P(J,N)*M(J,
     + N)))))**0.5))
      CA(J,N)=(2.0/(3.0*A*B*C))*M(J,N)
      CB(J,N)=(2.0/(3.0*A*B*C))*O(J,N)
```

```
      CC(J,N)=(2.0/(3.0*A*B*C))*P(J,N)
      RHOA(J,N)=2.0/((1.0/CB(J,N))+(1.0/CC(J,N)))
      RHOB(J,N)=2.0/((1.0/CA(J,N))+(1.0/CC(J,N)))
      RHOC(J,N)=2.0/((1.0/CA(J,N))+(1.0/CB(J,N)))
      DELA(J,N)=NU(J,N)/CA(J,N)
      DELB(J,N)=NU(J,N)/CB(J,N)
      DELC(J,N)=NU(J,N)/CC(J,N)
      TAU(J,N)=3.0/((1.0/CA(J,N))+(1.0/CB(J,N))+(1.0/CC(J,N)))
      PSI(J,N)=F(J,N)*((1.0/TAU(J,N))**(1.0/3.0))
      V(J,N)=NU(J,N)/TAU(J,N)
      X1(J,N)=0.5*((1.0/RHOB(J,N))+(1.0/RHOC(J,N))-(1.0/RHOA(J,N)))
      X2(J,N)=0.5*((1.0/RHOC(J,N))+(1.0/RHOA(J,N))-(1.0/RHOB(J,N)))
      X3(J,N)=0.5*((1.0/RHOA(J,N))+(1.0/RHOB(J,N))-(1.0/RHOC(J,N)))
      X4(J,N)=(X1(J,N)+X2(J,N)+X3(J,N))/3.0
      X5(J,N)=((X1(J,N)**2.0)+(X2(J,N)**2.0)+(X3(J,N)**2.0)-(X1(J,N)*X2
     +(J,N))-(X2(J,N)*X3(J,N))-(X3(J,N)*X1(J,N)))**0.5
      T1(J,N)=1.0/(X4(J,N)+X1(J,N))
      T2(J,N)=1.0/(X4(J,N)+X2(J,N))
      T3(J,N)=1.0/(X4(J,N)+X3(J,N))
      T4(J,N)=3.0/((6.0*X4(J,N))-(2.0*X5(J,N)))
      T5(J,N)=3.0/((6.0*X4(J,N))+(2.0*X5(J,N)))
      GAMMAA(J,N)=(1.0/2.0)*(F(J,N)**3.0)*((1.0/CB(J,N))+(1.0/CC(J,N)))
      GAMMAB(J,N)=(1.0/2.0)*(F(J,N)**3.0)*((1.0/CA(J,N))+(1.0/CC(J,N)))
      GAMMAC(J,N)=(1.0/2.0)*(F(J,N)**3.0)*((1.0/CA(J,N))+(1.0/CB(J,N)))
      MUA(J,N)=(CA(J,N)**(1.0/3.0))/F(J,N)
      MUB(J,N)=(CB(J,N)**(1.0/3.0))/F(J,N)
      MUC(J,N)=(CC(J,N)**(1.0/3.0))/F(J,N)
      DPLS(J,N)=6.0*TPLS(J,N)*NU(J,N)
      DMNS(J,N)=6.0*TMNS(J,N)*NU(J,N)
      GPLS(J,N)=6.0*TPLS(J,N)*(F(J,N)**3.0)
      GMNS(J,N)=6.0*TMNS(J,N)*(F(J,N)**3.0)
   70 CONTINUE
   80 CONTINUE
      CALL PAPER(1)
      CALL MAP(1.0,2.0,1.0,2.0)
      CALL SCALSI(0.1,0.1)
      CALL GPSTOP(21)
      CALL BORDER
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
C
C     (I)PLOT OF VISCOSITY INCREMENT AND PERRIN TRANSLATIONAL
C        FRICTIONAL FUNCTION
C
      H(1)=2.892
      CALL CONTRL(NU,1,21,21,1,21,21,H,1,1)
      CALL REDPEN
      H(1)=1.044
      CALL CONTRL(F,1,21,21,1,21,21,H,1,1)
C
C
C     (II)PLOT OF THE TRANSLATIONAL FUNCTIONS: THE VISCOSITY INCREMENT
C          THE PERRIN FUNCTION, THE BETA FUNCTION AND THE R FUNCTION, ALL
C          WITH +/-1% ASSUMED EXPERIMENTAL ERROR
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=2.92092
      CALL CONTRL(NU,1,21,21,1,21,21,H,1,1)
      H(1)=2.86308
      CALL CONTRL(NU,1,21,21,1,21,21,H,1,1)
      H(1)=2.14423
      CALL REDPEN
      CALL CONTRL(BETA,1,21,21,1,21,21,H,1,1)
      H(1)=2.10177
      CALL CONTRL(BETA,1,21,21,1,21,21,H,1,1)
      H(1)=1.05444
      CALL GRNPEN
      CALL CONTRL(F,1,21,21,1,21,21,H,1,1)
      H(1)=1.03356
      CALL CONTRL(F,1,21,21,1,21,21,H,1,1)
      H(1)=1.49379
      CALL BROKEN(4,8,8,8)
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
C
C     (III)PLOT OF THE R FUNCTION AND ROTATIONAL RELAXATION
C          TIME RATIOS
```

```
C
      CALL FRAME
      CALL FULL
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.433
      CALL CONTRL(RHOA,1,21,21,1,21,21,H,1,1)
      H(1)=1.115
      CALL REDPEN
      CALL CONTRL(RHOB,1,21,21,1,21,21,H,1,1)
      H(1)=1.093
      CALL GRNPEN
      CALL CONTRL(RHOC,1,21,21,1,21,21,H,1,1)
C
C     (IV)PLOT OF THE R FUNCTION WITH +/- 1% ASSUMED ERROR AND THE
C         ROTATIONAL RELAXATION TIME RATIOS WITH +/-2% ASSUMED ERROR
C
C
C     (IV)PLOT OF THE R FUNCTION, HARMONIC MEAN RELAXATION TIME
C        RATIO (TH/T0) THE PSI & LAMBDA FUNCTIONS
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.195
      CALL CONTRL(TAU,1,21,21,1,21,21,H,1,1)
      H(1)=.98378
      CALL REDPEN
      CALL CONTRL(PSI,1,21,21,1,21,21,H,1,1)
      H(1)=2.41886
      CALL GRNPEN
      CALL CONTRL(V,1,21,21,1,21,21,H,1,1)
C
C     (V)PLOT OF THE R FUNCTION (+/-1%) , THE HARMONIC MEAN
C         RELAXATION TIME RATIO (+/-1%) AND THE PSI FUNCTION
C        (+/- 2%) & THE LAMBDA FUNCTION (+/- 2%)
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.20695
      CALL CONTRL(TAU,1,21,21,1,21,21,H,1,1)
      H(1)=1.18305
      CALL CONTRL(TAU,1,21,21,1,21,21,H,1,1)
      H(1)=1.0034556
      CALL REDPEN
      CALL CONTRL(PSI,1,21,21,1,21,21,H,1,1)
      H(1)=0.9641044
      CALL CONTRL(PSI,1,21,21,1,21,21,H,1,1)
      CALL GRNPEN
      H(1)=2.4672372
      CALL CONTRL(V,1,21,21,1,21,21,H,1,1)
      H(1)=2.3704828
      CALL CONTRL(V,1,21,21,1,21,21,H,1,1)
C
C     (VI)PLOT OF R (+/-1%), DELTA1 (+/-1%), DELTA2 (+/-1%)
C     AND DELTA3 (+/-1%)
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
```

