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# ANALYSIS OF GRAN'S PLOT ACIDITY DATA

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NOVEMBER 1981

## Purpose

This program is an Fortran version of the Interactive Analysis of Gran's plot Acidity data program written by Paul Kluckner in June 1981 for the Ministry of Environment, Environmental Laboratory.

It accepts inputs of data from Gran's plot acidity titration used for the analysis of precipitation samples. Gran's functions are calculated and plotted for each data point. Data obtained on the acidity side of the inflection point can be analysed to detect the presence of strong acidity.

The program is also set up to enter the calculated values directly into the Laboratory Data Management data files located under the signon I.D. WQB6 if desired.

## Requirements

The current implementation is accessed by dialup terminals located in the Water Quality laboratory to an IBM 4341 located at Simon Fraser University. The program is written for use at MTS (Michigan Terminal System) facilities and may not be implemented directly at non-MTS facilities.

## Procedure

1. After signing on to MTS, type in 'SOU GRANS' to start the program running.
2. Input the normality of NaOH titrant, and the initial volume (ML).
3. Input the sample name (max 32 characters) and measured pH. If the data is to be added to the data file, enter the sample number instead

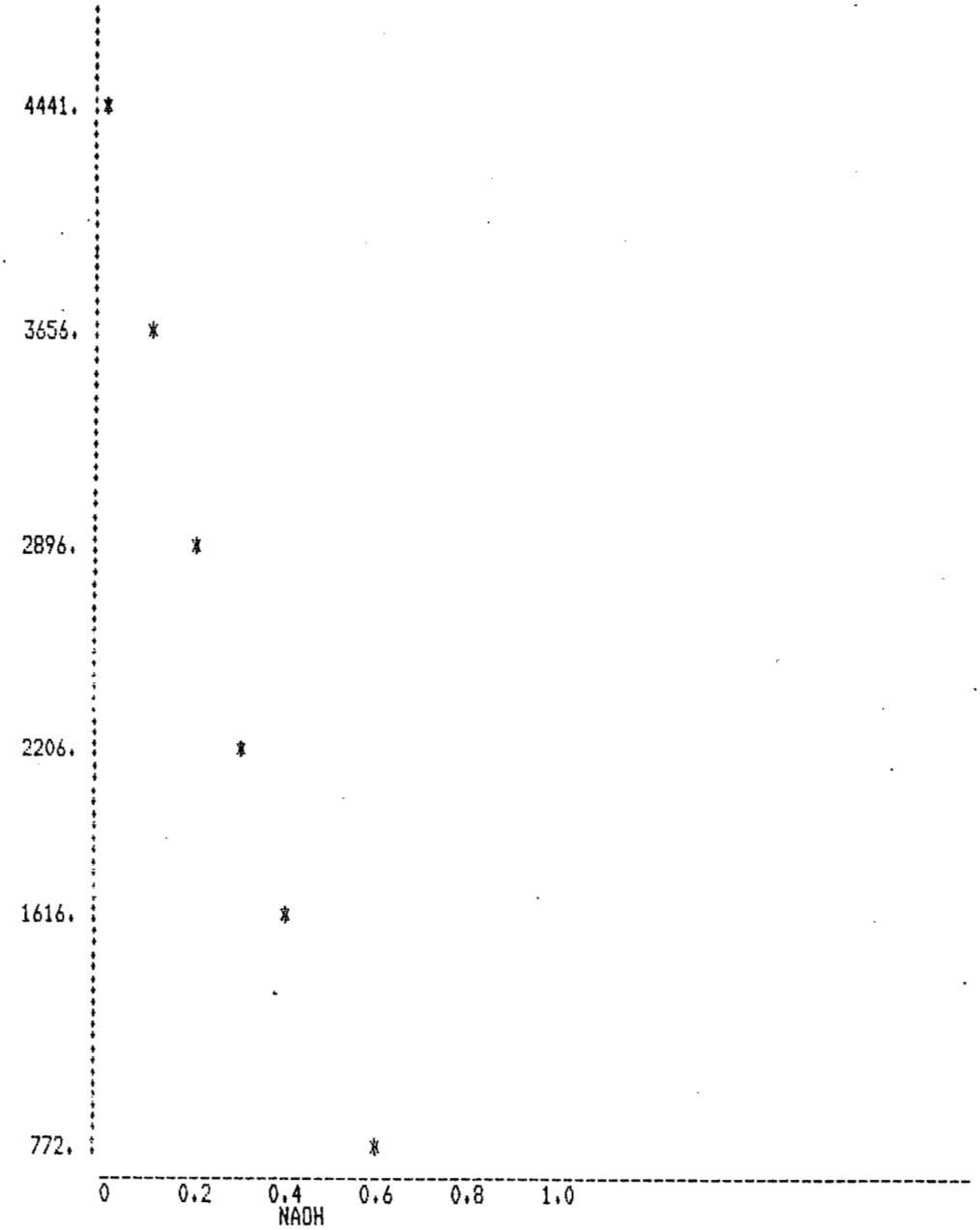
of the name, after which you will be prompted for the temperature and specific conductance as well as the usual information. Then input the pairs of the volume (ML) and meter readings (MV) for each point in the titration (max 20 pairs).

