NBS Technical Note 1224

Computer Software for the Acquisition and Treatment of Calorimetric Data

Steckler, Goldberg, Tewari, and Buckley

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Abstract

The computer software used for the acquisition and treatment of data from both heat-conduction microcalorimeters and an isoperibol solution calorimeter is described. For each program contained in this Technical Note there is documentation given which includes a listing of the program, comments, and an example of its use. The hardware used in the data acquisition is briefly described.

Keywords: chemical thermodynamics; computer software; data acquisition; enthalpy; heat-conduction microcalorimetry; isoperibol solution calorimetry; kinetics.

1. Introduction

The purpose of this Technical Note is to document the computer codes used for the acquisition and treatment of the data from both heat-conduction microcalorimeters and an isoperibol solution calorimeter. The descriptions of these calorimeters and the procedures used in their operation are contained in references [1,2]. Therefore, only a brief description of the hardware will be given herein.

Schematic diagrams showing the arrangements of the measuring apparatus is shown in figures 1 and 2. Note that, for the microcalorimeters, voltage is measured as a function of time for three separate calorimeters, while for the solution calorimeter, frequency is measured as a function of time. The microcomputer is an Apple IIe[1] with two floppy disk drives, a dot matrix printer, a color video monitor, and several cards. The cards in the microcomputer are: (1) clock, parallel, and serial interfaces, (2) an IEEE-488 communications bus controller [3], (3) 128 kbyte RAM memory, (4) 80 column display, and (5) a Z-80 microprocessor. All data recording electronics are IEEE-488 bus instruments. They are a digital voltmeter (Hewlett Packard 3456A), a digital counter (Hewlett Packard 5334A), and a scanner/ data acquisition/ control unit (Hewlett Packard 3457A).

For each program we have included a short description of its purpose, a listing with comments, and an example of its use. The programs written for data acquisition ("MCAL", "SOLNE", and "SOLNF") are written in Applesoft BASIC [4,5] and use the IEEE Bus command language [3].

---

[1]Certain commercial materials and apparatus are identified in this paper to specify adequately the experimental procedures. Such identification does not imply recommendation or endorsement by the National Bureau of Standards.

At the conclusion of an experiment, the voltages are written on a floppy disk using the Disk Operating System [4] on the Apple IIe. These data are then transferred to a CP/M disk using the utility program "APDOS" [6]. To save space on disks and to speed-up calculations, this ASCII data is then converted to a binary data file using the program "ASCBIN", a listing of which is given in this Technical Note. This program and the remainder of the calculations are done using GBASIC in the CP/M operating system [6,7]. In the examples, commands entered by the user have been underlined. Schematic overviews of the computational procedures are shown in figures 3 and 4.

Readers interested in obtaining computer readable copies of these programs should contact the authors.

References

[1] Steckler, D. K.; R. N. Goldberg; Y. B. Tewari; and T. J. Buckley, "High Precision Microcalorimetry: Apparatus, Procedures, and Biochemical Applications", J. Res. Nat. Bur. Stand., in press.

[2] Brunetti, A. P.; E. J. Prosen, and R. N. Goldberg, J. Res. Nat. Bur. Stand. 77A: 599 (1973).

[3] "Apple II IEEE-488 Interface User's Guide", Cupertino, CA: Apple Computer, Inc. (1981).

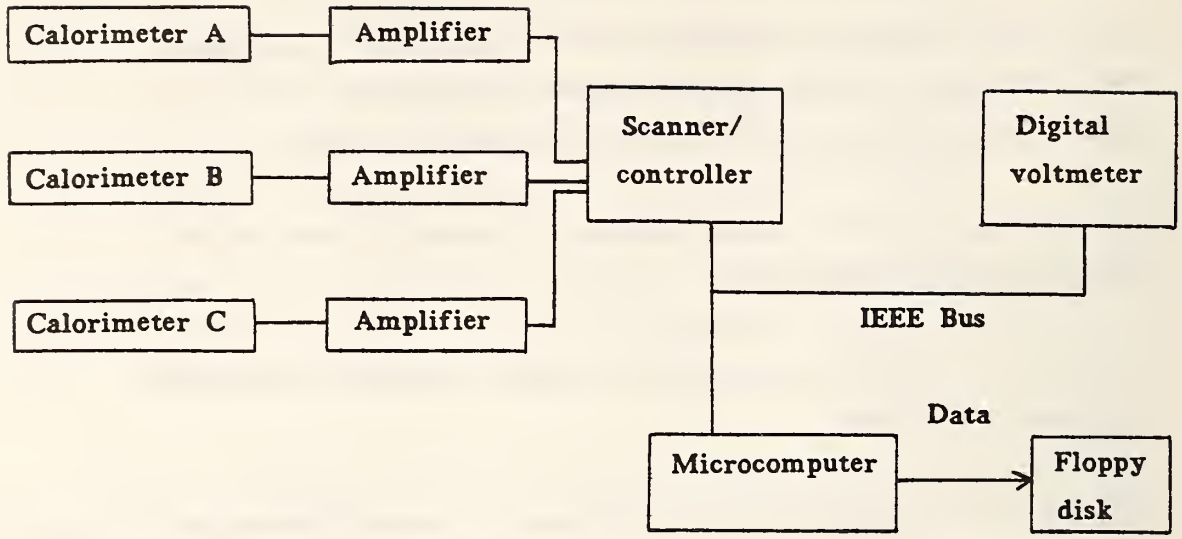
[4] "The DOS Manual: Apple II Disk Operating System", Cupertino, CA: Apple Computer, Inc. (1981).

[5] "Applesoft II Basic Programming Refernce Manual", Cupertino, CA: Apple Computer, Inc. (1978).

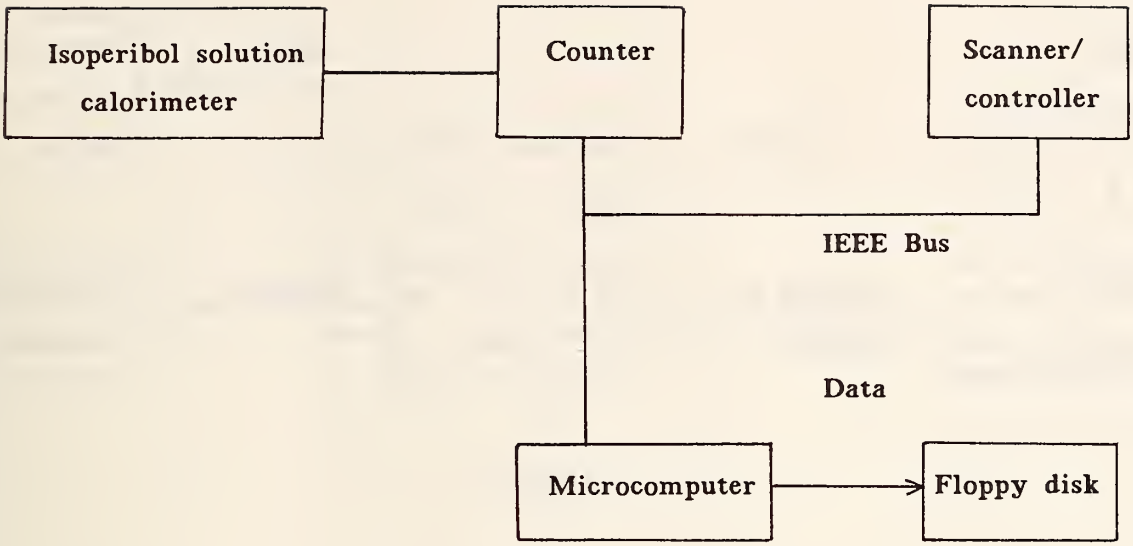
[6] "Microsoft Softcard System for Apple II", Bellevue, WA: Microsoft Corp. (1982).

[7] Hogan, T., "Osborne CP/M User Guide", Berkeley, CA: Osborne/McGraw Hill (1982).

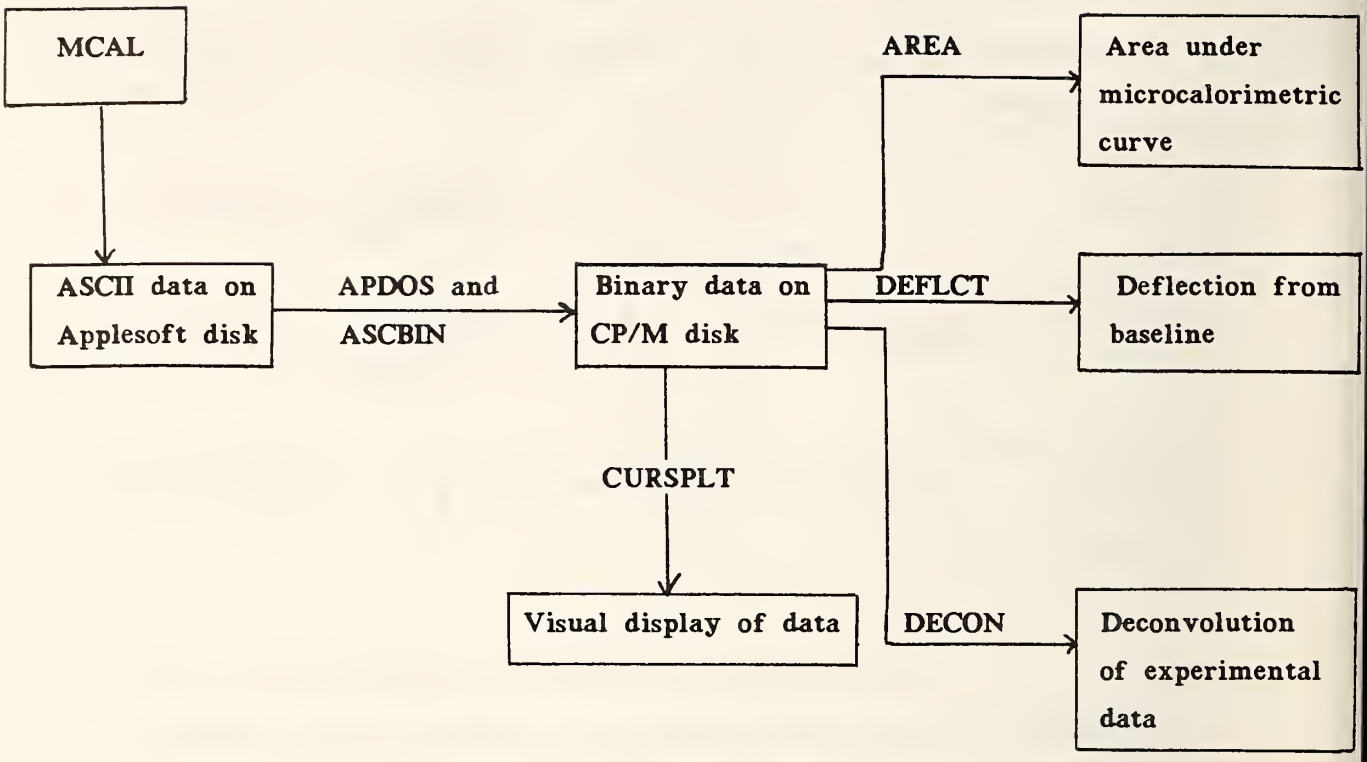
[8] Calvet, E., and H. Prat, "Recent Progress in Microcalorimetry", edited and translated from the French by H. A. Skinner, New York: The MacMillan Company (1963).



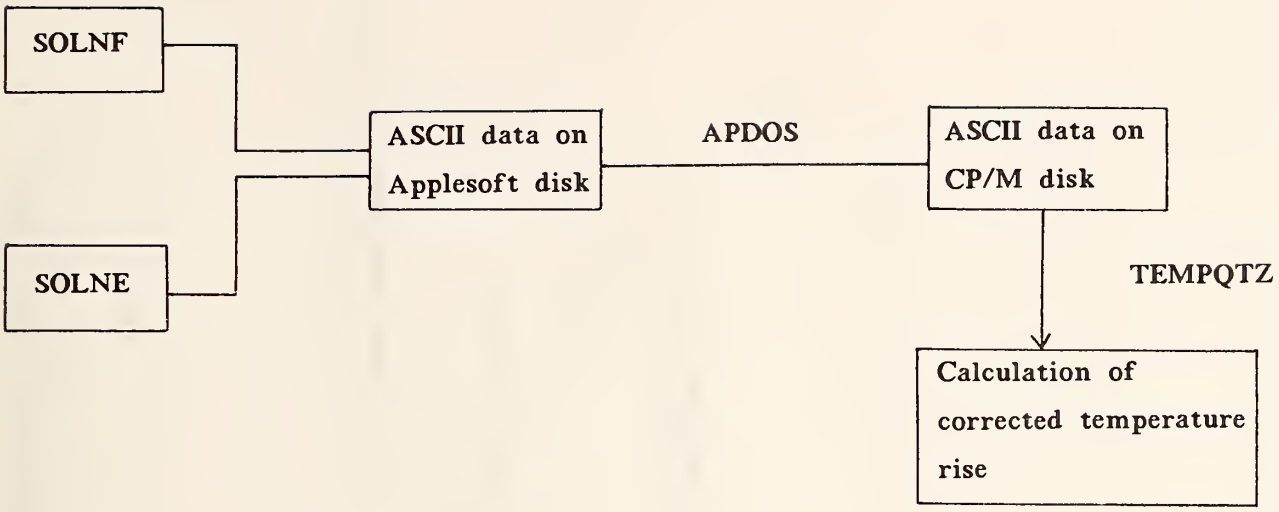
1. Schematic of data acquisition system for microcalorimeters.



2. Schematic of data acquisition system for isoperibol solution calorimeter.



3. Schematic of computational procedure by which microcalorimetric data is acquired (program "MCAL") and then treated. Auxiliary programs are "TEMP" for calculation of temperature and "ELCTRC" for treating the results of electrical calibrations.