```
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=3.2849
      CALL CONTRL(DELA,1,21,21,1,21,21,H,1,1)
      H(1)=3.1560802
      CALL CONTRL(DELA,1,21,21,1,21,21,H,1,1)
      H(1)=2.110
      CALL REDPEN
      CALL CONTRL(DELB,1,21,21,1,21,21,H,1,1)
      H(1)=2.072
      CALL CONTRL(DELB,1,21,21,1,21,21,H,1,1)
      H(1)=2.006
      CALL GRNPEN
      CALL CONTRL(DELC,1,21,21,1,21,21,H,1,1)
      H(1)=1.928
      CALL CONTRL(DELC,1,21,21,1,21,21,H,1,1)
C
C     (VII)PLOT OF THE R, GAMMAA, GAMMAB AND GAMMAC FUNCTIONS
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=0.795
      CALL CONTRL(GAMMAA,1,21,21,1,21,21,H,1,1)
      H(1)=1.022
      CALL REDPEN
      CALL CONTRL(GAMMAB,1,21,21,1,21,21,H,1,1)
      H(1)=1.042
      CALL GRNPEN
      CALL CONTRL(GAMMAC,1,21,21,1,21,21,H,1,1)
C
C     (VIII)PLOT OF R (+/-1%), GAMMAA (+/-1%), GAMMAB (+/-1%)
C     AND GAMMAC (+/-1%)
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=.81498
      CALL CONTRL(GAMMAA,1,21,21,1,21,21,H,1,1)
      H(1)=.78302
      CALL CONTRL(GAMMAA,1,21,21,1,21,21,H,1,1)
      H(1)=1.04244
      CALL REDPEN
      CALL CONTRL(GAMMAB,1,21,21,1,21,21,H,1,1)
      H(1)=1.00156
      CALL CONTRL(GAMMAB,1,21,21,1,21,21,H,1,1)
      CALL GRNPEN
      H(1)=1.06284
      CALL CONTRL(GAMMAC,1,21,21,1,21,21,H,1,1)
      H(1)=1.02116
      CALL CONTRL(GAMMAC,1,21,21,1,21,21,H,1,1)
C
C     (IX)PLOT OF THE R ,MUA, MUB AND MUC FUNCTIONS
C
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=.924
      CALL CONTRL(MUA,1,21,21,1,21,21,H,1,1)
      CALL REDPEN
      H(1)=1.071
      CALL CONTRL(MUB,1,21,21,1,21,21,H,1,1)
```

```
      CALL GRNPEN
      H(1)=1.089
      CALL CONTRL(MUC,1,21,21,1,21,21,H,1,1)
C
C
C     (X)PLOT OF R (+/-1%), MUA (+/-1%), MUB (+/-1%)
C     AND MUC (+/-1%)
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=.94248
      CALL CONTRL(MUA,1,21,21,1,21,21,H,1,1)
      H(1)=.90552
      CALL CONTRL(MUA,1,21,21,1,21,21,H,1,1)
      H(1)=1.90242
      CALL REDPEN
      CALL CONTRL(MUB,1,21,21,1,21,21,H,1,1)
      H(1)=1.04958
      CALL CONTRL(MUB,1,21,21,1,21,21,H,1,1)
      H(1)=1.11078
      CALL GRNPEN
      CALL CONTRL(MUC,1,21,21,1,21,21,H,1,1)
      H(1)=1.06722
      CALL CONTRL(MUC,1,21,21,1,21,21,H,1,1)
C
C
C     (XI)PLOT OF THE R, REDUCED THETA+ AND REDUCED
C     THETA - FUNCTIONS
C
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      CALL REDPEN
      H(1)=.163
      CALL CONTRL(TPLS,1,21,21,1,21,21,H,1,1)
      CALL GRNPEN
      H(1)=.116
      CALL CONTRL(TMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XII)PLOT OF THE R(+/-1%), REDUCED THETA+ (+/-1%)
C     AND REDUCED THETA- (+/-1%) FUNCTIONS
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      CALL REDPEN
      H(1)=.16463
      CALL CONTRL(TPLS,1,21,21,1,21,21,H,1,1)
      H(1)=.16137
      CALL CONTRL(TPLS,1,21,21,1,21,21,H,1,1)
      CALL GRNPEN
      H(1)=.11716
      CALL CONTRL(TMNS,1,21,21,1,21,21,H,1,1)
      H(1)=.11484
      CALL CONTRL(TMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XIII)PLOT OF THE R, DELTA+ AND DELTA- FUNCTIONS
C
C
```