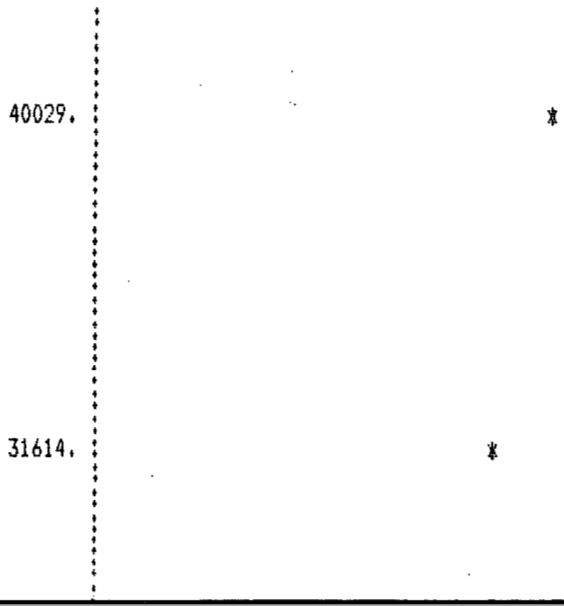
There should be a minimum of five points on the acid side and four points on the base side to permit accurate evaluation of the data. Note that negative MV readings must be entered as - xxx.

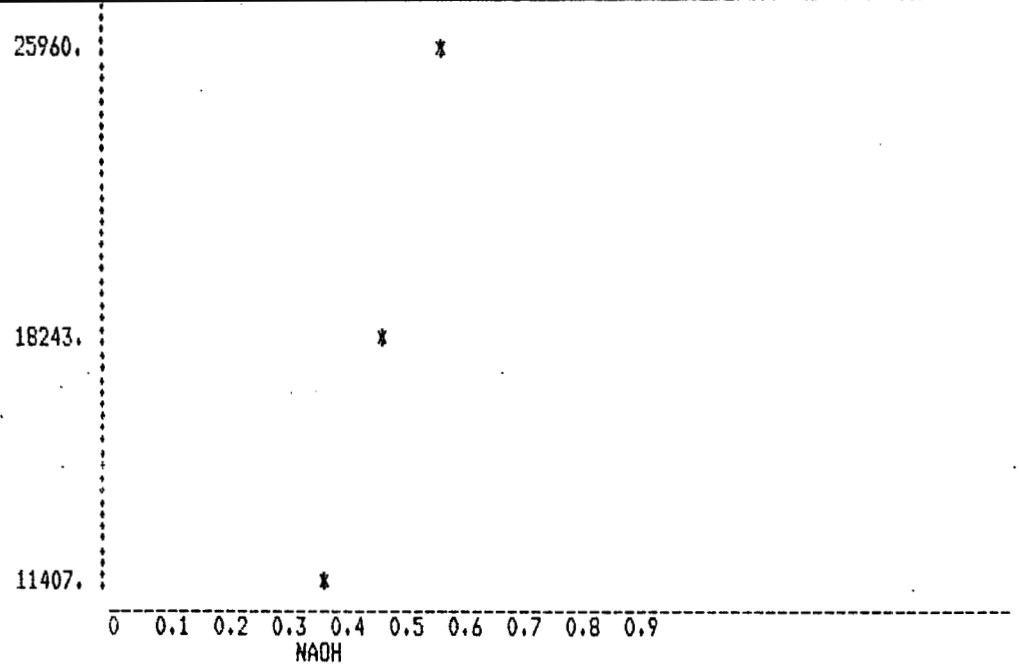
4. When all data points have been entered, enter o,o.
5. Edit data if desired. To finish INSERTing, DELETing or CORRECTing, enter a 'o' for the index of pair prompt.
6. If fewer than 4 acid points have been entered, the program will assume no strong acid and will not plot acid data.
7. If the correlation coefficient ($r^2$) of an exponential regression performed on the acid side is better (ie. closer to 1) than a linear regression, the program will assume that 15 ueq /L strong acid are present. If you agree, enter 'Y'es after the appropriate prompt. The program will then complete the analysis of this sample. Go to step 3 for the next sample or enter 'STOP' if no more samples are to be entered.
8. If you do not agree and there is evidence that the bottom part of the plot is curved, the plot can be edited by entering 'Y' in response to 'Remove points?', note that four points are normally necessary to accurrately determine the presence of strong acid. If the data is edited to the point where less than three points are available for the linear regression the program will override the editing, assume that 15 ueq /L of strong acid are present, and proceed with the analysis of the base side data.