4. Schematic of computational procedure by which data is acquired from an isoperibol solution calorimeter and then treated.

AREA

This program is used to calculate from the amplified thermopile voltages the area associated with either process or electrical heat. The integration is accomplished using the trapezoidal rule.

```
50 DEFDBL A-D, F-H, P-Z
100 DEFINT I-N: DEFSNG E
150 DEF FNT(N) = T0 + (N-1)*DT
200 DIM E(4000)
250 HOME: PRINT "MAKE SURE PRINTER IS ON"
300 PRINT: PRINT: FOR I = 1 TO 4: LPRINT: NEXT I
350 INPUT "DATE (MONTH DAY)";DA$
400 INPUT "SERIES (A,B,C, ETC.)";SE$
450 FOR LOOP = 0 TO 2                                   BEGIN LOOP (REPEATED ONCE FOR EACH OF 3 FILES)
500 FOR LF = 1 TO 4:LPRINT: NEXT LF
550 CAL$ = RIGHT$(STR$(LOOP), 1): D$ = "B:"
600 F$ = D$ + DA$ + SE$ + CAL$
650 LPRINT F$: LPRINT
700 OPEN "R", #1, F$, 4
750 FIELD #1, 4 AS ES$
800 GET #1, 1
850 NPTS = CVS(ES$)                                     READ IN VOLTAGE DATA FROM DISK FILE
900 FOR I = 2 TO NPTS+3
950     GET #1, I
1000     E(I) = CVS(ES$)
1050     NEXT I
1100 T0 = E(2): DT = E(3)
1150 IF LOOP > 0 THEN 1400
1200 PRINT: PRINT "NUMBER OF DATA POINTS = "; NPTS
1250 INPUT "ENTER 4 TIMES (TYPE CTRL-C TO STOP)"; K1, K2, K3, K4  REQUEST DATA POINT NUMBERS DEFINING
1300 PRINT K1, K2, K3, K4: LPRINT K1,K2,K3,K4                     INITIAL AND FINAL BASELINES
1350 REM CALL SUBROUTINE CURFIT1
1400 START = K1: FINISH = K2
1450 GOSUB 2950
1500 B0 = A0: B1 = A1                                   DETERMINE BY LEAST SQUARES, LINEAR EQUATIONS FOR THE BASELINES
1550 START = K3: FINISH = K4
1600 GOSUB 2950
1650 C0 = A0: C1 = A1
1700 PT1 = B0 + B1*FNT(K2)
1750 PT2 = C0 + C1*FNT(K3)
1800 PT3 = C0 + C1*FNT(K2)
1850 PT4 = B0 + B1*FNT(K3)
1900 PRINT " STARTING PT" TAB(14);
1950 PRINT USING "_ _ _ #.#####^^^^"; E(K2+3), PT1, PT3
2000 PRINT " END PT" TAB(14);                           PRINT PARAMETERS FROM THE LINEAR BASELINE FITS
2050 PRINT USING "_ _ _ #.#####^^^^"; E(K3+3), PT4, PT2
2100 SHIFT1 = PT3 - PT1
2150 SHIFT2 = PT2 - PT4
2200 SHIFT3 = E(K3+3) - E(K2+3)                         CALCULATE AND PRINT SHIFTS BETWEEN INITIAL AND
2250 PRINT " SHIFT =" TAB(14);                          FINAL BASELINES, BOTH CACULATED AND MEASURED
2300 PRINT USING "_ _ _ #.#####^^^^"; SHIFT1, SHIFT2, SHIFT3
2350 SLOPE = (PT2 - PT1) / (FNT(K3) - FNT(K2))
2400 PINCPT = PT1 - SLOPE*FNT(K2)                       CALCULATE, FROM THE 2 FITTED BASELINES, THE COEFFICIENTS
2450 PRINT: PRINT "...INTEGRATING...";                  OF A BASELINE CONNECTING LINE
2500 AREA = 0
```

```
2550 FOR I = K2 TO K3
2600       AA = (E(I+3) + E(I+4)) / 2
2601       AB = AA - PINCPT - SLOPE*(FNT(I) + FNT(I+1)) / 2
2602       AREA = AREA + AB*(FNT(I+1) - FNT(I))                    DETERMINE THE AREA, USING A RECTANGULAR APPROXIMATION,
2650      NEXT I                                                   BETWEEN THE VOLTAGE DATA CURVE AND THE BASELINE CONNECTING LINE
2700 BEEP 50,50
2750 PRINT: PRINT "AREA = ";: PRINT USING "#.#####^^^^"; AREA;
2751 PRINT " V-SEC": PRINT
2000 LPRINT: LPRINT "AREA = ";: LPRINT USING "#.#####^^^^"; AREA; PRINT THE CALCULATED AREA
2801 LPRINT " V-SEC"
2050 CLOSE #1: NEXT LOOP                                         END LOOP
2900 END
2950 REM *** SUBROUTINE CURFIT1 ***
3000 NU = FINISH - START + 1
3050 A = 0: B = 0: C = 0: D = 0: SUM = 0
3100 FOR I = START TO FINISH
3150      A = A + E(I+3)
3200      B = B + FNT(I)
3250      C = C + FNT(I)*E(I+3)                                  LINEAR LEAST SQUARES SUBROUTINE
3300      D = D + FNT(I)*FNT(I)
3350      NEXT I
3400 A0 = ((B*C) - (A*D)) / ((B*B) - (NU*D))
3450 A1 = (A - (A0*NU)) / B
3500 FOR I = START TO FINISH
3550      DEV = E(I+3) - (A0 +A1*FNT(I))
3600      SUM = SUM + DEV*DEV
3650      NEXT I
3700 STDDEV = SQR( SUM / NU )
3750 RETURN
3000 END
```

EXAMPLE

```
RUN

MAKE SURE PRINTER IS ON


DATE (MONTH DAY)? MAY13
SERIES (A,B,C, ETC.)? B

NUMBER OF DATA POINTS =  1000
ENTER 4 TIMES (TYPE CTRL-C TO STOP)? 1,10,900,910
 1             10             900            910

 STARTING PT     -.41787E-05    -.41871D-05    -.47044D-05
 END PT          -.38660E-05    -.38638D-05    -.38629D-05
 SHIFT =         -.51725D-06    0.84594D-09    0.31272D-06

...INTEGRATING...
AREA = -.39014D-02 V-SEC

 STARTING PT     -.25736E-05    -.25728D-05    -.46090D-05
 END PT          -.25079E-05    -.84251D-06    -.25040D-05
 SHIFT =         -.20362D-05    -.16623D-05    0.65770D-07

...INTEGRATING...
AREA = -.44877D-02 V-SEC

 STARTING PT     -.50243E-05    -.50199D-05    -.84839D-05
 END PT          -.44430E-05    -.36916D-05    -.44348D-05
 SHIFT =         -.34640D-05    -.74328D-06    0.58131D-06

...INTEGRATING...
AREA = -.35815D-02 V-SEC
```

ASCBIN

This program is used to convert data in ASCII format to data having a binary format.

```
50 DEFSNG A-H,P-Z DEFINT I-N
100 HOME
150 DIM V(4000)
200 ON ERROR GOTO 2150
250 DT = 5  GAIN = 10000!                                   DT = TIME BETWEEN DATA POINTS
300 PRINT "TIME BETWEEN POINTS  =  "; DT; "SEC"             GAIN = AMPLIFIER GAIN
350 PRINT  PRINT "AMPLIFIER GAIN = "; GAIN
400 PRINT: PRINT
450 INPUT "DATE(MONTH DAY)";DA$                             NAME FILES FROM DATE AND SERIES

500 PRINT: INPUT "SERIES"; SE$
550 FOR I = 0 TO 2
600 CAL$=RIGHT$(STR$(I),1)
650 FC$ = "B:"+DA$+SE$+CAL$
700 OPEN "I",#1,FC$
750 PRINT PRINT  FC$; " ALREADY EXISTS"                     CHECK TO SEE IF FILES NAMED BY ENTERED DATE
751 PRINT:PRINT "RENAME FILES SUFFIXED WITH "I" AND TRY AGAIN"   AND SERIES ALREADY EXIST ON DATA DISK
800 CLOSE #1: END
850 NEXT I
900 FOR LOOP=0 TO 2
950 CAL$=RIGHT$(STR$(LOOP),1)
1000 F$=DA$+SE$+CAL$+"I"
1050 OPEN "I",#1,F$
1100 PRINT F$
1150 INPUT#1,NPTS
1200 FOR I=1 TO NPTS                                        READ IN ASCII DATA FROM TEMPORARY FILE
1250 INPUT#1, V(I)                                          SUFFIXED WITH "I"
1300 V(I)=V(I)/GAIN
1350 NEXT I                                                 CALCULATE ACTUAL MEASURED VOLTAGE
1400 CLOSE #1                                               USING THE AMPLIFIER GAIN
1450 F1$="B:"+LEFT$(F$,7)
1500 RESET: OPEN "R",#2,F1$,4
1550 FIELD#2, 4 AS ES$                                                          MAIN LOOP
1600 LSET ES$=MKS$(NPTS): PUT #2,1                                              (REPEAT FOR 3 FILES)
1650 LSET ES$=MKS$(0): PUT #2,2
1700 LSET ES$=MKS$(OT): PUT #2,3
1750 FOR I = 1 TO NPTS
1800 LSET ES$=MKS$(V(I))                                    CREATE BINARY VOLTAGE DATA FILE
1850 PUT #2,I+3
1900 NEXT I
1950 CLOSE #2
2000 KILL F$                                                DELETE TEMPORARY ASCII FILE (SUFFIXED WITH "I")
2050 PRINT:PRINT "DONE"+STR$(LOOP)
2100 NEXT LOOP: END
2150 IF ERR = 53 THEN RESUME 850
2200 IF ERR = 61 OR ERR = 67 THEN PRINT: PRINT "DATA DISK FULL"   CHECK IF DATA DISK IS FULL          ERROR PROCESSING
2250 STOP
```

EXAMPLE

```
RUN

TIME BETWEEN POINTS  =  5 SEC

AMPLIFIER GAIN =  10000

DATE(MONTH DAY)? AUG22

SERIES? B
AUG22B0I

DONE 0
AUG22B1I

DONE 1
AUG22B2I

DONE 2
```

CURSPLT

This program is used for plotting a microcalorimetric thermogram. The use of a paddle control allows the user to determine the position of a given data point on the curve.

```
10 DEFINT I
20 DEFSNG P-Z
30 DIM E(2000)
40 TEXT: HOME: SUM = 0!
50  INPUT "INPUT NAME OF DATA FILE (CTRL-C TO STOP) "; I$
60 D$ = "E:": F$ = D$ + I$
70 OPEN "R", #1, F$, 4
80 FIELD #1, 4 AS ES$
90 GET #1, 1
100 NPTS = CVS(ES$)
110 YMAX = 0!
120 FOR I = 2 TO NPTS+3                                  READ VOLTAGE DATA FROM DISK FILE
130     GET #1, I
140     E(I) = CVS(ES$)
150     NEXT I
160 YMIN = E(4): YMAX = E(4)
165 PRINT: PRINT "...SCALING...";
170 FOR I = 5 TO NPTS+3                                  DETERMINE MAXIMUM AND MINIMUM VOLTAGES
180     IF E(I) < YMIN THEN YMIN = E(I)
190     IF E(I) > YMAX THEN YMAX = E(I)
200     NEXT I
210 T0 = E(2): DT = E(3)
220 XMAX = (NPTS-1)*DT
230 XSCALE = 279 / XMAX
240 YSCALE = 145 / (YMAX - YMIN)                         DETERMINE SCALE FACTORS BASED ON SCREEN SIZE
250 REM PRINT XSCALE, YSCALE                             AND MINIMUM AND MAXIMUM VOLTAGES
260 HGR 0,0: HCOLOR = 3
270 HPLOT 0, (159 - ((E(4)-YMIN)*YSCALE))
280 FOR I = 5 TO NPTS+3                                  PLOT CURVE ON SCREEN
290     PX = (I-4)*DT*XSCALE
300      PY = 159 - ((E(I)-YMIN)*YSCALE)
310      HPLOT TO PX,PY
320      NEXT I
330 VTAB 24: PRINT SPC(25) "TYPE <B> FOR INITIAL BASELINE"
335 VTAB 24: PRINT "POINT #" SPC(31) "TYPE <H> TO EXIT";
340 XVO = 10: FT = 1
350 X = 4*PDL(0)
360 KTES$=INKEY$                                         CHECK TO SEE IF KEY DEPRESSED
365 IF KTES$ = "H" THEN CLOSE #1: GOTO 40
370 IF KTES$ <> "B" THEN 410
372 VTAB 23: HTAB 26
373 PRINT "                                                ";
380 FOR I = 4 TO 13: SUM = SUM + E(I): NEXT I: AVG = SUM/10!
390 PX1 = 5*DT*XSCALE: PY1 = 159 - ((AVG-YMIN)*YSCALE)   EXTEND INITIAL BASELINE
400 HCOLOR = 3: HPLOT PX1,PY1 TO 279,PY1
410 FOR I = 1 TO 10: NEXT I
420 X = X + PDL(1) / 12.75
430 XS = NPTS / 1040                                     READ PADDLE VALUES AND DETERMINE
440 XV = INT((X*XS) + .5): IF XV = 0 THEN XV = 1         APPROPRIATE CURSOR POSITION
450 IF XV = XVO GOTO 350
460 IF FT = 1 THEN 530
470 HCOLOR = 0
480 IF (PXV < 0 OR PYV < 0) THEN 350
```

```
490 PXV = (279 / NPTS) * XVO
500 PYV = 159 - ((XVO+3)-YMIN)*YSCALE) - 5
510 FOR I = 0 TO 5: IF DOT(I) <> -1 THEN HPLOT PXV, PYV-1
520 NEXT I
530 HCOLOR =  3: FT = 0: XVO = XV
540 PXV = (279 / NPTS) * XV
550 PYV = 159 - ((E(XV+3)-YMIN)*YSCALE) - 5
560 IF (PXV < 0 OR PYV < 0) THEN 350
570 FOR I = 0 TO 5
580     DOT(I) = 0
590     IF HSCRN(PXV, PYV-I) = -1 THEN DOT(I) = -1
600     NEXT I
610 HPLOT PXV,PYV TO PXV,PYV-5
620 VTAB 24: HTAB 10: PRINT USING "####"; XV;
630 GOTO 350
```