```
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
     CALL REDPEN
      H(1)=2.821
      CALL CONTRL(DPLS,1,21,21,1,21,21,H,1,1)
     CALL GRNPEN
      H(1)=2.016
     CALL CONTRL(DMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XIV)PLOT OF R (;/-1%), DELTA+ (+/-2%) AND DELTA- (+/-2%)
C
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.49379
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
      H(1)=1.46421
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
     CALL REDPEN
      H(1)=2.87742
      CALL CONTRL(DPLS,1,21,21,1,21,21,H,1,1)
      H(1)=2.76458
      CALL CONTRL(DPLS,1,21,21,1,21,21,H,1,1)
     CALL GRNPEN
      H(1)=2.05632
      CALL CONTRL(DMNS,1,21,21,1,21,21,H,1,1)
      H(1)=1.97568
      CALL CONTRL(DMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XV)PLOT OF THE R, GAMMA+ AND GAMMA- FUNCTIONS
C
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.479
      CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
     CALL REDPEN
     H(1)=1.111
     CALL CONTRL(GPLS,1,21,21,1,21,21,H,1,1)
     CALL GRNPEN
     CALL CONTRL(GMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XVI)PLOT OF R(+/-1%), GAMMA+ (+/-2%) AND GAMMA- (+/-2%)
C
C
     CALL FRAME
     CALL BLKPEN
     CALL BORDER
     CALL CSPACE(0.0,1.0,0.0,1.0)
     CALL SCALSI(0.1,0.1)
     CALL CSPACE(0.0,0.0001,0.0,0.0001)
     H(1)=1.49379
     CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
     H(1)=1.46421
     CALL CONTRL(R,1,21,21,1,21,21,H,1,1)
     CALL REDPEN
     H(1)=1.13322
     CALL CONTRL(GPLS,1,21,21,1,21,21,H,1,1)
     H(1)=1.08878
     CALL CONTRL(GPLS,1,21,21,1,21,21,H,1,1)
     CALL GRNPEN
     H(1)=.80988
     CALL CONTRL(GMNS,1,21,21,1,21,21,H,1,1)
     H(1)=.77812
```

```
      CALL CONTRL(GMNS,1,21,21,1,21,21,H,1,1)
C
C
C     (XVII)PLOT OF THE 5 FLUORESCENCE ANISOTROPY RELAXATION TIME
C     RATIOS
C
      CALL FRAME
      CALL BLKPEN
      CALL BORDER
      CALL CSPACE(0.0,1.0,0.0,1.0)
      CALL SCALSI(0.1,0.1)
      CALL CSPACE(0.0,0.0001,0.0,0.0001)
      H(1)=1.02536
      CALL CONTRL(T1,1,21,21,1,21,21,H,1,1)
      H(1)=1.28883
      CALL REDPEN
      CALL CONTRL(T2,1,21,21,1,21,21,H,1,1)
      CALL GRNPEN
      H(1)=1.31877
      CALL CONTRL(T3,1,21,21,1,21,21,H,1,1)
      CALL BROKEN(4,8,8,8)
      H(1)=1.43405
      CALL CONTRL(T4,1,21,21,1,21,21,H,1,1)
      CALL BLKPEN
      H(1)=1.02497
      CALL CONTRL(T5,1,21,21,1,21,21,H,1,1)
      STOP
      END
```

```
C
C
C
      REAL FUNCTION FUN(X)
      COMMON/PARAM/A,C,NN
      B=1.0
      GOTO(10,20,30,40,50,60,70,80,90,100),NN
   10 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**0.5)
      RETURN
   20 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   30 FUN=1/((A*A+X)**0.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   40 FUN=1/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   50 FUN=1/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   60 FUN=1/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
   70 FUN=X/((A*A+X)**0.5*(B*B+X)**1.5*(C*C+X)**1.5)
      RETURN
   80 FUN=X/((A*A+X)**1.5*(B*B+X)**0.5*(C*C+X)**1.5)
      RETURN
   90 FUN=X/((A*A+X)**1.5*(B*B+X)**1.5*(C*C+X)**0.5)
      RETURN
  100 FUN=1.0/(((A*A+X)*(B*B+X)*(C*C+X))**0.5)
      RETURN
      END
```

Program 5

```
C
C NON-LINEAR LEAST SQUARES METHOD USING AN ALGORITHM OF GILL AND
C MURRAY (1976)
C
C GAMMA = BIREFRINGENCE (RADS), F = SUM OF SQUARES OF THE RESIDUALS
C DPLS = DELTA+, DMNS = DELTA-
C X(1) = CURRENT INITIAL GUESS FOR THETA+
C X(2) =       "         "      "   "    -
C X(3) =       "         "      "   "   A'+
C X(4) =       "         "      "   "   A'-
C X1 = CURRENT ESTIMATE FOR THETA+
C X2 =     "        "      "    "  -
C X3 =     "        "      "  A'+
C X4 =     "        "      "  A'-
C
C ******************************
C LINEAR TIME INCREASE, 100PTS.
C .001 DEGREES S.E.
C
C RANDOM NUMBER RUN 50
C
C     ****************************************
C      PROTEIN 3
C
C
C     ****************************************
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/GAMMA(101),T(101),R(101)
      REAL BL(4),BU(4),X(4),F,W(54)
      REAL Q1,Q2,Q3,Q4,Q5
      INTEGER IBOUND,IFAIL,J,LIW,LW,N
      INTEGER IW(6)
      P=-1.0
      DO21 I=1,101
      P=P+1.0
      R(I)=P
      T(I)=R(I)*1.0E-09
   21 CONTINUE
      WRITE(3,32)
   32 FORMAT( "   TIME(NS)      GAMMA")
C G05BBF REINITIALIZES THE STREAM OF THE RANDOM NUMBERS
      CALL G05BBF
C CALCULATE THE UNPERTURBED DECAY CURVE
      DO50 I=1,101
      GAMMA(I)=0.07*EXP(-T(I)*6.0*5.187243E06)+
     +0.05*EXP(-T(I)*6.0*4.167486E06)
C NOW PERTURB EACH OF THE 160 DATA POINTS USING A NORMAL PSEUDO-RANDOM
C NUMBER GENERATOR G05ADF
      GAMMA(I)=GAMMA(I)+((0.1*1.74555E-04)*G05ADF(Y))
      WRITE(3,33)R(I),GAMMA(I)
   33 FORMAT( F10.5,F8.5)
   50 CONTINUE
      N=4
      IBOUND=0
      Q1=1.0
C DO THE MINIMIZATION FOR 30 INITIAL GUESSES TO ATTEMPT TO AVOID
C SUBSIDIARY MINIMA
      DO10 I=1,30
C CALL RECTANGULAR PSEUDO RANDOM NUMBER ROUTINE G05AAF
      Z=G05AAF(X)
      X(1)=4.0+2.0*Z
      X(2)=3.0+2.0*Z
      X(3)=6.0+2.0*Z
      X(4)=4.0+2.0*Z
      BL(1)=4.0
      BL(2)=3.0
      BL(3)=6.0
      BL(4)=4.0
      BU(1)=6.0
      BU(2)=5.0
      BU(3)=8.0
      BU(4)=6.0
      LIW=6
      LW=54
      IFAIL=1
      CALL E04JAF(N,IBOUND,BL,BU,X,F,IW,LIW,W,LW,IFAIL)
      IF(IFAIL.NE.0)WRITE(3,100)IFAIL
      IF(IFAIL.EQ.1)GOTO 20
  100 FORMAT("ERROR EXIT TYPE",I3,"SEE ROUTINE MANUAL")
      WRITE(3,110)F
      WRITE(3,120)(X(J),J=1,4)
  110 FORMAT( " FUNCTION VALUE ON EXIT IS",F15.12)
```