SAMPLE RUN:

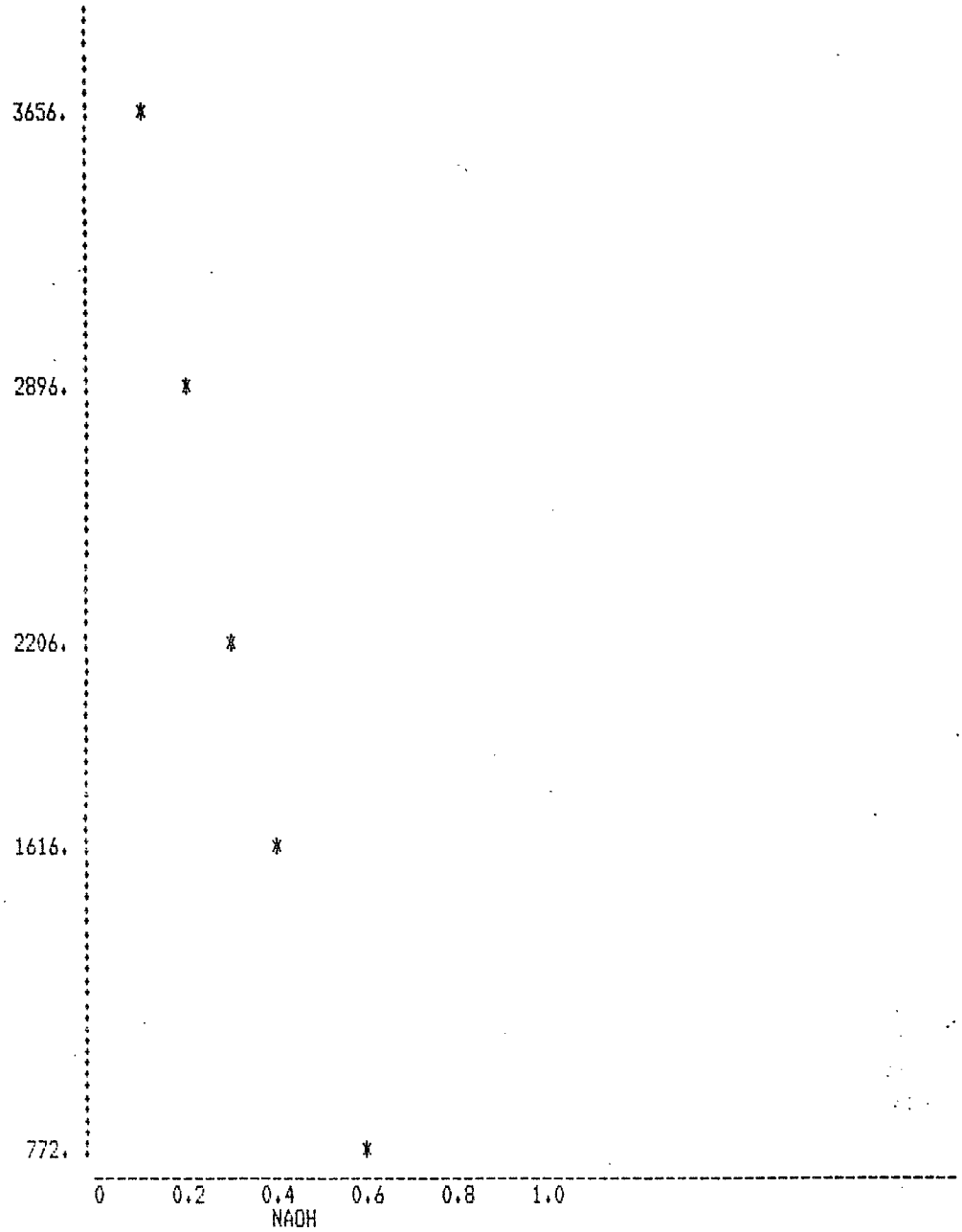
```
 SOU GRANS
#$R GRANS.MAIN+GRANS.LIB+UNSP:UBCLIB
#Execution Begins   10:48:38
 ENTER NORMALITY OF NAOH

?.009071
 ENTER SAMPLE VOLUME(ML)

?40
 ENTER SAMPLE NAME OR 'STOP'

?TEST
 ENTER MEASURED PH

?4.92
 ENTER ML,MV IN ORDER - MAX 20

 DATA PTS 0,0 TO END

?0,121
?.01,116
?.02,110
?.03,103
?.04,95
?.06,76
?.37,-145
?.47,-157
?.57,-166
?.67,-171
?.77,-177
?0,0
 DO YOU WANT TO VIEW GRAPHS?

?Y
```