ERASE PREVIOUS CURSOR IF CURSOR POSITION IS CHANGING

REDRAW CURSOR AT NEW POSITION

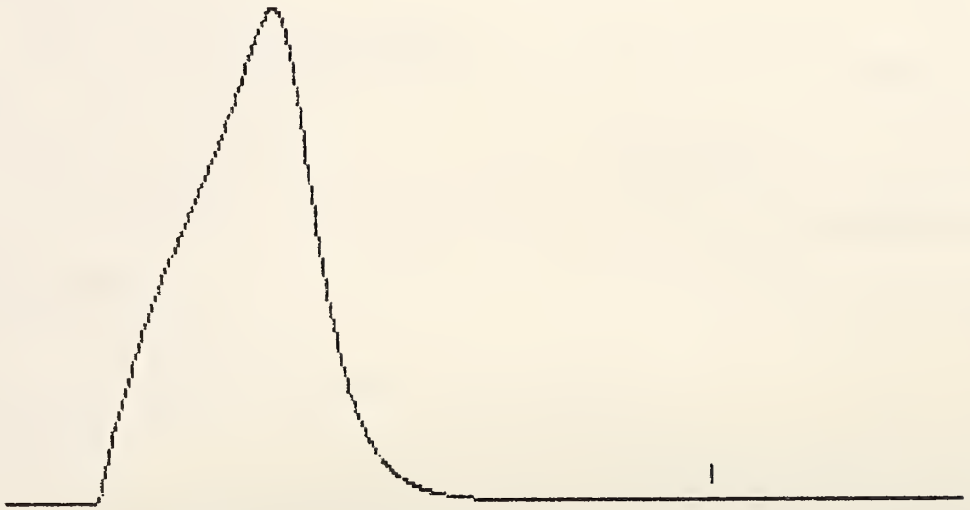
PRINT OUT DATA SET POINT NUMBER
WHICH CORRESPONDS TO CURSOR POSITION

EXAMPLE

```
RUN

INPUT NAME OF DATA FILE (CTRL-C TO STOP) ? AUG13B2

...SCALING...
```

```
POINT # 485

TYPE <B> FOR INITIAL BASELINE
TYPE <H> TO EXIT
```

DECON

This program is used to convert the time-voltage data into a deconvoluted curve showing power (dq/dt) as a function of time. It is based upon the method described in reference [8].

```
50 DEFINT I
100 DEFSNG P-Z
150 DIM E(2000), P(2000)
200 TEXT: HOME
250 F1 = 19.13: F2 = 2049                                   F1 = CALIBRATION FACTOR (J/(V*S))
300  INPUT "INPUT NAME OF DATA FILE (CTRL-C TO STOP)"; I$   F2 = FACTOR FROM AREA UNDER DECAY CURVE (J/V)
350 D$ = "B:": F$ = D$ + I$
400 OPEN "R", #1, F$, 4
450 FIELD #1, 4 AS ES$
500 GET #1, 1
550 NPTS = CVS(ES$)
600 YMAX = 0!
650 FOR I = 2 TO NPTS+3                                     READ VOLTAGE DATA FROM DISK FILE
700     GET #1, I
750     E(I) = CVS(ES$)
800     NEXT I
850 T0 = E(2): DT = E(3)
900 PRINT: PRINT "...DECONVOLUTING...";
950 FOR I = 5 TO NPTS+2                                     CALCULATE DERIVATIVE OF VOLTAGE WITH RESPECT
1050    DB = (E(I+1) - E(I)) / DT                           TO TIME AT EACH DATA POINT USING AN AVERAGE
1100    DD = (DA + DB) / 2                                  SLOPE TECHNIQUE
1000    DA = (E(I) - E(I-1)) / DT
1150    P(I-4) = (E(I)*F1) + (DD*F2)                        CALCULATE POWER AT EACH POINT IN TIME
1200    NEXT I
1250 YMIN = P(1): YMAX = P(1)
1300 PRINT: PRINT:  PRINT "...SCALING...";
1350 FOR I = 2 TO NPTS-2
1400     IF P(I) < YMIN THEN YMIN = P(I)                    DETERMINE SCALE FACTORS BASED ON SCREEN SIZE
1450     IF P(I) > YMAX THEN YMAX = P(I)                    AND MINIMUM AND MAXIMUM VOLTAGES
1500     NEXT I
1550 XMAX = (NPTS-2)*DT
1600 XSCALE = 279 / XMAX
1650 YSCALE = 145 / (YMAX - YMIN)
1700 REM PRINT XSCALE, YSCALE
1750 HGR 0,0: HCOLOR = 3
1800 HPLOT 0, (159 - ((P(1)-YMIN)*YSCALE))
1850 FOR I = 2 TO NPTS-2                                    PLOT POWER VS TIME CURVE ON SCREEN
1900     PX = I*DT*XSCALE
1950      PY = 159 - ((P(I)-YMIN)*YSCALE)
2000      HPLOT TO PX,PY
2050      NEXT I
2100 HTAB 1
2150 VTAB 24: PRINT "POINT #" SPC(31) "TYPE (H) TO EXIT";
2200 XVO = 10: FT = 1
2250 X = 4*PDL(0)
2300 KTES$ = INKEY$                                         CHECK TO SEE IF KEY DEPRESSED
2350 IF KTES$ = "H" THEN CLOSE #1: GOTO 200
2400 FOR I = 1 TO 10: NEXT I
2450 X = X + PDL(1) / 12.75
2500 XS = (NPTS-2) / 1040                                   READ PADDLE VALUES AND DETERMINE
2550 XV = INT((X*XS) + .5): IF XV = 0 THEN XV = 1           APPROPRIATE CURSOR POSITION
2600 IF XV = XVO GOTO 2250
2650 IF FT = 1 THEN 3000
2700 HCOLOR = 0
2750 IF (PXV < 0 OR PYV < 0) THEN 2250
2800 PXV = (279 / NPTS) * XVO                               ERASE PREVIOUS CURSOR IF CURSOR POSITION IS CHANGING
2850 PYV = 159 - ((P(XVO)-YMIN)*YSCALE) - 5
2900 FOR I = 0 TO 5: IF  DOT(I) <> -1 THEN HPLOT PXV, PYV-I
2950 NEXT I
3000 HCOLOR =  3: FT = 0: XVO = XV
3050 PXV = (279 / NPTS) * XV
3100 PYV = 159 - ((P(XV)-YMIN)*YSCALE) - 5                  REDRAW CURSOR AT NEW POSITION
3150 IF (PXV < 0 OR PYV < 0) THEN 2250
```

```
3200 FOR I = 0 TO 5
3250      DOT(I) = 0
3300      IF HSCRN(PXV, PYV-I) = -1 THEN DOT(I) = -1
3350      NEXT I
3400 HPLOT PXV,PYV TO PXV,PYV-5
3450 VTAB 24: HTAB 10: PRINT USING "####"; XV;
3500 GOTO 2250
```

PRINT OUT DATA SET POINT NUMBER
WHICH CORRESPONDS TO CURSOR POSITION

EXAMPLE

RUN

INPUT NAME OF DATA FILE (CTRL-C TO STOP)? JUL26B2

...DECONVOLUTING...

...SCALING...

POINT # 380

TYPE (H) TO EXIT

DEFLCT

This program is used to calculate the deflection of a thermogram from its baseline which is typically brought about by the steady-state input of electrical energy.

```
50 DEFDBL A-D, F-H, S, U-Z
100 DEFSNG E
150 DEF FNT(N) = T0 + (N-1)*DT
200 DIM E(2000)
250 HOME: INPUT " ENTER NAME OF DATA FILE"; I$
300 D$ = "B:": F$ = D$ + I$
350 OPEN "R", #1, F$,4
400 FIELD #1, 4 AS ES$
450 GET #1, 1: NPTS = CVS(ES$)
500 FOR I = 2 TO NPTS+3                                  READ IN VOLTAGE DATA FROM DISK FILE
550     GET #1, I
600       E(I) = CVS(ES$)
650     NEXT I
700 T0 = E(2): DT = E(3)
750 PRINT: PRINT " NUMBER OF DATA POINTS ="; NPTS
800 PRINT: PRINT "ENTER 6 TIMES (CTRL-C TO STOP)";
801 INPUT K1, K2, K3, K4, K5, K6                         REQUEST DATA POINT NUMBERS DEFINING BEGINNING
900 START = K1: FINISH = K2                              AND END OF FORE, MAIN, AND AFTER PERIODS
950 GOSUB 2200
1000 B1 = A1: B0 = A0: SD1 = STDDEV
1050 START = K3: FINISH = K4
1100 GOSUB 2200
1150 C1 = A1: C0 = A0: SD2 = STDDEV                      DETERMINE BY LEAST SQUARES, LINEAR EQUATIONS
1200 START = K5: FINISH = K6                             FOR EACH OF THE 3 PERIODS
1250 GOSUB 2200
1300 D1 = A1: D0 = A0: SD3 = STDDEV
1350 TA = (FNT(K1) + FNT(K2)) / 2
1400 TB = (FNT(K3) + FNT(K4))/ 2
1450 V1 = B0 + B1*TA                                     CALCULATE DEFLECTIONS FROM FITTED LINES
1500 V2 = C0 + C1*TA
1550 V3 = C0 + C1*TB
1600 V4 = D0 + D1*TB
1650 DE1 = V2 - V1                                       DEFLECTION 1 = DIFFERENCE BETWEEN MAIN AND FORE PERIODS
1700 DE2 = V3 - V4
1750 REM                                                 DEFLECTION 2 = DIFFERENCE BETWEEN MAIN AND AFTER PERIODS
1800 PRINT: PRINT TAB(18) "INTERCEPT" TAB(34) "SLOPE" TAB(44);
1801 PRINT "STD DEVIATION"
1849 PRINT " FORE PERIOD ";
1850  PRINT USING "_ _ _ #.#####^^^^"; B0, B1, SD1      PRINT PARAMETERS FROM THE LINEAR LEAST
1899 PRINT " MAIN PERIOD ";                              SQUARES FITS FOR THE 3 PERIODS
1900  PRINT USING "_ _ _ #.#####^^^^"; C0, C1, SD2
1949 PRINT " AFTER PERIOD";
1950  PRINT USING "_ _ _ #.#####^^^^"; D0, D1, SD3
2000 PRINT
2049  PRINT " DEFLECTIONS: ";                            PRINT BOTH DEFLECTIONS
```

```
2050  PRINT USING "_ _ _ #.#####^^^^_ _A_N_D_ "; DE1;
2100 PRINT USING "#.#####^^^^"; DE2;: PRINT " VOLTS"
2150 GOTO 800
2200 REM *** SUBROUTINE CURFIT ***
2250 NUM = FINISH - START + 1
2300 A = 0!: B = 0!: C = 0!: D = 0!: SUM = 0!
2350 FOR I = START TO FINISH
2400      A = A + E(I+3)
2450      B = B + FNT(I)
2500      C = C + FNT(I)*E(I+3)
2550      D = D + FNT(I)*FNT(I)
2600      NEXT I
2650 REM
2700 A0 = ((B*C) - (A*D)) / ((B*B) - (NUM*D))
2750 A1 = (A - (A0*NUM)) / B
2800 FOR I = START TO FINISH
2850      DEV = E(I+3) - (A0 + A1*FNT(I))
2900      SUM = SUM + DEV*DEV
2950      NEXT I
3000 REM
3050 STDDEV = SQR(SUM/NUM)
3100 RETURN
3150 END
```

LINEAR LEAST SQUARES SUBROUTINE

EXAMPLE

```
RUN

 ENTER NAME OF DATA FILE? APR26D2

 NUMBER OF DATA POINTS = 494

ENTER 6 TIMES (CTRL-C TO STOP)? 1,10,250,260,484,494

                  INTERCEPT        SLOPE      STD DEVIATION
 FORE PERIOD     -.36536D-05    -.15125D-10    0.10976D-07
 MAIN PERIOD      0.15026D-03    0.40749D-09    0.96677D-08
 AFTER PERIOD    -.26135D-05    -.44747D-09    0.76471D-08

 DEFLECTIONS:     0.15392D-03 AND 0.15396D-03 VOLTS
```