```
120 FORMAT( " THETA+",F10.7," THETA-",F10.7,"A ",F7.4,
   + " A- ",F7.4)
    IF(Q1.LE.F)GOTO 30
    Q1=F
    Q2=X(1)
    Q3=X(2)
    Q4=X(3)
    Q5=X(4)
 30 CONTINUE
    WRITE(3,130)
130 FORMAT( " ")
    WRITE(3,140)
140 FORMAT( " ")
 10 CONTINUE
    DPLS=0.50996303*Q2
    DMNS=0.50996303*Q3
    WRITE(3,141)
141 FORMAT( " ")
    WRITE(3,142)
142 FORMAT( " ")
    WRITE(3,143)
143 FORMAT( " ")
    WRITE(3,145)
145 FORMAT( " ")
    WRITE(3,150)Q1
150 FORMAT( " BEST LEAST SQUARES VALUE = ",F15.12)
    WRITE(3,160)Q2
160 FORMAT( "             THETA+ = ",F10.7)
    WRITE(3,170)Q3
170 FORMAT( "             THETA- = ",F10.7)
    WRITE(3,180)Q4
180 FORMAT( "                  A'+ = ",F7.4)
    WRITE(3,190)Q5
190 FORMAT( "                  A'- = ",F7.4)
    WRITE(3,200)DPLS
200 FORMAT( "            DELTA+   = ",F10.7)
    WRITE(3,210)DMNS
210 FORMAT( "            DELTA-   = ",F10.7)
 20 STOP
    END
```

```
C SUBROUTINE FOR CALCULATING THE SUM OF SQUARES OF THE RESIDUALS FOR THE
C CURRENT ESTIMATES OF THE ADJUSTABLE PARAMETERS
      SUBROUTINE FUNCT1(N,XC,FC)
      COMMON/PARAM/GAMMA(101),T(101),R(101)
      EXTERNAL FUN
      REAL Q,FC
      INTEGER N
      REAL XC(N)
      REAL X1,X2,X3,X4
      X1=XC(1)
      X2=XC(2)
      X3=XC(3)
      X4=XC(4)
      FC=0.0
      DO75 I=1,101
      Q=(GAMMA(I)-(0.01*X3*EXP(-6.0E06*X1*T(I))+0.01*X4
     + *EXP(-6.0E06*X2*T(I))))**2.0
      FC=FC+Q
   75 CONTINUE
      RETURN
      END
```

Program 6

```
C
C FOURIER TRANSFORM SOLUTION OF THE LAPLACE INTEGRAL EQUATION METHOD OF
C GARDNER, GARDNER, LAUSH AND MEINKE (1959)
C
C S = BIREFRINGENCE (RADS), GM = INTEGRAND OF EQUATION    , G = G(EXP(-Y))
C T = TIME (SEC), R = TIME (NS), EC AND ES ARE THE ERROR ESTIMATES IN FC
C AND FS RESPECTIVELY DUE TO THE NUMERICAL INTEGRATION IN EQN. 125
C AND ER IS THE ERROR ESTIMATE DUE TO THE NUMERICAL INTEGRATION IN
C EQN. 128
C
C ****************************************
C LOGARITHMIC TIME INCREASE, 140 DATA PTS.
C .001 DEGREES S.E.
C
C RANDOM NUMBER RUN 2
C
C      ***************************
C       PROTEIN 2
C
C      ***************************
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      EXTERNAL FUNXN
      REAL MMU(66),KC(66),KS(66),FC(66),FS(66),GM(66),MU
      REAL YYY,G(690),Y(690),EC(66),ES(66)
      INTEGER N,I,IFAIL
      INTEGER L
      REAL X(141),S(141),R(141),T(141),YC(141),YS(141)
      COMPLEX Z,C,K,CGAMMA
      P=-7.1
      DO21 I=1,141
      P=P+.1
      WRITE(3,500)
  500 FORMAT( " ")
      X(I)=P
      T(I)=(1.0E-09)*EXP(X(I))
      R(I)=T(I)*1.0E09
   21 CONTINUE
      WRITE(3,32)
   32 FORMAT( "   TIME(NS)     X       S(T) = S(EXP(-X))")
      WRITE(3,501)
  501 FORMAT( " ")
      WRITE(3,502)
  502 FORMAT( "************************************")
      WRITE(3,503)
  503 FORMAT( " ")
C G05BBF REINITIALIZES THE STREAM OF THE RANDOM NUMBERS
      CALL G05BBF
      DO50 I=1,141
C CALCULATE THE UNPERTURBED DECAY CURVE
      S(I)=0.07*EXP(-T(I)*4.6596278E07)+
     +0.05*EXP(-T(I)*3.137407E07)
C NOW PERTURB EACH OF THE 140 DATA PTS USING A NORMAL PSEUDO-RANDOM
C NUMBER GENERATOR
      S(I)=S(I)+((0.1*1.74555E-04)*G05ADF(Y))
      WRITE(3,33)R(I),X(I),S(I)
   33 FORMAT( F10.5,F6.2,F8.5)
   50 CONTINUE
      DO47 L=1,20
      WRITE(3,504)
  504 FORMAT( " ")
   47 CONTINUE
C THE NEXT PART OF THE PROGRAM EVALUATES THE FOURIER TRANSFORM OF THE DATA
      MU=-.1
      WRITE(3,99)
   99 FORMAT( "                 MU            KC                KS")
      WRITE(3,505)
  505 FORMAT( " ")
      WRITE(3,506)
  506 FORMAT( " ****************************************************")
      WRITE(3,507)
  507 FORMAT( " ")
      DO10 J=1,66
      MU=MU+.1
      MMU(J)=MU
      DO51 I=1,141
      YC(I)=(EXP(X(I)))*S(I)*COS(MU*X(I))
      YS(I)=(EXP(X(I)))*S(I)*SIN(MU*X(I))
      Y(I)=CMPLX(YC(I),YS(I))
   51 CONTINUE
      N=141
      IFAIL=1
```

