Supplementary Programme 1. “Intersection”

```
!     INTERSECTION AND ERROR
!
      REAL DH(2),SDH(2),DS(2),SDS(2),DV(2),SDV(2),K(2),SK(2)
      CHARACTER*1 YN,RET
      DATA RET/''/,R/8.31451/
      OPEN(5,FILE='EXAMPLE.DAT')
      OPEN(6,FILE='THERMOPT.RST')
!
      WRITE(6,5900)
5900  FORMAT('THERMODINAMIC DATA')
!
      READ(5,5000)
     *      (DH(I),SDH(I),DS(I),SDS(I),DV(I),SDV(I),K(I),SK(I),I=1,2)
5000  FORMAT(8F10.0)
      WRITE(6,6000)
     * (I,DH(I),SDH(I),DS(I),SDS(I),DV(I),SDV(I),K(I),SK(I),I=1,2)
6000  FORMAT('REACTION',5X,'dH',18X,'dS',18X,'dV',18X,'K'/
     * (I2,7X,2F10.0,6F10.4))
      PP=DH(2)*(DS(1)-R*ALOG(K(1)))-DH(1)*(DS(2)-R*ALOG(K(2)))
      XX=DV(2)*(DS(1)-R*ALOG(K(1)))-DV(1)*(DS(2)-R*ALOG(K(2)))
      TT=DV(2)*DH(1)-DV(1)*DH(2)
      T0=TT/XX-273.16
      P0=PP/XX
      DPDH1=-(DS(2)-R*ALOG(K(2)))/XX
      DPDH2=(DS(1)-R*ALOG(K(1)))/XX
      DPDS1=-PP
      DPDS1=DPDS1*(-DV(2))/XX/XX+DH(2)/XX
      DPDS2=-(DH(2)*(DS(1)-R*ALOG(K(1)))+DH(1)*(DS(2)-R*ALOG(K(2))))
      DPDS2=DPDS2*DV(1)/XX/XX-DH(1)/XX
      DPDV1=PP*(DS(2)-R*ALOG(K(2)))/XX/XX
      DPDV2=PP*(DS(1)-R*ALOG(K(1)))/XX/XX
      DPDK1=DH(2)*(-R)/K(1)/XX-PP/XX/XX*DV(2)*(-R)/K(1)
      DPDK2=-DH(2)*(-R)/K(2)/XX-PP/XX/XX*DV(1)*R/K(2)
      SIGMAP=       (DPDH1*SDH(1))**2+(DPDH2*SDH(2))**2
      SIGMAP=SIGMAP+(DPDS1*SDS(1))**2+(DPDS2*SDS(2))**2
      SIGMAP=SIGMAP+(DPDV1*SDV(1))**2+(DPDV2*SDV(2))**2
      SIGMAP=SIGMAP+(DPDK1*SK(1))**2+(DPDK2*SK(2))**2
      SIGMAP=SQRT(SIGMAP)
!
      DTDH1=DV(2)/XX
      DTDH2=-DV(1)/XX
      DTDS1=TT/XX/XX*(-DV(2))
      DTDS2=TT/XX/XX*(+DV(1))
      DTDV1=-DH(2)/XX+TT/XX/XX*DS(2)
      DTDV2=DH(1)/XX-TT/XX/XX*DS(1)
      DTDK1=TT/XX/XX*DV(2)*R/K(1)
      DTDK2=-TT/XX/XX*DV(1)*R/K(2)
!
      SIGMAT=       (DTDH1*SDH(1))**2+(PTDH2*SDH(2))**2
      SIGMAT=SIGMAT+(DTDS1*SDS(1))**2+(DTDS2*SDS(2))**2
      SIGMAT=SIGMAT+(DTDV1*SDV(1))**2+(DTDV2*SDV(2))**2
      SIGMAT=SIGMAT+(DTDK1*SK(1))**2+(DTDK2*SK(2))**2
      SIGMAT=SQRT(SIGMAT)
!
      WRITE(*,620) P0,SIGMAP
      WRITE(6,620) P0,SIGMAP
620   FORMAT('P(KBAR)=',F6.1,' +-',F6.1)
      WRITE(*,630) T0,SIGMAT
      WRITE(6,630) T0,SIGMAT
630   FORMAT('T(C)=   ',F6.0,' +-',F6.0)
      STOP
      END
```

EXAMPLE.DAT

```
-19832.   40.       -9.037    0.037     -99.79    0.79      2.18      0.18
-69203.   90.       -8.452    0.052     -1.15     0.15      703.      44.