ELECTRC

This program is used for the calculation of the calibration constant of a microcalorimeter.

```
50 DEFDBL A-Z
100 LPRINT:LPRINT:LPRINT TAB(6) "POWER" TAB(20) "HEAT" TAB(31);
101 LPRINT "RESISTANCE" TAB(45) "FACTOR(1)" TAB(59) "FACTOR(2)"
102 LPRINT
150 F$="B:ELCTRC.DAT"                                          READ IN DATA FROM DISK FILE "ELECTRIC.DAT"
200 OPEN "I",#1,F$
250 INPUT#1, EHTR, ESTD, TIME, AREA, DFLCT, TEMP, DVM
299 TD = (1+8*(TEMP-25) - .5*(TEMP-25)^2)
300 RSTD = 1000! + .001*TD                                     APPLY TEMPERATURE CORRECTION TO THE RESISTANCE
350 FACTOR = 1.01793 / DVM                                     OF THE 1000 OHM STANDARD RESISTOR
400 RSTNC = (EHTR / ESTD)*RSTD
450 PLEADS = ((ESTD/RSTD)*(ESTD/RSTD))*.0127                   CALCULATE POWER LOST IN THE HEATER LEADS FROM
500 POWER = (((FACTOR) * (FACTOR) * EHTR * (ESTD/RSTD))) - PLEADS CURRENT AND LEAD RESISTANCE
501 REM
502 REM                                                        CALCULATE POWER FROM THE VOLTAGE ACROSS THE HEATER
550 Q = POWER*TIME                                             AND THE CURRENT (SUBTRACT OUT THE POWER LOST IN THE LEADS)
600 ANS = Q / (AREA)
650 ANS1 = POWER / DFLCT                                       DETERMINE THE CALIBRATION CONSTANT (J/(V*S)) 2 WAYS:
700 LPRINT USING "_ #.######^^^^_ "; POWER, Q, RSTNC, ANS, ANS1
                                                               FACTOR 1 = POWER*TIME/AREA
750 IF EOF(1) THEN END ELSE GOTO 250                           FACTOR 2 = POWER/DEFLECTION
800 END
850 REM
900 REM  EHTR = VOLTAGE ACROSS HEATER
950 REM  ESTD = VOLTAGE ACROSS THE STANDARD RESISTOR
1000 REM TIME = TIME HEATER ON
1050 REM AREA = AREA UNDER THE VOLTAGE-TIME CURVE FOR
1100 REM        THE CALIBRATION RUN                            DEFINITIONS OF THE VALUES STORED IN THE DATA FILE
1150 REM DFLCT = DEFLECTION OF THE VOLTAGE DURING THE
1200 REM         CALIBRATION RUN
1250 REM TEMP = TEMPERATURE OF THE STANDARD RESISTOR
1300 REM DVM = DVM VOLTAGE READING OF 1.01793 VOLT STANDARD CELL
```

EXAMPLE

```
RUN
```

MCAL

This program is used for the acquisition of the amplified thermopile voltage data during a microcalorimetric experiment. Note that there is a set of single-key commands available during program execution. The available commands are:

R - start recording of data

H - end recording of data and write data to floppy disk

B - draw baseline from initial voltage readings

D - downscale the display

U - upscale the display

```
5000  PRINT  CHR$ (4)"MAXFILES 1": LOMEM: 16384:IV = 0
5005  GOSUB 5580
5010  FOR INDX = 1 TO 1000: GOSUB 5020: NEXT INDX
5011  IF IR = 1 THEN 5435
5020  PRINT "WT)";Z$;"AC0": PRINT "WT6";Z$;"X1"
5030  INPUT "SR";G$: IF G$ = "F" THEN 5030
5040  PRINT "SPV";Z$;: INPUT H$
5050  PRINT "WT6";Z$;"-3STRRER"
5060  PRINT "RDV";Z$;: INPUT V0$,V1$,V2$:IA = INDX                ACQUIRE VOLTAGE FROM 3 CALORIMETERS
5070 V(IA,0) =  VAL (V0$) * F:V(IA,1) =  VAL (V1$) * F
5071 V(IA,2) =  VAL (V2$) * F
5080 TI% = TI% + 5:PX%(0) = TI% - TC:PX%(1) = PX%(0) + 1
5081 PJ = 5
5090  FOR PI = 0 TO 2
5100  IF  ABS (V(IA,PI) * SY) <  = 80 THEN 5120
5110 A = 1: GOTO 5260                                                                    MAIN LOOP
5120 PY%(PI) = 80 - (V(IA,PI) * SY): HCOLOR= PJ + PI              PLOT 3 POINTS ON SCREEN
5130  IF PX%(0) <  = 279 THEN 5150                                WITH AUTOSCALE UP
5140 TC = TI%:PX%(0) = 0:PX%(1) = 1: HGR
5150  HPLOT PX%(0),PY%(PI) TO PX%(1),PY%(PI)
5160  NEXT PI
5180 A =  PEEK ( - 16384): IF A > 127 THEN  GOTO 5250             CHECK IF KEY COMMAND TYPED
5190  INPUT "SR";G$: IF G$ = "F" THEN 5190
5200  PRINT "SPI";Z$;: INPUT H$
5210  VTAB 1: RETURN
5250  POKE  - 16368,0:A = A - 128
5260  FOR S = 1 TO 30:X =  PEEK ( - 16336): NEXT S
5265  IF A = 1 THEN 5331
5268  IF A = 2 THEN 5341
5270  IF A = 68 THEN 5340
5280  IF A = 85 THEN 5340                                        DETERMINE KEYBOARD COMMAND AND BRANCH
5290  IF A = 66 THEN 5410
5310  IF A = 72 THEN 5430
5320  IF A = 82 THEN 5540
5330  GOTO 5190
5331  FOR ISEL = (SSEL + 1) TO 11
5332  IF  ABS (V(IA,PI)) <  = SCD(ISEL) THEN 5334                 AUTOSCALE UP
5333  NEXT ISEL
5334 SSEL = ISEL - 2
5340  IF A = 68 THEN SSEL = SSEL - 2
5341  IF SSEL = 10 THEN 5190                                      UPSCALE AND DOWNSCALE                    SCREEN SCALING
5350  PRINT D$;"PR#0"
5360 SSEL = SSEL + 1:SY = 80 / SCD(SSEL + 1): VTAB 24: HTAB 9
5380  PRINT SSEL + 1;" ";: VTAB 15: GOSUB 10000
5400  IF A = 1 THEN 5100
5401  IF A = 2 THEN 5410
5402  GOTO 5190
5410  FOR I = 0 TO 2:PY% = 80 - (VB(I) * SY): HCOLOR= PJ + I
```

```
5415  IF PY% ) 159 THEN A = 2: GOTO 5260                    DRAW BASELINE BASED ON DATA
5420  HPLOT 0,PY% TO 279,PY%: NEXT : GOTO 5190               FROM FORE PERIOD
5430  INPUT "SR";G$: IF G$ = "F" THEN 5430
5435  PRINT "WT)";Z$;"SE000": PRINT "CA": PRINT "WT6";Z$;"T4"
5440  PRINT "SPI";Z$;: INPUT H$: PRINT "LA"                  CLEAR BUS AND RESET INSTRUMENTS
5445  PRINT D$;"PR#0": PRINT D$;"IN#0"
5450  TEXT : HOME : PRINT "CREATING FILES:": PRINT
5460  FOR I = 0 TO 2                                                              HALT SECTION
5470 F$ = DA$ + SE$ +  STR$ (I): PRINT F$
5480  PRINT D$;"OPEN";F$
5490  PRINT D$;"WRITE";F$                                    CREATE 3 VOLTAGE DATA FILES
5500  PRINT IA
5510  FOR J = 1 TO IA: PRINT V(J,I): NEXT J
5520  PRINT D$;"CLOSE";F$: NEXT I: PRINT : PRINT "DONE": END
5540  PRINT D$;"PR#0":IR = 1:INDX = 0
5550  VTAB 24: HTAB 22: PRINT "TYPE (R) TO STOP ";
5555 VE(0) = V(IA,0):VB(1) = V(IA,1):VB(2) = V(IA,2)         BEGIN DATA LOGGING                    RUN SECTION
5560  VTAB 15: GOSUB 10000
5570  GOTO 5190
5500 D$ =  CHR$ (4):Z$ =  CHR$ (26)
5505  ONERR  GOTO 7000
5586  HOME
5590  IF IV ) 0 THEN 5612
5600  INPUT "DATE(MONTH DAY)?";DA$
5610  INPUT "SERIES(A,B,C,ETC.)";SE$                        TM = TIME INTERVAL BETWEEN DVM MEASUREMENTS
5611 IV = 0:IR = 0:TM = 5:PLC = 10
5612  IF IV ) 2 THEN 5620                                   PLC = INTEGRATION TIME OF DVM
5613 FT$ = DA$ + SE$ +  STR$ (IV): PRINT D$;"VERIFY";FT$          (IN POWER LINE CYCLES)
5614  PRINT
5615  PRINT "FILES NAMED BY ENTERED DATE AND SERIES ALREADY EXIST"
5616  PRINT " -- PLEASE TRY AGAIN": PRINT
5617  GOTO 5600
5620  HGR : HCOLOR= 3
5630  DIM V(1000,2),SCD(11),PY%(2),PX%(2)
5640 F = 1:IBEGIN = 0:TC = 0:TI% = 0
5650  FOR I = 1 TO 11: READ SCD(I): NEXT I
5660  DATA  5E-3,1E-2,2E-2,5E-2,1E-1,2E-1,5E-1,1,2,5,10     SCREEN SCALING CONSTANTS
5670  PRINT D$;"PR#5": PRINT D$;"IN#5"
5680  PRINT "CA": PRINT "RA": PRINT "LF1": PRINT "LL"
5682  PRINT "WT#";Z$;"INAU0GS1"                                                   INITIALIZATION SECTION
5690  PRINT "WT6";Z$;"F1R1Z1D1SM002" +  STR$ (PLC) + "STI"
5700  PRINT "WT6";Z$;"3STN.05STDRS1T4"                       INITIALIZE INSTRUMENTS ON THE BUS
5710  PRINT "WT)";Z$;"SD0AE1SE10AC0"
5720  PRINT "WT6";Z$;"L1RS1T3QX1"
5730  INPUT "SR";G$: IF G$ = "F" THEN 5730
5740  PRINT "WT6";Z$;"T4-3STRRER": PRINT "RDV";Z$;           READ FIRST 3 VOLTAGES
5741  INPUT V0$,V1$,V2$
5750 V(0,0) =  VAL (V0$) * F:V(0,1) =  VAL (V1$) * F
5751 V(0,2) =  VAL (V2$) * F
5760 QSY =  ABS (V(0,0)): FOR I = 1 TO 2
5761  IF  ABS (V(0,I)) ) QSY THEN QSY =  ABS (V(0,I))
5765  NEXT
5770  FOR SSEL = 10 TO 1 STEP  - 1
5779 T1 = SCD(SSEL):T2 = SCD(SSEL + 1)
5700  IF QSY ) T1 THEN  IF QSY (  = T2 GOTO 5800             DETERMINE INITIAL SCALE FACTORS
5790  NEXT
5800 SY = 80 / SCD(SSEL + 1)
5810  HOME : VTAB 24: PRINT D$;"PR#0"
5811  PRINT "SCALE = ";SSEL + 1;
5820  HTAB 22: PRINT "TYPE (R) TO START";
5830  VTAB 15: GOSUB 10000
5040  PRINT "WT)";Z$;"TI" +  STR$ (TM)
5850  RETURN
7000  IF  PEEK (222) = 6 THEN IV = IV + 1: GOTO 5005        MAKE SURE DISK FILE NAMES FOR DATA
7015  STOP                                                   SETS ARE NON-EXISTENT
7020 IV = IV + 1: GOTO 5005
10000  POKE 54,6: POKE 55,197: CALL 1002: RETURN             RESET SLOT 5 (IEEE INTERFACE)
```

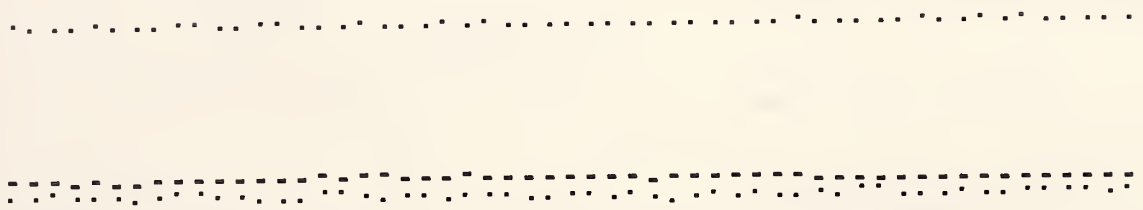
EXAMPLE

```
)RUN


DATE(MONTH DAY)?AUG22
SERIES(A,B,C,ETC.)A

FILES NAMED BY ENTERED DATE AND SERIES ALREADY EXIST -- PLEASE TRY AGAIN

DATE(MONTH DAY)?AUG22
SERIES(A,B,C,ETC.)B
```



```
SCALE = 3                    TYPE (H) TO STOP

H

CREATING FILES

AUG22B0
AUG22B1
AUG22B2

DONE
```