```
C CALL NUMERICAL INTEGRATION ROUTINE FROM THE UK NAG LIBRARY (MK 6)
      CALL D01GAF(X,YC,N,ANS,ER,IFAIL)
      FC(J)=((1.0/(2.0*3.141593))**0.5)*ANS
      EC(J)=((1.0/(2.0*3.141593))**0.5)*ER
      CALL D01GAF(X,YS,N,ANS,ER,IFAIL)
      FS(J)=((1.0/(2.0*3.141593))**0.5)*ANS
      ES(J)=((1.0/(2.0*3.141593))**0.5)*ER
C EVALUATE THE COMPLEX GAMMA FUNCTION FOR THE CURRENT VALUE OF MU USING
C THE SUBROUTINE BELOW
      Z=CMPLX(1.0,MU)
      C=CGAMMA(Z)
C DETERMINE THE EULER INTEGRAL OF THE COMPLEX GAMMA FUNCTION (EQN. 123 )
      K=((1.0/(2.0*3.141593))**0.5)*C
      KC(J)=REAL(K)
      KS(J)=AIMAG(K)
      C=CGAMMA(Z)
      WRITE(3,101)MU,K
  101 FORMAT( 7X,1F8.2,2E15.7)
   10 CONTINUE
      DO49 L=1,20
      WRITE(3,509)
  509 FORMAT( " ")
   49 CONTINUE
      WRITE(3,90)
   90 FORMAT( "      MU        FC              (ERR)              FS
     +     (ERR)")
      WRITE(3,510)
  510 FORMAT( " ")
      WRITE(3,511)
  511 FORMAT( "**********************************************
     +********")
      WRITE(3,512)
  512 FORMAT( " ")
      DO38 J=1,66
      WRITE(3,91)MMU(J),FC(J),EC(J),FS(J),ES(J)
   91 FORMAT( 1X,1F8.2,4E14.7)
   38 CONTINUE
      DO52 L=1,20
      WRITE(3,513)
  513 FORMAT( " ")
   52 CONTINUE
      WRITE(3,93)
   93 FORMAT( "           Y              G(EXP(-Y))           ERROR")
      WRITE(3,514)
  514 FORMAT( " ")
      WRITE(3,515)
  515 FORMAT( " ***********************************************")
      WRITE(3,516)
  516 FORMAT( " ")
      YYY=-.01
      DO31 M=1,690
      YYY=YYY+.01
      Y(M)=YYY
      DO29 J=1,66
C DIVIDE THE FOURIER TRANSFORM OF THE DATA BY THE EULER INTEGRAL FOR THE
C COMPLEX GAMMA FUNCTION
      GM(J)=((((FC(J)*KC(J))+(FS(J)*KS(J)))*COS(YYY*MMU(J)))/((KC(J)
     +*KC(J))
     ++(KS(J)*KS(J))))+((((FS(J)*KC(J))-(FC(J)*KS(J)))*SIN(YYY*MMU(J)))/
     +((KC(J)*KC(J))+(KS(J)*KS(J))))
   29 CONTINUE
      NN=66
C NOW G(EXP(-Y)) AS A FUNCTION OF Y IS FOUND FROM THE INVERSE FOURIER
C TRANSFORM USING THE SAME NUMERICAL INTEGRATION ROUTINE
      CALL D01GAF(MMU,GM,NN,ANS,ER,IFAIL)
      G(M)=(1.0/3.141593)*ANS
      ER=(1.0/3.141593)*ER
      WRITE(3,290)YYY,G(M),ER
      IF(IFAIL)241,261,241
  241 WRITE(3,289)
  261 CONTINUE
  290 FORMAT(/3X,F7.2,4X,1E15.7,4X,1E15.7)
  289 FORMAT(/28H LESS THAN 4 POINTS SUPPLIED)
   31 CONTINUE
C HENCE A PLOT OF G(EXP(-Y)) AGAINST Y IS OBTAINED
      CALL PAPER(1)
      CALL MAP(0.0,0.0,0.0,0.0)
      CALL CURVEO(Y,G,1,690)
      CALL SCALES
      CALL BORDER
      CALL GRAPHF(FUNXN)
```

```
      CALL GREND
      STOP
      END
```

```
C
      FUNCTION FUNXN(X)
      FUNXN=0.0
      RETURN
      END
```

```
C
C SUBROUTINE FOR CALCULATING THE COMPLEX GAMMA FUNCTION C = CGAMMA(Z) FOR
C THE CURRENT VALUE OF MU. THIS SUBROUTINE IS THAT GIVEN BY LUCAS AND
C TERRILL (1970)
      COMPLEX FUNCTION CGAMMA(Z)
      COMPLEX Z,ZM,T,TT,SUM,TERM,DEN,PI,A
      DIMENSION C(12)
      LOGICAL REFLEX
C SET IOUT FOR PROPER OUTPUT CHANNEL OF COMPUTER SYSTEM FOR
C ERROR MESSAGES
      IOUT=3
      PI=(3.141593,0.0)
      X=REAL(Z)
      Y=AIMAG(Z)
C TOL = LIMIT OF PRECISION OF COMPUTER SYSTEM IN SINGLE PRECISION
      TOL=1.0E-07
      REFLEX=.TRUE.
C DETERMINE WHETHER Z IS TOO CLOSE TO A POLE
C CHECK WHETHER TOO CLOSE TO ORIGIN
      IF(X.GE.TOL) GO TO 20
C FIND THE NEAREST POLE AND COMPUTE DISTANCE TO IT
      XDIST=X-INT(X-.5)
      ZM=CMPLX(XDIST,Y)
      IF(CABS(ZM).GE.TOL)GOTO 10
C IF Z IS TOO CLOSE TO A POLE, PRINT ERROR MESSAGE AND RETURN
C WITH CGAMMA=(1.E7,0.F0)
      WRITE (IOUT,900)Z
      CGAMMA=(1.E7,0.E0)
      RETURN
C FOR REAL(Z) NEGATIVE EMPLOY THE REFLECTION FORMULA
C         GAMMA(Z)=PI(SINPI*Z)*GAMMA(1-Z))
C
C AND COMPUTE GAMMA(1-Z). NOTE REFLEX IS A TAG TO INDICATE THAT
C THIS RELATION MUST BE USED LATER.
   10 IF(X.GE.0.0)GOTO 20
      REFLEX=.FALSE.
      Z=(1.0,0.0)-Z
      X=1.0-X
      Y=-Y
C IF Z IS NOT TOO CLOSE TO A POLE, MAKE REAL(Z)>10 AND ARG(Z)<PI/4
   20 M=0
   40 IF(X.GE.10.)GOTO 50
      X=X+1.0
      M=M+1
      GOTO 40
   50 IF(ABS(Y).LT.X)GOTO 60
      X=X+1.0
      M=M+1
      GOTO 50
   60 T=CMPLX(X,Y)
      TT=T*T
      DEN=T
```