```

TERMOPT.RST

```
THERMODINAMIC DATA
REACTION     dH                 dS                 dV                 K
 1          -19832.       40.   -9.0370    0.0370  -99.7900    0.7900    2.1800    0.1800
 2          -69203.       90.   -8.4520    0.0520   -1.1500    0.1500  703.0000   44.0000
P(KBAR)=  27.9 +-   9.4
T(C)   =  826. +-   12.
```

Supplementary Programme 2. “Weight-free *P–T* estimate”

```
C     Weight-free P-T Estimate
C     F=P-AT-B
C
      DOUBLE PRECISION F(3,100),A(3,3),UNKN(2),X(100),Y(100),SX(100)
      DOUBLE PRECISION SY(100),B(2,2),VAR(2),FL(100),FX(100),FY(100)
      DOUBLE PRECISION SIGMA(2),CORR(2),PSEC(100),TSEC(100)
      DOUBLE PRECISION SPSEC(100),STSEC(100)
      DOUBLE PRECISION S,DS,DF,PP,TT,SP,ST,SP1,SP2,SP3,PMEAN,TMEAN,XT,XP
      DIMENSION  L(2),M(2)
      DATA N/3/,NM1/2/,ERROR/1.0D-06/,UNKN/66.667,73.333/
!
      OPEN(5,FILE='PTdata.DAT')
      OPEN(6,FILE='PT_estimateNWT.RST')
!
      READ(5,5) NN     !   NN: NUMBER OF DATA SETS
5     FORMAT(I5)
      WRITE(6,6)
      WRITE(*,6)
6     FORMAT(1X,'No',4X,'A',9X,'+-',8X,'B',9X,'+-')
      DO 10 I=1,NN
          READ(5,500) X(I),SX(I),Y(I),SY(I)
500       FORMAT(4F10.0)
          WRITE(6,600) I,X(I),Y(I)
          WRITE(*,600) I,X(I),Y(I)
600       FORMAT(I3,F10.4,10x,F10.4)
10    CONTINUE
      WRITE(*,60)
      WRITE(6,60)
60    FORMAT(/' NCY',3X,'P (kbar)',7X,'T (C)',10X,'Delta P',8X,'Delta T'
     *)
      DO 1000 NCY=1,50
          DO 100 I=1,NN
              F(3,I)=UNKN(1)-X(I)*UNKN(2)-Y(I)
              F(2,I)=-X(I)
              F(1,I)=1.
              FX(I)=-UNKN(2)
              FY(I)=-1.
                  FL(I)=1.
100       CONTINUE
102    CONTINUE
       DO 50 I=1,N
        DO 40 J=1,N
         A(I,J)=0.
40      CONTINUE
50     CONTINUE
         DO 63 I=1,NN
            DO 62 J=1,N
              DO 61 K=1,N
                  A(J,K)=A(J,K)+F(J,I)*F(K,I)/FL(I)
61        CONTINUE
62     CONTINUE
63       CONTINUE
        DO 65 I=1,NM1
         DO 64 J=1,NM1
          B(I,J)=A(I,J)
64       CONTINUE
65      CONTINUE
      CALL GOJIRA(B,D,NM1,L,M,NM1)
      DO 76 I=1,NM1
       DO 74 J=1,NM1
        A(I,J)=B(I,J)
74     CONTINUE
76    CONTINUE
      DO 80 I=1,NM1
         CORR(I)=0.
80    CONTINUE
      DO 84 I=1,NM1
         DO 82 J=1,NM1
             CORR(I)=CORR(I)+A(I,J)*A(N,J)
82       CONTINUE
84    CONTINUE
         DS=0.