SOLNE

This program is used to acquire data during an electrical calibration of the isoperibol calorimeter. Note that, during execution, it also measures the voltages across the calorimeter heater and across the one ohm standard resistor in series with it.

```
50  DIM T(200),F(200)
100  DIM V(175,1),PV(175)
150 D$ =  CHR$ (4):Z$ =  CHR$ (26)
200  HOME : GOTO 20300                                          BRANCH TO INITIALIZATION ROUTINE
250 CV =  PEEK (37): PRINT D$;"PR#0": VTAB 24: PRINT  SPC( 4)COM$;
251  VTAB CV + 1: HTAB 1: IF IR = 1 THEN  PRINT                 RESET IEEE SLOT AND PRINT COMMENTS ON SCREEN
300 IR = 0: GOSUB 400: RETURN
350  POKE 56,3: POKE 57,197
400  POKE 54,6: POKE 55,197: CALL 1002: RETURN
450  PRINT "RDC";Z$;: INPUT FR$
500  IF JU = 1 THEN JU = 0: GOTO 450                            READ COUNTER
550 F(INDX) =  VAL ( RIGHT$ (FR$,18))
600 T(INDX) = (F(INDX) - A) / B
650  IF L2 = 1 THEN 950
700  IF L > 1 THEN 1000
750 TF = T(1):CT = TS - TF: IF CT <  = 0 THEN 19000
800  PRINT "WT#";Z$;"GA10RE"                                                          COUNTER READ AND
850 TT% =  INT (ES * CT / P)                                                          DISPLAY SECTION
900 MS = TT% / 60:MI =  INT (MS):SF = (MS - MI) * 60
901 T$ =  STR$ ((MI * 100) + SF)
950 DE = 0: GOTO 1050
1000 DE =  INT ((T(INDX) - T(INDX - 1)) * 1E+06)
1050 TP$ =  LEFT$ ( STR$ (T(INDX)),9):T(0) = T(1):L2 = 0          DETERMINE TEMPERATURE AND DELTA TEMP
1100  IF  LEN (TP$) = 9 THEN 1200                               AND PRINT BOTH ON SCREEN
1150 TP$ = TP$ + "0": GOTO 1100
1200  PRINT D$;"PR#0": PRINT TP$ SPC( 10)DE
1250  GOSUB 400
1300  IF CF = 1 THEN CF = 0: GOTO 2250
1350  RETURN
1400  FOR INDX = 1 TO 200
1450  PRINT "WT)";Z$;"TE": PRINT "RDI";Z$;: INPUT TE%
1500  IF TE% < (GT - 10) THEN 1650
1550  GOSUB 450
1600  PRINT "WT)";Z$;"TE0TE2":JU = 1: NEXT INDX: GOTO 30000                                MAIN DATA LOGGING LOOP
1650 K =  PEEK ( - 16384): IF K > 127 THEN 1750
1700  GOTO 1450
1750  POKE  - 16368,0:K = K - 128
1800  FOR S = 1 TO 30:X =  PEEK ( - 16336): NEXT S               CHECK KEYBOARD AND BRANCH
1850  IF K = 72 THEN 30000                                       IF COMMAND SELECTED
1900  IF K = 82 THEN 2050
1950  IF K = 67 THEN 2200
2000  GOTO 1450
2050  REI
2100 COM$ = "TYPE <C> TO CALIBRATE":IR = 1: GOSUB 250            BEGIN LOGGING DATA                    RUN SECTION
2150 T(0) = T(INDX - 1):INDX = 1:: GOTO 1450
2200 JU = 1:CF = 1:COM$ =  LEFT$ (SP$,22): GOSUB 250: GOTO 450
2250  PRINT "WT)";Z$;"SD0AE1SE00AC10AF10AL11TI" +  STR$ (TM)     INITIALIZE INSTRUMENTS TO READ VOLTAGES
2300 INDX = INDX + 1                                             ACROSS HEATER AND STANDARD RESISTOR AND
2350  PRINT "WT)";Z$;"DC4,0TE0TE2"                               TURN HEATER ON
2400  PRINT "WT6";Z$;"T2RS1"
2450 COM$ = "HEATER ON" +  LEFT$ (SP$,12): GOSUB 250                                    CALIBRATION SECTION
2451 IA = INDX - 1:JU = 1
2500 TL = TJ% - ((INDX - IA - 1) * GT)
2550  IF TL < (GT - 7) THEN 2650
2600  GOSUB 450:INDX = INDX + 1: GOTO 2500
2650  PRINT "WT)";Z$;"TE": PRINT "RDI";Z$;: INPUT TE%
```

```
2700  IF TE% < TJ% THEN 2650
2750  PRINT "WT6";Z$;"T4"
2800  PRINT "WT)";Z$;"DO4,0ACTI0"                                  TURN HEATER OFF WHEN APPROPRIATE
2850 COM$ = "TYPE (H) TO STOP": GOSUB 250                          TIME INTERVAL IS COMPLETE
2900  PRINT "SPI";Z$;: INPUT H$:JU = 1: GOTO 1550
10000 TL = TT% - ((L - 2) * 10.08)
10050  IF TL < (5.08) THEN 10400
10100  GOSUB 450
10150 L = L + 1: GOTO 10000
10200  PRINT "WT)";Z$;"DC4,0TI" + T$                               TURN HEATER ON
10250  PRINT "WT#";Z$;"RE"
10300 COM$ = "HEATER ON" +  LEFT$ (SP$,12): GOSUB 250
10350 L = L + 1: GOTO 10000
10400  PRINT "SPI";Z$;: INPUT H$
10450  IF H$ <  > "40" THEN 10400
10500  IF FL = 1 THEN 10750
10550  PRINT "WT)";Z$;"DO4,0"                                       TURN HEATER OFF WHEN TIME
10600 COM$ = "PAUSE FOR " +  STR$ (PA) + " MIN": GOSUB 250         INTERVAL IS COMPLETE
10650 L = 2:FL = 1:TT% = PA * 60
10700  PRINT "WT)";Z$;"TI" + FB$: PRINT "WT#";Z$;"RE": GOTO 10000 BEGIN PAUSE MODE
10750  PRINT "WT)";Z$;"SE0"
10000  PRINT D$;"PR#0": PRINT D$;"IN#0"
10850  POKE 32,0: POKE 33,40                                                                  INITIAL SOLUTION
10900  POKE 34,0: POKE 35,23                                                                  WARM-UP SECTION
10950  VTAB 24: HTAB 7: PRINT SP$                                                             (GATE TIME = 10 SEC)
11000  HOME : PRINT "CALIBRATION": PRINT
11001  PRINT "RESET HP-5325B COUNTER"
11002  PRINT "HIT THE SPACE BAR TO CONTINUE";: POKE  - 16368,0
11050 K =  PEEK ( - 16304): POKE  - 16368,0
11051 IF K <  > 32 THEN 11050
11100  PRINT : PRINT "SELECT:": PRINT                               REQUEST CALIBRATION SPECIFICS
11150  PRINT "1 - TIME HEATER ON"
11200  PRINT "2 - DESIRED DELTA T"
11250  PRINT "3 - HEAT DELIVERED"
11300  INPUT HT
11350  IF HT = 1 THEN 11500
11400  IF HT = 2 THEN 11550
11450  HOME : PRINT "MAX Q INPUT = ";(TM * 175 * P);" J": PRINT
11451  INPUT "ENTER DESIRED HEAT (J)";QH:TH = QH / P: GOTO 11600
11500  HOME : PRINT "MAX TIME = ";(TM * 175);" SECONDS": PRINT
11501  INPUT "ENTER TIME HEATER ON IN SECONDS";TH: GOTO 11600
11550  HOME : PRINT "MAX DELTA T = ";(TM * 175 * P / ES);" K"
11551  PRINT: INPUT "ENTER DESIRED DELTA T";TD:TH = ES * TD / P
11600 NRD =  INT (TH / TM)
11650 TJ% = TH
11651  PRINT
11700  IF NRD > 175 THEN   PRINT "TIME TOO LARGE -- TRY AGAIN"
11701  IF NRD > 175 THEN  PRINT : GOTO 11100
11750  VTAB 1: PRINT SP$ + "                          ": HOME
11751  GOSUB 20000: GOSUB 350
11000  PRINT "WT#";Z$;"GA" +  STR$ (T1) + "RE"                       PROGRAM INSTRUMENTS WITH CALIBRATION PARAMETERS
11850  PRINT "WT)";Z$;"TE0TE2"
11900 COM$ = "TYPE (R) TO RUN": GOSUB 250:L2 = 1: GOTO 1400
19000  PRINT D$;"PR#0": PRINT D$;"IN#0": POKE 34,0: POKE 35,23
19050  POKE 32,0: POKE 33,40: HOME                                  INITIAL SPECIFIED TEMPERATURE TOO LOW
19051  PRINT "DESIRED TEMPERATURE LOWER THAN SOLUTION TEMPERATURE"
19100  PRINT : PRINT "SOLN TEMP = ";TF: PRINT
19101  PRINT : PRINT "EXECUTION HALTED": END
20000  POKE 32,7
20050  POKE 33,30                                                    DEFINE TEXT WINDOW FOR TEMPERATURE DISPLAY
20100  POKE 34,4
20150  POKE 35,22
20200  VTAB 3: PRINT "TEMP (C)"; SPC( 6)"DELTA (MICRODEG)"
20250  RETURN
```

```
20300  PRINT "ELECTRICAL CALIBRATION:": PRINT
20350 T1 = 29.999:T2 = .08:GT = T1 + T2                    T1 = GATE TIME, T2 = DEAD TIME
20400 PLC = 1!:TM = 2!                                     TM = TIME BETWEEN DVM MEASUREMENTS
20450 PA = .3:FL = 0:L2 = 0:JU = 0:CF = 0                  PLC = INTEGRATION TIME OF DVM
20500  PRINT : PRINT "GATE TIME = ";T1;" SEC"                    (IN POWER LINE CYCLES)
20550  PRINT : PRINT "TIME BETWEEN DVM RDGS = ";TM;" SEC"
20600  PRINT : PRINT "PAUSE FOR ";PA;" MIN"                PA = PAUSE TIME (IN MINUTES)
20650  PRINT
20651  PRINT "SEE LINES 20350-20450 TO ALTER THESE VALUES"
20652  PRINT : PRINT                                                          INITIALIZATION SECTION
20700  PRINT : PRINT
20750  PRINT "DATE (MONTH DAY)";: INPUT DA$: PRINT
20800  PRINT "SERIES";: INPUT SE$: HOME
20850 FI$ = DA$ + SE$
20900 R1 = 82.3:RT = 83.4                                  SYSTEM RESISTANCES FOR POWER ESTIMATION
20950 ES = 460!                                            ES = SYSTEM ENERGY EQUIVALENT (J/K)
21000  PRINT : PRINT "ENTER DESIRED INITIAL TEMPERATURE";
21001  INPUT TS
21050  PRINT : PRINT "ENERGY EQUIVALENT = ";ES;"J/K - (Y OR N)";  REQUEST INITIAL SOLUTION WARM-UP PARAMETERS
21100  INPUT R$: IF R$ = "Y" THEN 21200
21150  INPUT "ENTER ENERGY EQUIVALENT (J/K)";ES
21200  PRINT : INPUT "ENTER EMF OF THE POWER SUPPLY?";EP
21250 P = (EP * 2 / RT * 2) * R1
21300 A = 8226!:B = 921.8
21350 MS = PA:MI =  INT (MS):SF = (MS - MI) * 60
21351 PB$ =  STR$ ((MI * 100) + SF)
21400 SF$ = "                          _       "
21450  HOME
21500  GOSUB 20000
21550  PRINT D$;"PR#5": PRINT D$;"IN#5"
21600  PRINT "CA": PRINT "RA": PRINT "LL": PRINT "LF1"
21601  PRINT "WT6";Z$;"T4"
21650 SU$ = "INFN1SM0WA0GA2"                               INITIALIZE INSTRUMENTS ON THE BUS
21700  PRINT "WT#";Z$;SU$
21750  PRINT "WT#";Z$;"AZ0MO-28.2E6AU0"
21800  PRINT "WT6";Z$;"F1R1Z1D1SM000" +  STR$ (PLC) + "STI"
21850  PRINT "WT6";Z$;"2STN.05STDRS1T4"
21900  PRINT "WT)";Z$;"SD0SE10"
21950  PRINT "WT#";Z$;"RE"
22000 L = 1:INDX = 1: GOSUB 450
22050  GOTO 10200
30000  POKE 32,0: POKE 33,40
30050  POKE 34,0: POKE 35,24
30100  PRINT "CL";"#";Z$:
30150  HOME : PRINT D$;"PR#0"
30200  PRINT "CREATING:": PRINT : PRINT FI$
30250  PRINT D$;"OPEN";FI$: PRINT D$;"WRITE";FI$           CREATE DISK FILE TO STORE FREQUENCY DATA
30300  PRINT INDX - 1:NPTS = INDX - 1
30350  FOR J = 1 TO INDX - 1
30400  PRINT F(J): NEXT J
30450  PRINT D$;"CLOSE";FI$
30500  PRINT D$;"PR#1": PRINT : PRINT
30550  PRINT  CHR$ (9);"132N"
30600  PRINT FI$ + ":": PRINT
30650  PRINT "POINT" TAB( 11)"TIME" TAB( 22)"TEMP (C)" TAB( 22);
30651  PRINT "DELTA (MICRODEG)"
30700  FOR I = 1 TO NPTS                                   LIST TIME-TEMPERATURE DATA ON PRINTER
30750 TIME = (I - 1) * (T1 + T2)
30800 S1 = (9 -  LEN ( STR$ (TIME))) + 16
30850 S2 = (10 -  LEN ( STR$ (T(I)))) + 26
30900  IF I = 1 THEN DE = 0: GOTO 31000
30950 DE =  INT ((T(I) - T(I - 1)) * 1E+06)
31000  IF I - 1 < 10 THEN  PRINT "  "I - 1 TAB( 12);: GOTO 31100
31050  PRINT " ";I - 1; TAB( 12)
```

```
31100  PRINT TIME SPC( S1)T(I) SPC( S2)DE: NEXT I
31150  HOME : GOSUB 400
31200  FOR J = 0 TO 1: FOR I = J TO 2 * NRD - 1 STEP 2
31250 SV$ = "T4" +  STR$ (2 * NRD - I) + "STRRER"
31300  PRINT "WT6";Z$;SV$: PRINT "RDV";Z$;: INPUT V$                READ VOLTAGE DATA STORED IN DVM MEMORY
31301 V(I - J) / 2,J) =  VAL (V$): NEXT I: NEXT J
31350  PRINT "CA": PRINT "WT6";Z$;"T4": PRINT "LA"
31351  PRINT D$;"PR#0": PRINT D$;"IN#0"
31400 F$ = FI$ + "E"
31450  PRINT "CREATING:": PRINT : PRINT F$                          CREATE DISK FILE TO STORE VOLTAGE DATA
31500  PRINT D$;"OPEN";F$
31550  PRINT D$;"WRITE";F$
31600  PRINT NRD
31650  FOR I = 0 TO NRD - 1
31700 PV(I) = V(I,0) * V(I,1)
31750  PRINT V(I,0);",";V(I,1);",";PV(I)
31800  NEXT I: PRINT D$;"CLOSE";F$
31850 SPV = 0:SH = 0:SS = 0:RPV = 0:RH = 0:RS = 0                                                  HALT SECTION
31900 Z1PV = PV(0):Z2V0 = V(0,0):Z3V1 = V(0,1)                     CALCULATE AND PRINT MAXIMUM,
31950 A1PV = PV(0):A2V0 = V(0,0):A3V1 = V(0,1)                     MINIMUM, AND AVERAGE VOLTAGES
32000  FOR I = 0 TO NRD - 1                                        AND STANDARD DEVIATIONS
32050 SPV = SPV + PV(I)
32100 SH = SH + V(I,0)
32150 SS = SS + V(I,1)
32200  IF PV(I) > Z1PV THEN Z1PV = PV(I)
32250  IF V(I,0) > Z2V0 THEN Z2V0 = V(I,0)
32300  IF V(I,1) > Z3V1 THEN Z3V1 = V(I,1)
32350  IF PV(I) < A1PV THEN A1PV = PV(I)
32400  IF V(I,0) < A2V0 THEN A2V0 = V(I,0)
32450  IF V(I,1) < A3V1 THEN A3V1 = V(I,1)
32500  NEXT I
32550 PAVG = SPV / NRD:HAVG = SH / NRD:SAVG = SS / NRD
32600  FOR I = 0 TO NRD - 1
32650 PDE = PAVG - PV(I)
32700 HDE = HAVG - V(I,0)
32750 SDE = SAVG - V(I,1)
32800 RPV = RPV + PDE ^ 2
32850 RH = RH + HDE ^ 2
32900 RS = RS + SDE ^ 2
32950  NEXT I
33000 DIV = NRD * (NRD - 1)
33050 PSDM =  SQR (RPV / DIV):HSDM =  SQR (RH / DIV)
33051 SDM =  SQR (RS / DIV)
33100  PRINT D$;"PR#1": PRINT  CHR$ (9);"132N"
33150  PRINT : PRINT : PRINT
33200  PRINT  SPC( 19)"MIN" SPC( 13)"MAX" SPC( 13)"AVG" SPC( 14)"SDM"
33250  PRINT "(EHTR)*(ESTD)",A1PV,Z1PV,PAVG,PSDM
33300  PRINT "EHTR",A2V0,Z2V0,HAVG,HSDM
33350  PRINT "ESTD",A3V0,Z3V1,SAVG,SDM
33400  PRINT D$;"PR#0": HOME : PRINT "DONE"
33450  END
```