```
C COEFFICIENTS IN STIRLING'S APPROXIMATION FOR LN(GAMMA(T))
      C(1)=1./12.
      C(2)=-1./360.
      C(3)=1./1260.
      C(4)=-1./1680.
      C(5)=1./1188.
      C(6)=-691./360360.
      C(7)=1./156.
      C(8)=-3617./122400.
      C(9)=43867./244188.
      C(10)=-174611./125400.
      C(11)=77683./5796.
      SUM=(T-(.5,0.0))*CLOG(T)-T*CMPLX(.5*ALOG(2.*3.14159),0.0)
      J=1
   70 TERM=C(J)/DEN
C TEST REAL AND IMAGINARY PARTS OF LN(GAMMA(Z))SEPARATELY FOR
C CONVERGENCE. IF Z IS REAL SKIP IMAGINARY PART OF CHECK.
      IF(ABS(REAL(TERM)/REAL(SUM)).GE.TOL)GOTO 80
      IF(Y.EQ.0.0)GOTO 100
      IF(ABS(AIMAG(TERM)/AIMAG(SUM)).LT.TOL)GOTO 100
   80 SUM=SUM+TERM
      J=J+1
      DEN=DEN*TT
C TEST FOR CONVERGENCE
      IF(J.EQ.12)GOTO 90
      GOTO 70
C STIRLINGS SERIES DID NOT CONVERGE. PRINT ERROR MESSAGE AND
C PROCEDE
   90 WRITE(IOUT,910)Z
C RECURSION RELATION USED TO OBTAIN LN(GAMMA(Z))
C           LN(GAMMA(Z))=LN(GAMMA(Z+M)/(Z*(Z+1)*...*(Z+M-1)))
C                       =LN(GAMMA(Z+M)-LN(Z)-LN(Z+1)-...-LN(Z+M-1)
  100 IF(M.EQ.0)GOTO 120
      DO110 I=1,M
      A=CMPLX(I*1.-1.,0.0)
  110 SUM=SUM-CLOG(Z+A)
C CHECK TO SEE IF REFLECTION FORMULA SHOULD BE USED
  120 IF(REFLEX)GOTO 130
      SUM=CLOG(PI/CSIN(PI*Z))-SUM
      Z=(1.0,0.0)-Z
  130 CGAMMA=CEXP(SUM)
      RETURN
  900 FORMAT(1X,2F14.7,10X,49HARGUMENT OF GAMMA FUNCTION IS TOO CLOSE TO
     + A POLE)
  910 FORMAT(44H ERROR - STIRLING'S SERIES HAS NOT CONVERGED/14X,4H7    ,
     +2E14.7)
      END
```

Program 7

```
C
C R-CONSTRAINED NON-LINEAR LEAST SQUARES METHOD (HARDING)
C
C GAMMA = BIREFRINGENCE (RADS), FC = SUM OF SQUARES OF THE RESIDUALS
C X(1) = CURRENT INITIAL GUESS FOR A/B
C X(2) =    "       "      "    "  A+
C X(3) =    "       "      "    "  A-
C ON EXIT, X(1), X(2), X(3) CONTAIN THE BEST ESTIMATES FOR THESE PARAMETERS
C XC(1) = A = CURRENT ESTIMATE FOR A/B
C D = 1/C = VALUE OF B/C                    CORRESPONDING TO THIS ESTIMATE
C      S   =    "   "  VISCOSITY INCREMENT       "          "   "     "
C      V   =    "   "           DELTA+           "          "   "     "
C      W   =    "   "           DELTA-           "          "   "     "
C  THPLUS  =    "   "           THETA+           "          "   "     "
C  THMNUS  =    "   "           THETA-           "          "   "     "
C XC(2) = CURRENT ESTIMATE FOR A+
C XC(3) =    "       "      "  A-
C AA1,AA2,....AA6 ARE THE A/B COORDINATES FOR 6 PTS ON THE R-CURVE
C AD1,AD2,....AD6  "   "  B/C     "        "  "  "   "   "    "
C THE VALUE FOR B/C CORRESPONDING TO THE CURRENT ESTIMATE FOR A/B CAN THEN
C BE FOUND USING A CUBIC POLYNOMIAL INTERPOLATION PROCEDURE BETWEEN THE
C SIX GIVEN POINTS.THIS IS DONE USING A LIBRARY ROUTINE E01LF1
C
C ***********
C  PROTEIN 1
C ***********
C LINEAR TIME INCREASE, 100PTS.
C CUT OFF TIME: 100NS
C STREAM OF RANDOM NUMBERS: 3
C 0.1 DEG STANDARD ERROR ON EACH DATA PT.
C
      PROGRAM MAIN(INPUT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
      COMMON/PARAM/GAMMA(101),T(101),A,C,D,NN,AA(6),AD(6)
      REAL R(101)
      REAL AA1,AA2,AA3,AA4,AA5,AA6,AD1,AD2,AD3,AD4,AD5,AD6
      REAL BL(3),BU(3),X(3),F,W(39)
      INTEGER IBOUND,IFAIL,J,LIW,LW,N
      INTEGER IW(5)
      REAL Q1,Q2,Q3,Q4
      WRITE(3,37)
   37 FORMAT( " PROTEIN 1,  0.1 DEG. STANDARD ERROR")
      WRITE(3,38)
   38 FORMAT( "
     + 100NS, 100PTS")
      WRITE(3,39)
   39 FORMAT( "
     +STREAM 3")
      P=-1.1
      DO21 I=1,101
      P=P+1.1
      R(I)=P
      T(I)=R(I)*1.0E-09
      R(I)=T(I)*1.0E09
   21 CONTINUE
C G05BAF(0.X) SPECIFIES THE XTH STREAM OF THE RANDOM NUMBERS
      CALL G05BAF(0.3)
      DO50 I=1,101
C CALCULATE THE UNPERTURBED DECAY CURVE
      GAMMA(I)=0.07*EXP(-T(I)*6.0*5.815383E06)+
     +0.05*EXP(-T(I)*6.0*4.1564612E06)
C NOW PERTURB EACH OF THE 100 DATA POINTS USING A NORMAL PSEUDO RANDOM
C NUMBER GENERATOR G05ADF
      GAMMA(I)=GAMMA(I)+((1.74555E-03)*G05ADF(Y))
   50 CONTINUE
C READ IN THE VALUES FOR THE LOWER LIMITS FOR THE INITIAL GUESSES OF THE
C A/B, A+, A- (X100), THE LOWER AND UPPER LIMITS FOR THE COMPUTER ESTIMATES
C THE COORDINATES OF THE A/B VALUES AND THEN THE COORDINATES OF THE B/C
C FOR THE R-CURVE TO WHICH THESE ESTIMATES ARE CONSTRAINED
      READ(2,*)XX1,XX2,XX3,BBL1,BBL2,BBL3,BBU1,BBU2,BBU3,
     +AA1,AA2,AA3,AA4,AA5,AA6,AD1,AD2,AD3,AD4,AD5,AD6
      AA(1)=AA1
      AA(2)=AA2
      AA(3)=AA3
      AA(4)=AA4
      AA(5)=AA5
      AA(6)=AA6
      AD(1)=AD1
      AD(2)=AD2
      AD(3)=AD3
      AD(4)=AD4
      AD(5)=AD5
```