          DO 85 I=1,NM1
           DS=DS+A(N,I)*CORR(I)
85        CONTINUE
         S=A(N,N)-DS
         DO 86 I=1,NM1
          UNKN(I)=UNKN(I)-CORR(I)
86       CONTINUE
        WRITE(6,640) NCY,(UNKN(I),I=1,NM1),(CORR(I),I=1,NM1)
```

```
        WRITE(*,640) NCY,(UNKN(I),I=1,NM1),(CORR(I),I=1,NM1)
640     FORMAT(I3,6D15.5)
       DO 88 I=1,NM1
          IF(DABS(CORR(I)).GE.ERROR) GO TO 1000
88     CONTINUE
          GO TO 1500
1000  CONTINUE
1500  CONTINUE
      DF=S/FLOAT(NN-NM1)
      DO 90 I=1,NM1
         VAR(I)=DF*A(I,I)
         SIGMA(I)=DSQRT(VAR(I))
90    CONTINUE
      WRITE(*,6000) (UNKN(I),SIGMA(I),I=1,NM1)
      WRITE(6,6000) (UNKN(I),SIGMA(I),I=1,NM1)
6000  FORMAT(/'Result of Least Squares'/
     *      'P (kbar) =',F8.2,'  +-',F8.2/'T (C)    =',F8.1,'  +-',F8.1)
!
!     L-coefficient
!
      WRITE(*,7)
      WRITE(6,7)
7     FORMAT(/1X,'No',4X,'A',9X,'+-',8X,'B',9X,'+-',8X,'1/L')

      DO 190 I=1,NN
          WRITE(*,6150) I,X(I),Y(I),1./FL(I)
          WRITE(6,6150) I,X(I),Y(I),1./FL(I)
6150      FORMAT(I3,F10.4,10X,F10.4,10X,D15.5)
190   CONTINUE
!
!     INTERSECTION
!
      WRITE(*,6170)
      WRITE(6,6170)
6170  FORMAT(/'Intersection'/11X,'P (kbar)',15X,'T (C)')
      NSEC=0
      DO 200 I=1,NN
          DO 180 J=1,NN
              IF(J.LE.I) GO TO 180
              NSEC=NSEC+1
              TT=-(Y(I)-Y(J))/(X(I)-X(J))
              PP=(X(I)*Y(J)-Y(I)*X(J))/(X(I)-X(J))
              PSEC(NSEC)=PP; TSEC(NSEC)=TT
                  WRITE(*,6160) I,J,PP,TT
                  WRITE(6,6160) I,J,PP,TT
6160              FORMAT(2I3,F10.2,13X,F10.1)
                  SPSEC(NSEC)=-1.; STSEC(NSEC)=-1.
180       CONTINUE
200   CONTINUE
!
      PMEAN=0.; TMEAN=0.; SP=0.; ST=0.; XP=0.; XT=0.
      DO 300 I=1,NSEC
          PMEAN=PMEAN+PSEC(I)
          TMEAN=TMEAN+TSEC(I)
          XP=REAL(I)
          XT=REAL(I)
 300   CONTINUE
          PMEAN=PMEAN/XP
          TMEAN=TMEAN/XT
       SP=0.; ST=0.; XP=0.; XT=0.
      DO 310 I=1,NSEC
         SP=SP+(PMEAN-PSEC(I))**2
         ST=ST+(TMEAN-TSEC(I))**2
310   CONTINUE
          SP=SQRT(SP/REAL(NSEC))
          ST=SQRT(ST/REAL(NSEC))
          WRITE(6,6300)PMEAN,SP,TMEAN,ST
          WRITE(*,6300)PMEAN,SP,TMEAN,ST
6300      FORMAT(/'Average'/'P (kbar) =',F10.2,' +-',F10.2/
     *      'T (C)    =',F10.1,' +-',F10.1)
      STOP
      END
C-------------------------------------------------------------------------------
      SUBROUTINE GOJIRA(A,D,N,L,M,IA)
C-------------------------------------------------------------------------------
      DOUBLE PRECISION A(N,IA),D,BA,HOLD
      DIMENSION L(N),M(N)
      D=1.