EXAMPLE

```
]RUN

ELECTRICAL CALIBRATION:

GATE TIME = 20 SEC

TIME BETWEEN DVM RDGS = 2 SEC
```

```
PAUSE FOR 2 MIN

SEE LINES 20350-20450 OF PROGRAM TO ALTER THESE VALUES


DATE (MONTH DAY)?AUG23

SERIES?B

ENTER DESIRED INITIAL TEMPERATURE?22.52

ENERGY EQUIVALENT = 460J/K - (Y OR N)?Y

ENTER EMF OF THE POWER SUPPLY?5.000

CALIBRATION

RESET HP-5325B COUNTER



HIT THE SPACE BAR TO CONTINUE
SELECT:

1 - TIME HEATER ON
2 - DESIRED DELTA T
3 - HEAT DELIVERED
?1
MAX TIME = 350 SECONDS

ENTER TIME HEATER ON IN SECONDS? 60



          TEMP (C)       DELTA (MICRODEG)

          22.536417            813
          22.537209            791
          22.537936            726
          22.538652            716
          22.539412            759
          22.540138            726
          22.540865            726
          22.541625            759
          22.542395            770
          22.543100            705
          22.543859            759
          22.544532            672
          22.545205            672
          22.545834            629
          22.546474            640
          22.547092            618
          22.547743            650

              TYPE (H) TO STOP
```

H

AUG23B:

POINT	TIME	TEMP (C)	DELTA (MICRODEG)
0	0	22.4977978	0
1	20.08	22.4986006	802
2	40.16	22.4993817	781
3	60.24	22.5001627	781
4	80.32	22.5008679	705
5	100.4	22.5016381	770
6	120.48	22.50243	791
7	140.56	22.5031569	726
8	160.64	22.5038729	715
9	180.72	22.5046539	781
10	200.8	22.5053482	694
11	220.88	22.5060425	694
12	240.96	22.5067585	716
13	261.04	22.5074203	661
14	281.12	22.5082339	813
15	301.2	22.5095357	1301
16	321.28	22.5117705	2234
17	341.36	22.5149165	3146
18	361.44	22.5184313	3514
19	381.52	22.5215774	3146
20	401.6	22.5240074	2430
21	421.68	22.5259601	1952
22	441.76	22.5276741	1714
23	461.84	22.5292146	1540
24	481.92	22.5305706	1356
25	502	22.5317965	1225
26	522.08	22.5328813	1084
27	542.16	22.533836	954
28	562.24	22.5347364	900
29	582.32	22.5356043	867
30	602.4	22.5364179	813
31	622.48	22.5372098	791
32	642.56	22.5379366	726
33	662.64	22.5386526	716
34	682.72	22.539412	759
35	702.8	22.5401389	726
36	722.88	22.5408657	726
37	742.96	22.5416251	759
38	763.04	22.5423953	770
39	783.12	22.5431005	705
40	803.2	22.5438599	759
41	823.28	22.5445324	672
42	843.36	22.545205	672
43	863.44	22.5458342	629
44	883.52	22.5464743	640
45	903.6	22.5470926	618
46	923.68	22.5477436	650

	MIN	MAX	AVG	SDM
(EHTR)*(ESTD)	.288528982	.28854858	.288536869	9.4127059E-07
EHTR	.0592062	.0592101	.0592078467	1.80531875E-07
ESTD	4.87328	4.8733	4.87328766	1.41278412E-06

SOLNF

This program is used to acquire data from a process heat measurement using the isoperibol solution calorimeter.

```
50  DIM T(200),F(200)
100  DIM V(175,1),FV(175)
150 D$ =  CHR$ (4):Z$ =  CHR$ (26)
200  HOME : GOTO 20300                                  BRANCH TO INITIALIZATION ROUTINE
250 CV =  PEEK (37): PRINT D$;"PR#0": VTAB 24: PRINT  SPC( 4)COM$;
251  VTAB CV + 1: HTAB 1: IF IR = 1 THEN  PRINT         RESET IEEE SLOT AND PRINT COMMENTS ON SCREEN
300 IR = 0: GOSUB 400: RETURN
350  POKE 56,3: POKE 57,197
400  POKE 54,6: POKE 55,197: CALL 1002: RETURN
450  PRINT "RDC";Z$;: INPUT FR$                         READ COUNTER
500  IF JU = 1 THEN JU = 0: GOTO 450
550 F(INDX) =  VAL ( RIGHT$ (FR$,18))
600 T(INDX) = (F(INDX) - A) / B
650  IF L2 = 1 THEN 950
700  IF L > 1 THEN 1000
750 TF = T(1):CT = TS - TF: IF CT <  = 0 THEN 19000
800  PRINT "WT#";Z$;"GA10RE"                                                    COUNTER READ AND
850 TT% =  INT (ES * CT / P)                                                    DISPLAY SECTION
900 MS = TT% / 60:MI =  INT (MS):SF = (MS - MI) * 60
901 T$ =  STR$ ((MI * 100) + SF)
950 DE = 0: GOTO 1050
1000 DE =  INT ((T(INDX) - T(INDX - 1)) * 1E+06)
1050 TP$ =  LEFT$ ( STR$ (T(INDX)),9):T(0) = T(1):L2 = 0   DETERMINE TEMPERATURE AND DELTA TEMP
1100  IF  LEN (TP$) = 9 THEN 1200                         AND PRINT BOTH ON SCREEN
1150 TP$ = TP$ + "0": GOTO 1100
1200  PRINT D$;"PR#0": PRINT TP$ SPC( 10)DE
1250  GOSUB 400
1300  IF CF = 1 THEN CF = 0: GOTO 2250
1350  RETURN
1400  FOR INDX = 1 TO 200
1450  PRINT "WT)";Z$;"TE": PRINT "RDI";Z$;: INPUT TE%
1500  IF TE% < (GT - 10) THEN 1650
1550  GOSUB 450
1600  PRINT "WT)";Z$;"TE0TE2":JU = 1: NEXT INDX: GOTO 30000                    MAIN DATA LOGGING LOOP
1650 K =  PEEK ( - 16384): IF K > 127 THEN 1750
1700  GOTO 1450
1750  POKE  - 16368,0:K = K - 128
1800  FOR S = 1 TO 30:X =  PEEK ( - 16336): NEXT S      CHECK KEYBOARD AND BRANCH
1850  IF K = 72 THEN 30000                              IF COMMAND SELECTED
1900  IF K = 82 THEN 2000
1950  GOTO 1450
2000  REM
2050 COM$ = "TYPE (H) TO STOP":IR = 1: GOSUB 250        BEGIN LOGGING DATA                 RUN SECTION
2100 T(0) = T(INDX - 1):INDX = 1:: GOTO 1450
10000 TL = TT% - ((L - 2) * 10.08)
10050  IF TL < (5.08) THEN 10400
10100  GOSUB 450
10150 L = L + 1: GOTO 10000
10200  PRINT "WT)";Z$;"DC4,0TI" + T$                    TURN HEATER ON
```

```
10250  PRINT "WT#";Z$;"RE"
10300 COM$ = "HEATER ON" +  LEFT$ (SP$,12): GOSUB 250
10350 L = L + 1: GOTO 10000
10400  PRINT "SPI";Z$;: INPUT H$
10450  IF H$ (  ) "48" THEN 10400                                                    INITIAL SOLUTION
10500  IF FL = 1 THEN 10750                                                          WARM-UP SECTION
10550  PRINT "WT)";Z$;"DO4,0"                                                        (GATE TIME = 10 SEC)
10600  COM$ = "PAUSE FOR " +  STR$ (PA) + " MIN": GOSUB 250
10650 L = 2:FL = 1:TT% = PA * 60
10700  PRINT "WT)";Z$;"TI" + PB$: PRINT "WT#";Z$;"RE": GOTO 10000 BEGIN PAUSE MODE
10750  PRINT "WT)";Z$;"SE0"
10800  PRINT "WT#";Z$;"GA" +  STR$ (T1) + "RE"
10850  PRINT "WT)";Z$;"TE0TE2"
10900  HOME
10950 COM$ = "TYPE (R) TO RUN  ": GOSUB 250:L2 = 1: GOTO 1400
19000  PRINT D$;"PR#0": PRINT D$;"IN#0": POKE 34,0: POKE 35,23
19050  POKE 32,0: POKE 33,40: HOME                          INITIAL SPECIFIED TEMPERATURE TOO LOW
19051  PRINT "DESIRED TEMPERATURE LOWER THAN SOLUTION TEMPERATURE"
19100  PRINT : PRINT "SOLN TEMP = ";TF
19101  PRINT : PRINT "EXECUTION HALTED": END
20000  POKE 32,7
20050  POKE 33,30                                            DEFINE TEXT WINDOW FOR TEMPERATURE DISPLAY
20100  POKE 34,4
20150  POKE 35,22
20200  VTAB 3: PRINT "TEMP (C)"; SPC( 6)"DELTA (MICRODEG)"
20250  RETURN
20300  PRINT "CHEMICAL RUN:": PRINT
20350 T1 = 29.999:T2 = .08:GT = T1 + T2                     T1 = GATE TIME, T2 = DEAD TIME
20400 PLC = 1!:TM = 2!                                      TM = TIME BETWEEN DVM MEASUREMENTS
20450 PA =  3:FL = 0:L2 = 0:JU = 0:CF = 0                   PLC = INTEGRATION TIME OF THE DVM
20500  PRINT : PRINT "GATE TIME = ";T1;" SEC"                      (IN POWER LINE CYCLES)
20550  PRINT : PRINT "PAUSE FOR ";PA;" MIN"
20599  PRINT                                                PA = PAUSE TIME (IN MINUTES)
20600  PRINT "SEE LINES 20350-20450 TO ALTER THESE VALUES"
20601  PRINT : PRINT
20650  PRINT : PRINT
20700  PRINT "DATE (MONTH DAY)";: INPUT DA$: PRINT                                   INITIALIZATION SECTION
20750  PRINT "SERIES";: INPUT SE$: HOME
20800 FI$ = DA$ + SE$
20850 R1 = 82.3:RT = 83.4                                   SYSTEM RESISTANCES FOR POWER ESTIMATION
20900 ES = 460!                                             ES = SYSTEM ENERGY EQUIVALENT (J/K)
20950  PRINT : PRINT "ENTER DESIRED INITIAL TEMPERATURE";
20951  INPUT TS
21000  PRINT : PRINT "ENERGY EQUIVALENT = ";ES;"J/K - (Y OR N)";
21050  INPUT R$: IF R$ = "Y" THEN 21150                     REQUEST INITIAL SOLUTION WARM-UP PARAMETERS
21100  INPUT "ENTER ENERGY EQUIVALENT (J/K)";ES
21150  PRINT : INPUT "ENTER EMF OF THE POWER SUPPLY  ";EP
21200 P = (EP ^ 2 / RT ^ 2) * R1
21250 A = 8226!:B = 921.8
21300 MS = PA:MI =  INT (MS):SF = (MS - MI) * 60
21301 PB$ =  STR$ ((MI * 100) + SF)
21350 SP$ = "                                "
21400  HOME
21450  GOSUB 20000
```

```
21500  PRINT D$;"PR#5": PRINT D$;"IN#5"
21550  PRINT "CA": PRINT "RA": PRINT "LL": PRINT "LF1"
21551  PRINT "WT6";Z$;"T4"
21600 SU$ = "INFN1SM0WA0GA2"                                  INITIALIZE INSTRUMENTS ON THE BUS
21650  PRINT "WT#";Z$;SU$
21700  PRINT "WT#";Z$;"AZ0MO-28.2E6AU0"
21750  PRINT "WT6";Z$;"T4"
21800  PRINT "WT)";Z$;"SD0SE10"
21850  PRINT "WT#";Z$;"RE"
21900 L = 1:INDX = 1: GOSUB 450
21950  GOTO 10200
30000  POKE 32,0: POKE 33,40
30050  POKE 34,0: POKE 35,24
30100  PRINT "CL";"#";Z$:
30150  HOME : PRINT D$;"PR#0"
30200  PRINT "CREATING:": PRINT : PRINT FI$                   CREATE DISK FILE TO STORE FREQUENCY DATA
30250  PRINT D$;"OPEN";FI$: PRINT D$;"WRITE";FI$
30300  PRINT INDX - 1:NPTS = INDX - 1
30350  FOR J = 1 TO INDX - 1
30400  PRINT F(J): NEXT J
30450  PRINT D$;"CLOSE";FI$
30500  PRINT D$;"PR#1": PRINT : PRINT
30550  PRINT  CHR$ (9);"132N"
30600  PRINT FI$ + ":": PRINT                                                    HALT SECTION
30650  PRINT "POINT" TAB( 11)"TIME" TAB( 22)"TEMP (C)" TAB( 22);
30651  PRINT "DELTA (MICRODEG)"
30700  FOR I = 1 TO NPTS                                      LIST TIME-TEMPERATURE DATA ON PRINTER
30750 TIME = (I - 1) * (T1 + T2)
30800 S1 = (9 -  LEN ( STR$ (TIME))) + 16
30850 S2 = (10 -  LEN ( STR$ (T(I)))) + 26
30900  IF I = 1 THEN DE = 0: GOTO 31000
30950 DE =  INT ((T(I) - T(I - 1)) * 1E+06)
31000  IF I - 1 < 10 THEN  PRINT "  "I - 1 TAB( 12);: GOTO 31100
31050  PRINT " ";I - 1; TAB( 12)
31100  PRINT TIME SPC( S1)T(I) SPC( S2)DE: NEXT I
31150  HOME : PRINT D$;"PR#0": PRINT D$;"IN#0"
```