```
      AD(6)=AD6
      N=3
      IBOUND=0
      Q1=1.0
      DO10 I=1,3
      Z=G05AAF(X)
      X(1)=XX1+0.2*Z
      X(2)=XX2+2.0*Z
      X(3)=XX3+2.0*Z
      BL(1)=BBL1
      BL(2)=BBL2
      BL(3)=BBL3
      BU(1)=BBU1
      BU(2)=BBU2
      BU(3)=BBU3
      LIW=5
      LW=39
      IFAIL=1
      CALL E04JAF(N,IBOUND,BL,BU,X,F,IW,LIW,W,LW,IFAIL)
      IF(IFAIL.NE.0)WRITE(3,100)IFAIL
      IF(IFAIL.EQ.1)GOTO 20
  100 FORMAT("ERROR EXIT TYPE",I3,"SEE ROUTINE MANUAL")
      X(2)=X(2)*.01
      X(3)=X(3)*.01
      WRITE(3,110)F
      WRITE(3,120)(X(1),X(2),X(3))
  110 FORMAT( " FUNCTION VALUE ON EXIT IS",F15.12)
  120 FORMAT( " A/B= ",F8.5,"   A+=",F15.12,
     +"   A-=",F15.12)
      IF(Q1.LE.F)GOTO 30
      Q1=F
      Q2=X(1)
      Q3=X(2)
      Q4=X(3)
   30 CONTINUE
      WRITE(3,130)
  130 FORMAT( " ")
      WRITE(3,140)
  140 FORMAT( " ")
   10 CONTINUE
      WRITE(3,150)Q1
  150 FORMAT( " BEST LEAST SQUARES VALUE = ",F15.12)
      WRITE(3,160)Q2
  160 FORMAT( "                         A / B = ",F8.5)
      WRITE(3,170)Q3
  170 FORMAT( "                         B / C = ",F8.5)
      WRITE(3,180)Q3
  180 FORMAT( "                            A+ = ",F7.4)
      WRITE(3,190)Q4
  190 FORMAT( "                            A- = ",F7.4)
   20 STOP
      END
```

```
C
C
C SUBROUTINE FOR CALCULATING THE SUM OF THE SQUARES OF THE RESIDUALS FOR
C CURRENT ESTIMATES OF A/B, A+ AND A-
C KB = BOLTZMANNS CONSTANT, NA = AVOGADROS NUMBER
C
      SUBROUTINE FUNCT1(N,XC,FC)
      COMMON/PARAM/GAMMA(101),T(101),A,C,D,NN,AA(6),AD(6)
      EXTERNAL FUN
      REAL Q,FC
      INTEGER N
      DIMENSION ALPHA(9)
      REAL XC(N)
      REAL X2,X3
      REAL THPLUS,THMNUS,TEMP,ETA,M,O,P,KB,NA,MW
      NN=0
      A=XC(1)
      NM=6
      IEXIT=0
C CALL LIBRARY ROUTINE FOR THE CUBIC POLYNOMIAL FIT TO THE R-CURVE POINTS
C A LISTING OF THIS IS GIVEN BELOW
      CALL E01LF1(NM,AA,AD,A,D,IEXIT)
      C=1.0/D
      B=1.0
      DO45 K=1,9
      AZ=0.0
      BZ=1000000
      NN=NN+1
      MAXDIV=50
      EPS=1.0E-08
      ACC=0.0
      IFAIL=0
      CALL D01AGF(AZ,BZ,FUN,MAXDIV,EPS,ACC,ANS,ERROR,NOFUN,IFAIL)
      ALPHA(NN)=ANS
   45 CONTINUE
      S=(1.0/(A*B*C))*((4.0/15.0)*((ALPHA(7)+ALPHA(8)
     + +ALPHA(9))/(ALPHA(8)*ALPHA(9)+ALPHA(9)*ALPHA
     + (7)+ALPHA(7)*ALPHA(8)))+(1.0/5.0)*(((ALPHA(2)
     + +ALPHA(3))/(ALPHA(4)*(B*B*ALPHA(2)+C*C*ALPHA(3)
     + )))+((ALPHA(3)+ALPHA(1))/(ALPHA(5)*(C*C*ALPHA(3)
     + +A*A*ALPHA(1))))+((ALPHA(1)+ALPHA(2))/(ALPHA(6)
     + *(A*A*ALPHA(1)+B*B*ALPHA(2))))))
      M=(B*B+C*C)/(B*B*ALPHA(2)+C*C*ALPHA(3))
      O=(C*C+A*A)/(C*C*ALPHA(3)+A*A*ALPHA(1))
      P=(A*A+B*B)/(A*A*ALPHA(1)+B*B*ALPHA(2))
      Z=((A*B*C)/(12.0))*((((1.0/M)+(1.0/O)+(1.0/P
     + ))-(((1.0/M**2.0)+(1.0/O**2.0)+(1.0/P**2.0))-
     + ((1.0/(M*O))+(1.0/(O*P))+(1.0/(P*M
     + ))))**0.5))
      U=((A*B*C)/(12.0))*((((1.0/M)+(1.0/O)+(1.0/P
     + ))+(((1.0/M**2.0)+(1.0/O**2.0)+(1.0/P**2.0))-
     + ((1.0/(M*O))+(1.0/(O*P))+(1.0/(P*M
     + ))))**0.5))
      V=6.0*U*S
      W=6.0*Z*S
C     ENTER INTRINSIC VISCOSITY
      ETA=2.746
C     ENTER TEMPERATURE
      TEMP=293.0
C     ENTER MOLECULAR WEIGHT
      MW=71744.0
      KB=1.38046E-16
      NA=6.0248E23
      THPLUS=(NA*KB*100.0/6.0)*(TEMP/(ETA*MW))*V
      THMNUS=(NA*KB*100.0/6.0)*(TEMP/(ETA*MW))*W
      X2=XC(2)
      X3=XC(3)
      FC=0.0
      DO75 I=1,101
      Q=(GAMMA(I)-(0.01*X2*EXP(-6.0*THPLUS*T(I))+0.01*X3*EXP
     + (-6.0*THMNUS*T(I))))**2.0
      FC=FC+Q
   75 CONTINUE
      RETURN
      END
```