      DO 80 K=1,N
      L(K)=K
      M(K)=K
      BA=A(K,K)
      DO 20 J=K,N
```

```
      DO 20 I=K,N
      IF(DABS(BA)-DABS(A(I,J))) 15,20,20
   15 BA=A(I,J)
      L(K)=I
      M(K)=J
   20 CONTINUE
      J=L(K)
      IF(J-K) 35,35,25
   25 DO 30 I=1,N
      HOLD=A(K,I)
      A(K,I)=A(J,I)
   30 A(J,I)=HOLD
      D=-D
   35 I=M(K)
      IF(I-K) 45,45,38
   38 DO 40 J=1,N
      HOLD=A(J,K)
      A(J,K)=A(J,I)
   40 A(J,I)=HOLD
      D=-D
   45 IF(BA) 48,46,48
   46 D=0.
      RETURN
   48 DO 55 I=1,N
      IF(I-K) 50,55,50
   50 A(I,K)=A(I,K)/(-BA)
   55 CONTINUE
      DO 65 I=1,N
      HOLD=A(I,K)
      DO 65 J=1,N
      IF(I-K) 60,65,60
   60 IF(J-K) 62,65,62
   62 A(I,J)=HOLD*A(K,J)+A(I,J)
   65 CONTINUE
      DO 75 J=1,N
      IF(J-K) 70,75,70
   70 A(K,J)=A(K,J)/BA
   75 CONTINUE
      D=D*BA
      A(K,K)=1./BA
   80 CONTINUE
      K=N
  100 K=K-1
      IF(K) 150,150,105
  105 I=L(K)
      IF(I-K) 120,120,108
  108 DO 110 J=1,N
      HOLD=A(J,K)
      A(J,K)=A(J,I)
  110 A(J,I)=HOLD
  120 J=M(K)
      IF(J-K) 100,100,125
  125 DO 130 I=1,N
      HOLD=A(K,I)
      A(K,I)=A(J,I)
  130 A(J,I)=HOLD
      GO TO 100
  150 RETURN
      END
```

Results of weight-free least-squares fitting

$n = 3$

```
 No    A          +-         B          +-
  1    0.0300              -18.0000          a
  2    0.0150               -7.0000          b
  3    0.0600              -46.0000          c

NCY   P (kbar)        T (C)           Delta P         Delta T
  1    0.70000D+01    0.87619D+03    0.59667D+02   -0.80286D+03
  2    0.70000D+01    0.87619D+03    0.37007D-16   -0.98017D-12

Result of Least Squares
P (kbar) =    7.00  +-    1.96
T (C)    =   876.2  +-    49.5

Intersection
          P (kbar)               T (C)
a-b       4.00                  733.3
a-c      10.00                  933.3
b-c       6.00                  866.7

Average
P (kbar) =    6.67 +-    2.49
T (C)    =   844.4 +-    83.1
```

$n = 4$

```
 No    A          +-         B          +-
  1    0.0300              -18.0000          a
  2    0.0150               -7.0000          b
  3    0.0600              -46.0000          c
  4   -0.1500              130.0000          d

NCY   P (kbar)        T (C)           Delta P         Delta T
  1    0.53853D+01    0.83242D+03    0.61282D+02   -0.75909D+03
  2    0.53853D+01    0.83242D+03    0.27690D-14   -0.16719D-12

Result of Least Squares
P (kbar) =    5.39  +-    0.77
T (C)    =   832.4  +-     9.3

Intersection
          P (kbar)               T (C)
a-b       4.00                  733.3
a-c      10.00                  933.3
a-d       6.67                  822.2
b-c       6.00                  866.7
b-d       5.45                  830.3
c-d       4.29                  838.1

Average
P (kbar) =    6.07 +-    1.99
T (C)    =   837.3 +-    59.4
```

$n = 5$

```
 No    A          +-         B          +-
  1    0.0300              -18.0000          a
  2    0.0150               -7.0000          b
  3    0.0600              -46.0000          c
  4   -0.1500              130.0000          d
  5    0.1500             -127.5000          e

NCY   P (kbar)        T (C)           Delta P         Delta T
  1    0.42382D+01    0.85420D+03    0.62429D+02   -0.78087D+03
  2    0.42382D+01    0.85420D+03   -0.34156D-14   -0.27307D-13

Result of Least Squares
P (kbar) =    4.24  +-    1.53
T (C)    =   854.2  +-    15.4

Intersection
          P (kbar)               T (C)
a-b       4.00                  733.3
a-c      10.00                  933.3
a-d       6.67                  822.2
a-e       9.38                  912.5
```

b-c	6.00	866.7
b-d	5.45	830.3
b-e	6.39	892.6
c-d	4.29	838.1
c-e	8.33	905.6
d-e	1.25	858.3

Average
P (kbar) = 6.18 +- 2.51
T (C) = 859.3 +- 54.9

Supplementary Programme 3. “Weighted *P–T* estimate”

```
C     Weighted P-T Estimate
C     F=P-AT-B
C
      DOUBLE PRECISION F(3,100),A(3,3),UNKN(2),X(100),Y(100),SX(100)
      DOUBLE PRECISION SY(100),B(2,2),VAR(2),FL(100),FX(100),FY(100)
      DOUBLE PRECISION SIGMA(2),CORR(2),PSEC(100),TSEC(100)
      DOUBLE PRECISION SPSEC(100),STSEC(100)
      DOUBLE PRECISION S,DS,DF,PP,TT,SP,ST,SP1,SP2,SP3,PMEAN,TMEAN,XT,XP
      DIMENSION  L(2),M(2)
      DATA N/3/,NM1/2/,ERROR/1.0D-06/,UNKN/66.667,73.333/
!