EXAMPLE

```
]RUN

CHEMICAL RUN:

GATE TIME = 20 SEC

PAUSE FOR 2 MIN

SEE LINES 20260-20264 OF PROGRAM TO ALTER THESE VALUES
```

DATE (MONTH DAY)?AUG22

SERIES?D

ENTER DESIRED INITIAL TEMPERATURE?22.37

ENERGY EQUIVALENT = 460J/K - (Y OR N)?Y

ENTER EMF OF THE POWER SUPPLY?5.000

TEMP (C)	DELTA (MICRODEG)
22.370785	303
22.371197	412
22.371544	347
22.371957	412
22.372315	358
22.372716	401
22.373063	347
22.373389	325
22.373833	444
22.374365	531
22.374994	629
22.375602	607
22.376242	640
22.376882	640
22.377424	542
22.377934	509

TYPE (H) TO STOP

AUG22D:

POINT	TIME	TEMP (C)	DELTA (MICRODEG)
0	0	22.3715448	0
1	20.08	22.371957	412
2	40.16	22.372315	358
3	60.24	22.3727164	401
4	80.32	22.3730636	347
5	100.4	22.373389	325
6	120.48	22.3738338	444
7	140.56	22.3743654	531
8	160.64	22.3749946	629
9	180.72	22.3756021	607
10	200.8	22.3762421	640
11	220.88	22.3768822	640
12	240.96	22.3774246	542
13	261.04	22.3779345	509

TEMP

This program is used to calculate the resistance of a platinum resistance thermometer from the reading of a six dial resistance bridge. Using the calibration constants of the thermometer, the temperature is then calculated.

```
50 DEFDBL A-C, E-H, P-Z
100 DEFINT D, I-N
150 HOME
200 REM
250 DIM DGT(6,3), DGTIN$(6,3), DAT$(3), DAT(3), D(7), R(7)
300 INPUT "IS DATA IN A DATA FILE (Y,N)"; ANS$
350 IF ANS$ = "Y"  GOTO 600                                   DATA ENTERED EITHER FROM KEYBOARD OR FROM A FILE
399 PRINT: PRINT
400 PRINT "ENTER THREE TEMPERATURE READINGS (CTRL-C TO STOP)"
401 PRINT "(DO NOT INCLUDE DECIMAL POINTS)": PRINT
402 INPUT DAT$(1), DAT$(2), DAT$(3)
500 GOTO 900
550 REM
600 INPUT "ENTER NAME OF DATA FILE"; I$
650 D$ = "B:": F$ = D$ + I$
700 OPEN "I", #1, F$
750 IF EOF(1) THEN END
800 INPUT#1, DAT$(1), DAT$(2), DAT$(3)
850 REM
900 PRINT: PRINT DAT$(1), DAT$(2), DAT$(3)
950 FOR J = 1 TO 3
1000      FOR I = 1 TO 6
1050          DGTIN$(I,J) = MID$(DAT$(J), I, 1)
1100          NEXT I
1150      NEXT J
1200 FOR J = 1 TO 3                                           BRIDGE CONTAINS AN "X" DIAL -- THIS SECTION DEALS WITH THAT DIAL
1250      FOR I = 1 TO 6
1300          IF (DGTIN$(I,J))="0")AND(DGTIN$(I,J)(="9") GOTO 1450
1350          DGT(I,J) = 10
1400          GOTO 1500
1450          DGT(I,J) = VAL(DGTIN$(I,J))
1500          NEXT I
1550      NEXT J
1600 REM
1650 FOR K = 1 TO 3                                           CALL SUBROUTINE TO MAKE DIAL CORRECTIONS
1700      D(1) = DGT(1,K): D(2) = DGT(2,K): D(3) = DGT(3,K)
1750      D(4) = DGT(4,K): D(5) = DGT(5,K): D(6) = DGT(6,K)
1800      GOSUB 3150
1850      R(K) = R
1900      NEXT K
1950 ZN = .001415                                             ZERO CORRECTIONS FOR BRIDGE
2000 ZR = .001435
2050 FCTR = 1!
2100 RN = ((R(1) + R(3)) / 2!) - ZN                           CALCULATE AVERAGE RESISTANCE
2150 RR = R(2) - ZR
2200 RST = (RN + RR) * FCTR / 2!
2250 A1 = .0039244323#
2300 D1# = 1.49716716#                                        PARAMETERS FOR PLATINUM RESISTANCE THERMOMETER
2350 R0 = 25.53885412#
2400 A2 = -.0001*A1*R0*D1#
2450 B1 = (A1 * R0) + (A1 * R0 * D1# * .01)
2500 C1 = R0 - RST
2550 S1 = SQR (B1 * B1 - 4! * A2 * C1)
2600 T = (-B1 + S1) / (2! * A2)                               CALCULATE TEMPERATURE
2650 CORR = (.045) * (T/100!) * ((T/100!)-1!) * ((T/419.58)-1!)
```

```
2651 CORR = CORR*((T/630.74)-1)
2700 TEMP = T + CORR
2750 REM
2798 PRINT: PRINT
2799 PRINT "RESISTANCE = ";
2800 PRINT USING  "### ###_ _O_H_M_S"; RST                    PRINT RESISTANCE AND TEMPERATURE
2849 PRINT "TEMPERATURE = ";
2850 PRINT USING "###.###_ _D_E_G_R_E_E_S_ _C"; TEMP
2900 IF ANS$ = "Y" GOTO 750
2950 GOTO 399
3000 END
3050 REM
3100 REM
3150 REM *** SUBROUTINE RSTNCE ***
3200 R = 0!: D(7) = 0                                        SUBROUTINE FOR APPLYING DIAL CORRECTIONS
3250 FOR J = 1 TO 7: FOR I = 1 TO 10
3300         READ C(I,J)
3350         NEXT I: NEXT J
3400 FOR J = 1 TO 7
3450     FOR I = 1 TO 10
3500          IF I = D(J) GOTO 3600
3550          GOTO 3700
3600          R = R + D(J) * 10!^(2!-J) + C(I,J) * .000001
3650          GOTO 3750
3700          NEXT I
3750     NEXT J
3800 REM
3850 DATA 3452, 8014, 12244, 16806, 18993, 23175, 27429      DIAL CORRECTIONS FOR THE BRIDGE
3900 DATA 31104, 35341, 39099, 521, 1007, 1463, 1961, 2437, 2936
3901 DATA 3382, 3885
3950 DATA 4376, 4792, 190, 429, 654, 813, 1070, 1237, 1455, 1605
3951 DATA 1765, 1911
4000 DATA 1, 2, 8, 14, 20, 21, 27, 33, 39, 45
4050 DATA 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
4100 DATA 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
4150 DATA 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
4200 REM
4250 RESTORE
4300 RETURN
4350 END
4400 REM TEMP OF THERMOM #2 IS EQUAL TO TCALC+.14
```

EXAMPLE

```
RUN

IS DATA IN A DATA FILE (Y,N)? N

ENTER THREE TEMPERATURE READINGS (CTRL-C TO STOP)? 295479,296016,295479

295479         296016         295479


RESISTANCE = 0.295869D+02 OHMS
TEMPERATURE = 0.40020D+02 DEGREES C
```

TEMPQTZ

This program, based upon the one initially written by Dr. R. L. Nuttall [2], is used to calculate the corrected temperature rise from the time-temperature data obtained from the isoperibol solution calorimeter.

```
50 DEFDBL A-H,P-S,U-Z: DEFINT I-L,N-O: DEFSNG M, T
100 ON ERROR GOTO 11250
150 HOME
200 DIM T(200), Y(200), F(2,200), P(200), FR(200)
250 DIM G(3,3), C(3,3), B(3), D(3,3), H(3,0), E(3,0), INDEX(3,2)
300 DIM CC(3), LZ(3)
350 DATA 3,3,.0001
400 DATA 99.999, 0.08, 8.226E3, 9.218E2
450 DATA 12345678
500 READ F, E1, A2
550 READ T1, T2, AF, BF
600 PRINT: PRINT "MAKE SURE PRINTER IS ON":PRINT :PRINT
650 PRINT "GATE TIME = "; T1
700 PRINT: PRINT "DEAD TIME = "; T2
750 PRINT: PRINT "JACKET TEMP = "; V+20!; " C"
800 LPRINT CHR$(25);"132N"
850 PRINT: INPUT "ENTER NAME OF DATA FILE"; FM1$
900 FM$ = "B:" + FM1$
950 OPEN "I", #1, FM$
1000 INPUT#1, NPTS
1050 NM = NPTS - 1
1100 FOR I = 0 TO NM
1150     INPUT#1, FR(I): T(I) = I*(T1+T2)
1200     Y(I) = ((FR(I) - AF) / BF) - 20: NEXT I
1250 CLOSE #1
1300 LPRINT: LPRINT FM$
1350 PRINT: PRINT
1400 PRINT "ENTER STARTING AND ENDING POINT OF MAIN PERIOD";
1401 INPUT LM, M(F)
1450 FOR I = (F-1) TO 1 STEP -1
1500     M(I) = M(I+1) - 1: NEXT I
1550 READ A3
1600 LPRINT
1650 LPRINT "CORRECTED TEMP CHANGES FOR SELECTED END POINTS:"
1700 IF A3 = 12345678# THEN 1850
1750 PRINT "DATA ERROR"
1800 GOTO 8400
1850 FOR J = 1 TO F
1900 Z6 = -T(M(J)) + T(NM)
1950 Z7 = T(LM) - T(0)
2000 R(1) = (Y(NM) - Y(M(J))) / Z6
2050 R(2) = (Y(LM) - Y(0)) / Z7
2100 R(3) = (Y(NM) + Y(M(J))) / 2
2150 R(4) = (Y(LM) +Y(0)) / 2
2200 A = (R(2) - R(1)) / (R(3) - R(4))
2250 A1 = A
2300 Z8 = (1 - EXP(-A*Z6)) / (A*EXP(-A*Z6))
2350 Z9 = (1 - EXP(-A*Z7)) / (A*EXP(-A*Z7))
2400 A = (R(2)*Z7/Z9 - R(1)*Z6/Z8) / (Y(NM) - Y(LM))
2450 IF ABS (A - A1) >= A2 THEN 2250
2500 DENOM1 = (1 - EXP(-A*(T(M(J)) - T(NM))))
2550 B = Y(NM) + (Y(M(J)) - Y(NM)) / DENOM1
```

F = NUMBER OF CALCS OF A CORRECTED TEMP RISE DESIRED, EACH WITH A DIFFERENT TIME SELECTED AS THE END OF THE MAIN PERIOD

T1 = GATE TIME (SEC), T2 = DEAD TIME (SEC)

V = JACKET TEMP (DEG C)

AF, BF = PARAMETERS FROM RELATIONSHIP BETWEEN FREQUENCY AND TEMPERATURE (FROM THE CALIBRATION OF THE QUARTZ PROBE)