```
C LEICESTER UNIVERSITY COMPUTER LIBRARY SUBROUTINE FOR A CUBIC
C POLYNOMIAL FIT TO A SET OF POINTS (K. BRODLIE)
C
      SUBROUTINE E01LF1(N,AX,AY,X,Y,IEXIT)
      DIMENSION AX(N),AY(N)
C  CHECK DATA POINTS ARE MONOTONICALLY INCREASING
      IEXIT=1
      DO 5 I=2,N
      IF(AX(I).LE.AX(I-1))RETURN
    5 CONTINUE
C  CHECK THAT X IS A VALID POINT
      IEXIT=2
      IF((AX(1)-X)*(AX(N)-X).GT.0)RETURN
C  LOCATE INTERVAL IN WHICH X LIES -
C             AX(J-1).LT.X.LE.AX(J)
      IEXIT=0
      Y=AY(1)
      IF(X.EQ.AX(1))RETURN
      DO 10 I=2,N
      J=I
      IF(X.LE.AX(I))GOTO 20
   10 CONTINUE
   20 CONTINUE
      Y=AY(J)
      IF(X.EQ.AX(J))RETURN
C  ESTIMATE SLOPE AT AX(J-1)
      CALL E011A(N,AX,AY,J-1,G1)
C  ESTIMATE SLOPE AT AX(J)
      CALL E011A(N,AX,AY,J,G2)
C  CONSTRUCT INTERPOLATING CUBIC POLYNOMIAL IN INTERVAL
      D=AY(J-1)
      C=G1
      H=AX(J)-AX(J-1)
      S=(AY(J)-AY(J-1))/H
      B=(3.0*S-2.0*G1-G2)/H
      A=(G1+G2-2.0*S)/H/H
C  EVALUATE POLYNOMIAL AT POINT
      H=X-AX(J-1)
      Y=((A*H+B)*H+C)*H+D
      RETURN
      END
      SUBROUTINE E011A(N,AX,AY,J,G)
      DIMENSION AX(N),AY(N)
C  CALCULATE SLOPES ON EITHER SIDE OF DATA POINT
      JM1=J-1
      JP1=J+1
      IF(J.NE.1)GO TO 20
C  END-POINT IS DIFFERENT
      H1=AX(2)-AX(1)
      S1=2.0*(AY(2)-AY(1))/H1-(AY(3)-AY(2))/(AX(3)-AX(2))
      GO TO 30
   20 CONTINUE
      H1=AX(J)-AX(J-1)
      S1=(AY(J)-AY(JM1))/H1
   30 CONTINUE
      IF(J.NE.N)GO TO 40
C  END-POINT IS DIFFERENT
      H2=AX(N)-AX(N-1)
      S2=2.0*(AY(N)-AY(N-1))/H2-(AY(N-1)-AY(N-2))/(AX(N-1)-AX(N-2))
      GO TO 50
   40 CONTINUE
      H2=AX(JP1)-AX(J)
      S2=(AY(JP1)-AY(J))/H2
   50 CONTINUE
      S12=S1*S2
C  IF DATA IS NOT MONOTONIC SET SLOPE TO ZERO
      IF(S12.GT.0.0)GO TO 10
      G=0.0
      RETURN
   10 CONTINUE
C  WHEN DATA IS MONOTONIC USE WEIGHTED AVERAGE OF NORMAL SLOPES
      T1=2.0*H1+H2
      T2=H1+2.0*H2
      T=(T1*S2+T2*S1)/(3.0*(H1+H2))
      G=S12/T
      RETURN
      END
```

```
C
C
C SUBROUTINE FOR CALCULATING THE ELLIPTIC INTEGRALS USED FOR DETERMINING
C THE S VALUE FROM THE CURRENT GUESS FOR A/B
C
      REAL FUNCTION FUN(Y)
      COMMON/PARAM/GAMMA(101),T(101),A,C,D,NN,AA(6),AD(6)
      B=1.0
      GOTO(10,20,30,40,50,60,70,80,90),NN
   10 FUN=1.0/((A*A+Y)**1.5*(B*B+Y)**0.5*(C*C+Y)**0.5)
      RETURN
   20 FUN=1.0/((A*A+Y)**0.5*(B*B+Y)**1.5*(C*C+Y)**0.5)
      RETURN
   30 FUN=1.0/((A*A+Y)**0.5*(B*B+Y)**0.5*(C*C+Y)**1.5)
      RETURN
   40 FUN=1.0/((A*A+Y)**0.5*(B*B+Y)**1.5*(C*C+Y)**1.5)
      RETURN
   50 FUN=1.0/((A*A+Y)**1.5*(B*B+Y)**0.5*(C*C+Y)**1.5)
      RETURN
   60 FUN=1.0/((A*A+Y)**1.5*(B*B+Y)**1.5*(C*C+Y)**0.5)
      RETURN
   70 FUN=Y/((A*A+Y)**0.5*(B*B+Y)**1.5*(C*C+Y)**1.5)
      RETURN
   80 FUN=Y/((A*A+Y)**1.5*(B*B+Y)**0.5*(C*C+Y)**1.5)
      RETURN
   90 FUN=Y/((A*A+Y)**1.5*(B*B+Y)**1.5*(C*C+Y)**0.5)
      RETURN
      END
```

<u>Results</u>:

```
PROTEIN 1,   0.1 DEG. ABSOLUTE ERROR
                                                        110NS,  100PTS
                                                        STREAM3

FUNCTION VALUE ON EXIT IS   .000399962998
A/B=  1.48309   A+=   .070458728408   A-=   .048831535604


FUNCTION VALUE ON EXIT IS   .000399962998
A/B=  1.48309   A+=   .070458845275   A-=   .048831534073


FUNCTION VALUE ON EXIT IS   .00399962998
A/B=  1.48309   A+=   .070458881237   A-=   .048831534081


BEST LEAST SQUARES VALUE =   .000399962998
                   A / B =   1.48309
                      A+ =   .0707
                      A- =   .0488
```