      OPEN(5,FILE='PTDATA.DAT')
      OPEN(6,FILE='PT_ESTIMATEWT.RST')
!
      READ(5,5) NN     !   NN: NUMBER OF DATA SETS
5     FORMAT(I5)
      WRITE(6,6)
      WRITE(*,6)
6     FORMAT(1X,'No',4X,'A',9X,'+-',8X,'B',9X,'+-')
      DO 10 I=1,NN
          READ(5,500) X(I),SX(I),Y(I),SY(I)
500       FORMAT(4F10.0)
         WRITE(6,600) I,X(I),SX(I),Y(I),SY(I)
          WRITE(*,600) I,X(I),SX(I),Y(I),SY(I)
600       FORMAT(I3,4F10.4)
10    CONTINUE
      WRITE(*,60)
      WRITE(6,60)
60    FORMAT(/' NCY',3X,'P (kbar)',7X,'T (C)',10X,'Delta P',8X,'Delta T'
     *)
      DO 1000 NCY=1,50
          DO 100 I=1,NN
              F(3,I)=UNKN(1)-X(I)*UNKN(2)-Y(I)
              F(2,I)=-X(I)
              F(1,I)=1.
              FX(I)=-UNKN(2)
              FY(I)=-1.
              FL(I)=(FX(I)*SX(I))**2+(FY(I)*SY(I))**2
100       CONTINUE
102    CONTINUE
       DO 50 I=1,N
        DO 40 J=1,N
         A(I,J)=0.
40       CONTINUE
50     CONTINUE
         DO 63 I=1,NN
            DO 62 J=1,N
              DO 61 K=1,N
                  A(J,K)=A(J,K)+F(J,I)*F(K,I)/FL(I)
61          CONTINUE
62     CONTINUE
63       CONTINUE
        DO 65 I=1,NM1
         DO 64 J=1,NM1
          B(I,J)=A(I,J)
64       CONTINUE
65      CONTINUE
      CALL GOJIRA(B,D,NM1,L,M,NM1)
      DO 76 I=1,NM1
       DO 74 J=1,NM1
        A(I,J)=B(I,J)
74     CONTINUE
76    CONTINUE
      DO 80 I=1,NM1
         CORR(I)=0.
80    CONTINUE
      DO 84 I=1,NM1
         DO 82 J=1,NM1
             CORR(I)=CORR(I)+A(I,J)*A(N,J)
82       CONTINUE
84    CONTINUE
         DS=0.
          DO 85 I=1,NM1
           DS=DS+A(N,I)*CORR(I)
85        CONTINUE
         S=A(N,N)-DS
         DO 86 I=1,NM1
          UNKN(I)=UNKN(I)-CORR(I)
86       CONTINUE
        WRITE(6,640) NCY,(UNKN(I),I=1,NM1),(CORR(I),I=1,NM1)
```

```
        WRITE(*,640) NCY,(UNKN(I),I=1,NM1),(CORR(I),I=1,NM1)
640     FORMAT(I3,6D15.5)
       DO 88 I=1,NM1
          IF(DABS(CORR(I)).GE.ERROR) GO TO 1000
88     CONTINUE
          GO TO 1500
1000   CONTINUE
1500   CONTINUE
       DF=S/FLOAT(NN-NM1)
       DO 90 I=1,NM1
          VAR(I)=DF*A(I,I)
          SIGMA(I)=DSQRT(VAR(I))
90     CONTINUE
       WRITE(*,6000) (UNKN(I),SIGMA(I),I=1,NM1)
       WRITE(6,6000) (UNKN(I),SIGMA(I),I=1,NM1)
6000   FORMAT(/'Result of Least Squares'/
     *      'P (kbar) =',F8.2,'  +-',F8.2/'T (C)    =',F8.1,'  +-',F8.1)
!