E = NUMBER OF ITERATIONS USED IN CALCULATING PARAMETERS

A2 = TOLERANCE LIMIT FOR PARAMETER APPROXIMATION

READ IN FREQUENCY DATA FROM DISK FILE AND CONVERT TO TEMPS

CALCULATE PARAMETERS IN THE LINEARIZED EQUATIONS REPRESENTING TEMPERATURE VS TIME

Y = TEMPERATURE
B = CONVERGENCE TEMPERATURE (theta(inf))
C = INITIAL TEMPERATURE (theta(init))
D = FINAL TEMPERATURE (theta(fin))

```
2600 C = Y(LM)
2650 D = Y(M(J))
2700 IF J < F THEN 3000
2750 LPRINT
2800 LPRINT "k (1/sec)"TAB(17)"Theta(inf)"TAB(29)"Theta(init)";
2850 LPRINT TAB(42) "Theta(fin)"
2900 LPRINT USING "#.######^^^^"; A;
2950 LPRINT USING "_ _ _ _ _ #.#####"; B; C; D
3000 Z3 = 0
3050 FOR I = 0 TO 3: E(I,0) = 0: NEXT I
3100 FOR I = 0 TO 3: FOR J1 = 0 TO 3
3150       G(I,J1) = 0: C(I,J1) = 0: D(I,J1) = 0
3200       NEXT J1: NEXT I
3250 Z5 = 0
3300 FOR I = 0 TO NM                                    PERFORM LEAST SQUARES ON LINEARIZED EQUATIONS
3350    IF I < (LM+1) THEN 3900
3400    IF I > (M(J) - 1) THEN 4300
3450    GOTO 3800
3500    E(0,0) = F(1,I)*F(2,I) + E(0,0)
3550    G(0,0) = F(2,I)^2 + G(0,0)
3600    G(0,1) = -F(2,I)*P(I) + G(0,1)
3650    G(1,1) = P(I)^2 + G(1,1)
3700    E(1,0) = -P(I)*F(1,I) + E(1,0)
3750    Z5 = F(1,I)^2 + Z5
3800    NEXT I
3850 GOTO 4700
3900 P(I) = 1 - EXP(-A*(T(I) - T(LM)))                  CALCULATE THE COEFFICIENTS OF THE NORMAL EQUATIONS
3950 F(1,I) = Y(I) - C - (B-C)*P(I)
4000 F(2,I) = (B-C)*(T(I) - T(LM))*(P(I) - 1)
4050 G(0,2) = F(2,I)*(P(I) - 1) + G(0,2)
4100 G(1,2) = -P(I)*(P(I) - 1) + G(1,2)
4150 G(2,2) = (P(I) - 1)^2 + G(2,2)
4200 E(2,0) = (P(I) - 1)*F(1,I) + E(2,0)
4250 GOTO 3500
4300 P(I) = 1 - EXP(-A*(T(I) - T(M(J))))
4350 F(1,I) = Y(I) - D - (B-D)*P(I)
4400 F(2,I) = (B-D)*(T(I) - T(M(J)))*(P(I) - 1)
4450 G(0,3) = F(2,I)*(P(I) - 1) + G(0,3)
4500 G(1,3) = -P(I)*(P(I) - 1) + G(1,3)
4550 G(3,3) = (P(I) - 1)^2 + G(3,3)
4600 E(3,0) = (P(I) - 1)*F(1,I) + E(3,0)
4650 GOTO 3500
4700 FOR I = 0 TO 3
4750    FOR K = I+1 TO 3
4800       G(K,I) = G(I,K)
4850       NEXT K
4900   NEXT I
4950 GOSUB 8450                                         SOLVE EQUATIONS BY MATRIX INVERSION USING SUBROUTINE
5000 FOR I = 0 TO 3: H(I,0) = 0: NEXT I
5050 FOR I = 0 TO 3: FOR J1 = 0 TO 3
5100       H(I,0) = H(I,0) + C(I,J1)*E(J1,0)
5150       NEXT J1: NEXT I
5200    A = A - H(0,0)
5250    B = B - H(1,0)
5300    C = C - H(2,0)
5350    D = D - H(3,0)
5400 IF J < F THEN 5550
5450 LPRINT USING "#.######^^^^"; A;
5500 LPRINT USING "_ _ _ _ _ #.#####"; B; C; D
5550 Z3 = Z3 + 1
```

```
5600 IF Z3 < E1 THEN 3050
5650 A4 = A*60
5700 U1 = A4*(B-V)                                          CALCULATE THE STIRRING ENERGY
5750 W = 0
5800 T2 = (T(M(J)) - T(LM)) / (M(J) - LM) - T1
5850 FOR I = LM+1 TO M(J)
5900    W = W + Y(I)*(T(I) - T(I-1))
5950    NEXT I
6000 W = W - T2*(Y(M(J)) - Y(LM)) / 2                       CALCULATE THE CORRECTION ON THE OBSERVED TEMP RISE (Z1)
6050 Z1 = A*(B*(T(M(J)) - T(LM)) - W)
6100 Z2 = (C-D)*A*T1 / (EXP(A*T1) - 1)                      CALCULATE THE OBSERVED TEMP RISE (Z2)
6150 IF J = F THEN 6350
6200 LPRINT USING "#.######"; -Z2-Z1
6250 IF J < F THEN 6650
6300 LPRINT
6350 LPRINT "MEAN TEMP = ";: LPRINT USING "#.######"; (C+D)/2
6400 LPRINT USING "_O_B_S_V_ _R_I_S_E_ #.######"; -Z2
6450 LPRINT USING "_C_O_R_R_ _O_N_ #.######****"; Z1        PRINT CALCULATED RESULTS
6500 LPRINT "THE CORRECTED TEMP CHANGE ..... ";
6550 LPRINT USING "#.######"; -Z2-Z1
6600 LPRINT USING "_U_ _=_ #.#####****"; U1
6650 NEXT J
6700 LPRINT
6750 LPRINT "TIME(SEC)      OBSVD TEMP    OBSVD-CALC TEMP";
6800 LPRINT " (MICRODEG)   "
6850 LPRINT
6900 FOR I = 0 TO LM                                        PRINT TIME-TEMP DATA AND THE DIFFERENCES BETWEEN CALCULATED
6950 LPRINT USING "####.#"; T(I) - T(0);                    AND OBSERVED TEMPERATURES AT EACH MEASUREMENT POINT IN THE
7000 LPRINT USING "_ _ _ _ _ _ _ _ _ #.######"; Y(I);       FORE AND AFTER PERIODS
7050 LPRINT "         ";
7100 LPRINT USING "#####.#"; (Y(I)-C-(B-C)*P(I))*1E+06
7150 NEXT I
7200 LPRINT
7250 FOR I = M(F) TO NM
7300 P(I) = 1 - EXP(-A*(T(I) - T(M(F))))
7350 LPRINT USING "####.#"; T(I) - T(0);
7400 LPRINT USING "_ _ _ _ _ _ _ _ _ #.######"; Y(I);
7450 LPRINT "          ";
7500 LPRINT USING "#####.#"; (Y(I)-D-(B-D)*P(I))*1E+06
7550 NEXT I
7600 LPRINT
7650 LPRINT "ERROR MATRIX"
7700 LPRINT: FOR I = 0 TO 3                                 PRINT VARIANCE-COVARIANCE MATRIX WHICH CONTAINS INFORMATION
7750 LPRINT USING "#.#####****_ _ ";C(I,0);C(I,1);C(I,2);C(I,3)   ON THE VARIANCE OF THE FITTED CURVE AND OF THE ADJUSTED PARAMETERS
7800 NEXT I
7850 S=Z5-E(0,0)*H(0,0)-E(1,0)*H(1,0)-E(2,0)*H(2,0)-E(3,0)*H(3,0)
7900 LPRINT : LPRINT USING "#.#####****"; S
7950 S1 = S / (LM+NM-M(F)-2)
8000 S2 = S1*C(0,0)
8050 S3 = S1*C(1,1)                                         CALCULATE AND PRINT THE STANDARD
8100 S4 = S1*C(2,2)                                         DEVIATIONS OF THE CALCULATED PARAMETERS
8150 S5 = S1*C(3,3)
8200 LPRINT "SIGMA"TAB(20)"SIGMA(k)"TAB(39)"SIGMA(Theta(inf))";
8250 LPRINT TAB(58)"SIGMA(Theta(init))"TAB(77)"SIGMA(Theta(fin))"
8300 LPRINT USING "#.######****_ _ _ _ _ _ _ _ "; SQR(S1); SQR(S2);
8350 LPRINT USING "#.######****_ _ _ _ _ _ _ _ "; SQR(S3); SQR(S4);
8351 LPRINT USING "#.######****_ _ _ _ _ _ _ _ "; SQR(S5)
8400 END
8450 DELTA = 1: EPS = .00001
8500 NEROR = 0: N = 3
```

```
8550 FOR J1 = 0 TO N
0600    LZ(J1) = J1: NEXT J1
8650 FOR I = 0 TO N
8700    K = I
8750    YY = G(I,I)
0800    L = I-1
8850    LP = I+1
0900    IF (N-LP) < 0 THEN 9250
8950    FOR J1 = LP TO N
9000       WW = G(I,J1)
9050       IF (ABS(WW) - ABS(YY)) <= 0 THEN 9200
9100       K = J1
9150       YY = WW
9200       NEXT J1
9250    DELTA = DELTA*YY
9300    FOR J1 = 0 TO N                                    MATRIX INVERSION SUBROUTINE
9350       CC(J1) = G(J1,K)
9400       G(J1,K) = G(J1,I)
9450       G(J1,I) = -CC(J1) / YY
9500       G(I,J1) = G(I,J1) / YY
9550       B(J1) = G(I,J1): NEXT J1
9600    G(I,I) = 1 / YY
9650    J1 = LZ(I)
9700    LZ(I) = LZ(K)
9750    LZ(K) = J1
9000    FOR K = 0 TO N
9850       IF (I-K) = 0 THEN 10100
9900       FOR J1 = 0 TO N
9950          IF (I-J1) = 0 THEN 10050
10000          G(K,J1) = G(K,J1) - B(J1)*CC(K)
10050          NEXT J1
10100       NEXT K
10150    NEXT I
10200 IF (ABS(DELTA) - EPS) > 0 THEN 10300
10250 NEROR = 1: PRINT "**********************": GOTO 11200
10300 FOR I = 0 TO N
10350    IF (I-LZ(I)) = 0 THEN 11050
10400    K = I+1
10450    IF (I-N) >= 0 THEN 11050
10500    FOR J1 = K TO N
10550       IF (I-LZ(J1)) <> 0 THEN 11000
10600       MM = LZ(I)
10650       LZ(I) = LZ(J1)
10700       LZ(J1) = MM
10750       DELTA = -DELTA
10800       FOR L = 0 TO N
10850          CC(L) = G(I,L)
10900          G(I,L) = G(J1,L)
10950          G(J1,L) = CC(L): NEXT L
11000       NEXT J1
11050    NEXT I
11100 FOR I = 0 TO 3: FOR J1 = 0 TO 3: C(I,J1) = G(I,J1): NEXT J1
11150 NEXT I
11200 RETURN
11250 PRINT ERR, ERL: STOP
```

EXAMPLE

RUN

MAKE SURE PRINTER IS ON

```
GATE TIME =  100

DEAD TIME =  1.6

ENTER JACKET TEMP (DEG C) ? 25.2203

ENTER NAME OF DATA FILE? CALTEMP.DAT


ENTER STARTING AND ENDING POINT OF MAIN PERIOD? 14,20

CORRECTED TEMP CHANGES FOR SELECTED END POINTS:
0.282412
0.282427

k (1/sec)          Theta(inf)  Theta(init)  Theta(fin)
0.102927D-03        5.20177      4.82820      5.12050
0.102955D-03        5.20161      4.82822      5.12049
0.102955D-03        5.20161      4.82822      5.12049
0.102956D-03        5.20161      4.82822      5.12049

MEAN  TEMP = 4.974352
OBSV RISE 0.290771
CORR ON 0.834891D-02
THE  CORRECTED TEMP CHANGE..... 0.282422
U = -.11547D-03

TIME(SEC)      OBSVD TEMP     OBSVD-CALC TEMP (MICRODEG)

   0.0          4.769310            -19.3
 101.6          4.773810            -17.4
 203.2          4.778270             -8.8
 304.8          4.782690              6.1
 406.4          4.787060             16.9
 508.0          4.791370             13.1
 609.6          4.795640             14.1
 711.2          4.799870             19.6
 812.8          4.804030             -1.0
 914.4          4.808170              1.9
1016.0          4.812270              7.9
1117.6          4.816320              6.4
1219.2          4.820320             -2.8
1320.8          4.824270            -20.4
1422.4          4.828200            -16.6

2032.0          5.120500             12.0
2133.6          5.121340              7.9
2235.2          5.122170              2.6
2336.8          5.122990             -4.1
2438.4          5.123800            -12.1
2540.0          5.124600            -21.6
2641.6          5.125410            -12.7
2743.2          5.126210             -5.5
2844.8          5.127010             10.0
2946.4          5.127800             23.7

ERROR MATRIX

0.14410D-04  -.45915D-01  0.66756D-03  0.16339D-02
-.45915D-01  0.17157D+03  -.27136D+00  -.63881D+01
0.66756D-03  -.27136D+00  0.22457D+00  -.11115D-01
0.16339D-02  -.63881D+01  -.11115D-01  0.35023D+00

0.43338D-08
SIGMA              SIGMA(k)            SIGMA(Theta(inf))  SIGMA(Theta(init))  SIGMA(Theta(fin))
0.143656E-04       0.545327E-07        0.188165E-03       0.680762E-05        0.850151E-05
```

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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

The computer software used for the acquisition and treatment of data from both heat-conduction microcalorimeters and an isoperibol solution calorimeter is described. For each program contained in this Technical Note there is documentation given which includes a listing of the program, comments, and an example of its use. The hardware used in the data acquisition is briefly described.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

chemical thermodynamics; computer software; data acquisition; enthalpy; heat-conduction microcalorimetry; isoperibol solution calorimetry; kinetics.

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