!      L-coefficient
!
       WRITE(*,7)
       WRITE(6,7)
7      FORMAT(/1X,'No',4X,'A',9X,'+-',8X,'B',9X,'+-',8X,'1/L',12X,'L')
!
       DO 190 I=1,NN
           WRITE(*,6150) I,X(I),SX(I),Y(I),SY(I),1./FL(I),FL(I)
           WRITE(6,6150) I,X(I),SX(I),Y(I),SY(I),1./FL(I),FL(I)
6150       FORMAT(I3,4F10.4,2D15.5)
190    CONTINUE
!
!      INTERSECTION
!
       WRITE(*,6170)
       WRITE(6,6170)
6170   FORMAT(/'Intersection'/11X,'P (kbar)',15X,'T (C)')
       NSEC=0
       DO 200 I=1,NN
           DO 180 J=1,NN
               IF(J.LE.I) GO TO 180
               NSEC=NSEC+1
               TT=-(Y(I)-Y(J))/(X(I)-X(J))
               PP=(X(I)*Y(J)-Y(I)*X(J))/(X(I)-X(J))
               PSEC(NSEC)=PP; TSEC(NSEC)=TT
             ST=(SX(I)*SX(I)+SX(J)*SX(J))/(X(I)-X(J))/(X(I)-X(J))
              ST=ST+(SY(I)*SY(I)+SY(J)*SY(J))/(Y(I)-Y(J))/(Y(I)-Y(J))
               ST=ABS(TT)*SQRT(ST)
              SP1=((X(I)*SY(J))**2+(X(J)*SY(I))**2)/(X(I)-X(J))**2
             SP2=(Y(J)-(X(I)*Y(J)-X(J)*Y(I))/(X(I)-X(J)))/(X(I)-X(J))
              SP2=SP2*SP2*SX(I)*SX(I)
               SP3=(-Y(I)+(X(J)*Y(I)-X(I)*Y(J))/(X(I)-X(J)))/(X(I)-X(J))
                 SP3=SP3*SP3*SX(J)*SX(J)
                 SP=SQRT(SP1+SP2+SP3)
                WRITE(*,6180) I,J,PP,SP,TT,ST
               WRITE(6,6180) I,J,PP,SP,TT,ST
6180           FORMAT(2I3,F10.2,' +-',F10.2,F10.1,' +-',F10.1)
             PSEC(NSEC)=PP; TSEC(NSEC)=TT; SPSEC(NSEC)=SP; STSEC(NSEC)=ST
180        CONTINUE
200    CONTINUE
!
       PMEAN=0.; TMEAN=0.; SP=0.; ST=0.; XP=0.; XT=0.
       DO 300 I=1,NSEC
               PMEAN=PMEAN+PSEC(I)/SPSEC(I)/SPSEC(I)
               TMEAN=TMEAN+TSEC(I)/STSEC(I)/STSEC(I)
               XP=XP+1./SPSEC(I)/SPSEC(I)
               XT=XT+1./STSEC(I)/STSEC(I)
 300    CONTINUE
             PMEAN=PMEAN/XP
             TMEAN=TMEAN/XT
       SP=0.; ST=0.; XP=0.; XT=0.
       DO 310 I=1,NSEC
               SP=SP+(PMEAN-PSEC(I))**2/SPSEC(I)/SPSEC(I)
               ST=ST+(TMEAN-TSEC(I))**2/STSEC(I)/STSEC(I)
               XP=XP+1./SPSEC(I)/SPSEC(I)
               XT=XT+1./STSEC(I)/STSEC(I)
310    CONTINUE
           SP=DSQRT(SP/XP/REAL(NSEC))
           ST=DSQRT(ST/XT/REAL(NSEC))
           WRITE(6,6300)PMEAN,SP,TMEAN,ST
           WRITE(*,6300)PMEAN,SP,TMEAN,ST
6300       FORMAT(/'Average'/'P (kbar) =',F10.2,' +-',F10.2/
     *      'T (C)    =',F10.1,' +-',F10.1)
       STOP
```

```
      END
C-------------------------------------------------------------------------------
      SUBROUTINE GOJIRA(A,D,N,L,M,IA)
C-------------------------------------------------------------------------------
      DOUBLE PRECISION A(N,IA),D,BA,HOLD
      DIMENSION L(N),M(N)
      D=1.
      DO 80 K=1,N
      L(K)=K
      M(K)=K
      BA=A(K,K)
      DO 20 J=K,N
      DO 20 I=K,N
      IF(DABS(BA)-DABS(A(I,J))) 15,20,20
   15 BA=A(I,J)
      L(K)=I
      M(K)=J
   20 CONTINUE
      J=L(K)
      IF(J-K) 35,35,25
   25 DO 30 I=1,N
      HOLD=A(K,I)
      A(K,I)=A(J,I)
   30 A(J,I)=HOLD
      D=-D
   35 I=M(K)
      IF(I-K) 45,45,38
   38 DO 40 J=1,N
      HOLD=A(J,K)
      A(J,K)=A(J,I)
   40 A(J,I)=HOLD
      D=-D
   45 IF(BA) 48,46,48
   46 D=0.
      RETURN
   48 DO 55 I=1,N
      IF(I-K) 50,55,50
   50 A(I,K)=A(I,K)/(-BA)
   55 CONTINUE
      DO 65 I=1,N
      HOLD=A(I,K)
      DO 65 J=1,N
      IF(I-K) 60,65,60
   60 IF(J-K) 62,65,62
   62 A(I,J)=HOLD*A(K,J)+A(I,J)
   65 CONTINUE
      DO 75 J=1,N
      IF(J-K) 70,75,70
   70 A(K,J)=A(K,J)/BA
   75 CONTINUE
      D=D*BA
      A(K,K)=1./BA
   80 CONTINUE
      K=N
  100 K=K-1
      IF(K) 150,150,105
  105 I=L(K)
      IF(I-K) 120,120,108
  108 DO 110 J=1,N
      HOLD=A(J,K)
      A(J,K)=A(J,I)
  110 A(J,I)=HOLD
  120 J=M(K)
      IF(J-K) 100,100,125
  125 DO 130 I=1,N
      HOLD=A(K,I)
      A(K,I)=A(J,I)
  130 A(J,I)=HOLD
      GO TO 100
  150 RETURN
      END
```

Reals of weighted least-squares fitting

$n = 3$

```
 No     A          +-         B          +-
  1     0.0300     0.0016   -18.0000     0.9004          a
  2     0.0150     0.0008    -7.0000     0.3503          b
  3     0.0600     0.0031   -46.0000     2.3031          c

NCY    P (kbar)        T (C)           Delta P         Delta T
  1     0.53448D+01     0.81541D+03     0.61322D+02    -0.74207D+03
  2     0.55769D+01     0.82727D+03    -0.23207D+00    -0.11864D+02
  3     0.55794D+01     0.82740D+03    -0.25157D-02    -0.12861D+00
  4     0.55794D+01     0.82740D+03    -0.26966D-04    -0.13785D-02
  5     0.55794D+01     0.82740D+03    -0.28902D-06    -0.14775D-04
  6     0.55794D+01     0.82740D+03    -0.30976D-08    -0.15835D-06

Result of Least Squares
P (kbar) =     5.58  +-     1.42
T (C)    =   827.4   +-    66.6

 No     A          +-         B          +-         1/L             L
  a     0.0300     0.0016   -18.0000     0.9004     0.40029D+00     0.24982D+01
  b     0.0150     0.0008    -7.0000     0.3503     0.19693D+01     0.50780D+00
  c     0.0600     0.0031   -46.0000     2.3031     0.85670D-01     0.11673D+02

Intersection
          P (kbar)                T (C)
a-b       4.00 +-       1.77     733.3 +-      106.7
a-c      10.00 +-       4.22     933.3 +-      134.8
b-c       6.00 +-       1.25     866.7 +-       79.6

Average
P (kbar) =     5.59 +-     0.81
T (C)    =   839.9 +-     42.0
```

$n = 4$

```
 No     A          +-         B          +-
  1     0.0300     0.0076   -18.0000     0.1529          a
  2     0.0150     0.0079    -7.0000     0.0090          b
  3     0.0600     0.0081   -46.0000     0.0135          c
  4    -0.1500     0.0083   130.0000     0.0180          d

NCY    P (kbar)        T (C)           Delta P         Delta T
  1     0.54077D+01     0.83239D+03     0.61259D+02    -0.75905D+03
  2     0.54380D+01     0.83221D+03    -0.30366D-01     0.17550D+00
  3     0.54380D+01     0.83221D+03     0.10515D-06    -0.60762D-06

Result of Least Squares
P (kbar) =     5.44  +-     0.78
T (C)    =   832.2   +-     9.8

 No     A          +-         B          +-         1/L             L
  a     0.0300     0.0076   -18.0000     0.1529     0.24723D-01     0.40449D+02
  b     0.0150     0.0079    -7.0000     0.0090     0.23312D-01     0.42896D+02
  c     0.0600     0.0081   -46.0000     0.0135     0.22062D-01     0.45328D+02
  d    -0.1500     0.0083   130.0000     0.0180     0.20859D-01     0.47942D+02

Intersection
          P (kbar)                T (C)
a-b       4.00 +-       9.24     733.3 +-      536.3
a-c      10.00 +-      14.43     933.3 +-      346.2
a-d       6.67 +-       5.26     822.2 +-       51.6
b-c       6.00 +-       9.10     866.7 +-      217.4
b-d       5.45 +-       5.94     830.3 +-       57.6
c-d       4.29 +-       5.12     838.1 +-       46.3

Average
P (kbar) =     5.53 +-     0.54
T (C)    =   831.9 +-      5.3
```

$n = 5$

```
 No     A          +-         B          +-
  1     0.0300     0.0076   -18.0000     0.1529          a
  2     0.0150     0.0079    -7.0000     0.0090          b
  3     0.0600     0.0081   -46.0000     0.0135          c
  4    -0.1500     0.0083   130.0000     0.0180          d
```

```
  5    0.1500    0.0085 -127.5000    0.0225         e

NCY   P (kbar)       T (C)          Delta P        Delta T
  1    0.43758D+01    0.85358D+03    0.62291D+02   -0.78025D+03
  2    0.44233D+01    0.85353D+03   -0.47492D-01    0.49242D-01
  3    0.44233D+01    0.85353D+03    0.43121D-07   -0.44851D-07

Result of Least Squares
P (kbar) =    4.42  +-    1.52
T (C)    =   853.5  +-    15.8

 No    A         +-        B         +-        1/L            L
  a    0.0300    0.0076  -18.0000    0.1529    0.23504D-01    0.42547D+02
  b    0.0150    0.0079   -7.0000    0.0090    0.22162D-01    0.45122D+02
  c    0.0600    0.0081  -46.0000    0.0135    0.20973D-01    0.47680D+02
  d   -0.1500    0.0083  130.0000    0.0180    0.19829D-01    0.50430D+02
  e    0.1500    0.0085 -127.5000    0.0225    0.18821D-01    0.53132D+02

Intersection
         P (kbar)              T (C)
a-b      4.00 +-      9.24     733.3 +-     536.3
a-c     10.00 +-     14.43     933.3 +-     346.2
a-d      6.67 +-      5.26     822.2 +-      51.6
a-e      9.38 +-      8.74     912.5 +-      87.1
b-c      6.00 +-      9.10     866.7 +-     217.4
b-d      5.45 +-      5.94     830.3 +-      57.6
b-e      6.39 +-      7.81     892.6 +-      76.8
c-d      4.29 +-      5.12     838.1 +-      46.3
c-e      8.33 +-     12.72     905.6 +-     118.4
d-e      1.25 +-      5.17     858.3 +-      34.1

Average
P (kbar) =    5.15 +-    0.75
T (C)    =   852.2 +-     8.3
```