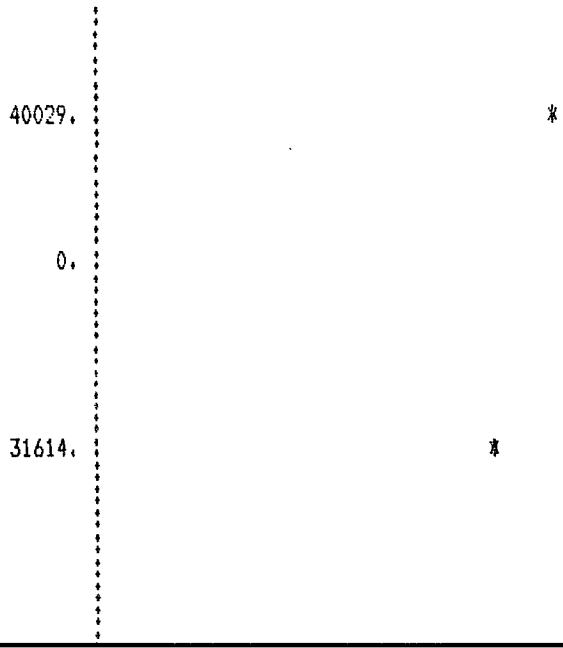

4441.
3656.
2896.
2206.
1616.
772.
0
0.2
0.4
0.6
0.8
1.0
NAOH


40029.
31614.




```
DO YOU WISH TO EDIT? (Y/N)

?Y
 ENTER ONE OF 'CORRECT','INSERT','DELETE'

?INSERT
 INDEX OF PAIR TO INSERT

?1
 ENTER NEW ML,MV

?.015,119
 INDEX OF PAIR TO INSERT

?0
 MORE EDITING? (Y/N)
?Y
 ENTER ONE OF 'CORRECT','INSERT','DELETE'

?DELETE
 INDEX OF PAIR TO DELETE

?1
 DELETE   0.0150 119.0000
 INDEX OF PAIR TO DELETE

?0
 MORE EDITING? (Y/N)
?N
 CALCULATION NECESSARY - STANDBY

 DO YOU WANT TO VIEW GRAPHS?

?NO
 DO YOU WISH TO EDIT? (Y/N)

?N
 SAMPLE IDENT

 TEST

 MEASURED PH   4.920

 #     ML      MV      GRAN'S FN

  1   0.01   116.      36.6E+02
  2   0.02   110.      29.0E+02
  3   0.03   103.      22.1E+02
  4   0.04    95.      16.2E+02
  5   0.06    76.      77.2E+01
  6   0.37  -145.      11.4E+03
  7   0.47  -157.      18.2E+03
  8   0.57  -166.      26.0E+03
  9   0.67  -171.      31.6E+03
 10   0.77  -177.      40.0E+03
 11   0.00     0.      40.0E+00
```


3656.
2896.
2206.
1616.
772.
0
0.2
0.4
0.6
0.8
1.0
NAOH


40029.
0.
31614.

```
>     1     C
>     2     C*********************************************************************************
>     3     C
>     4     C  PLOT FUNCTIONS
>     5     C   THESE THREE SUBROUTINES CALCUTE THE APPROPRIATE FUNCTION FOR THE
>     6     C   GRAN'S FUNCTION. THEY ARE CALLED BY 'MAIN'.
>     7     C
>     8     C*********************************************************************************
>     9     C
>    10           REAL FUNCTION FNV(Y,X)
>    11           REAL Y(20,4),X
>    12           FNV=EXP(Y(1,2)+Y(1,3)*X)
>    13           RETURN
>    14           END
>    15     C
>    16           REAL FUNCTION FNV2(Y,X,F3)
>    17           REAL Y(20,4),X
>    18           INTEGER F3
>    19           FNV2=Y(F3,2)+Y(F3,3)*X
>    20           RETURN
>    21           END
>    22     C
>    23           REAL FUNCTION FND(J,VV1,VV2,V1)
>    24           REAL V1,VV1(20),VV2(20)
>    25           FND=(V1+VV1(J))*10**(ABS(VV2(J))/59.157)
>    26           RETURN
>    27           END
>    28
>    29
>    30     C
>    31     C*********************************************************************************
>    32     C
>    33     C DOES LINEAR REGRESSION CALCULATIONS USING GRAN'S FUNCTION CALCULATIONS
>    34     C AND INPUT VOLUMES. CALLED  BY 'MAIN'
>    35     C
>    36     C*********************************************************************************
>    37     C
>    38           SUBROUTINE LIN(A,M,N1,F3,F5,GG2,VV1,Y,S,N,V1)
>    39           REAL GG2(20),VV1(20),M(5),S,A(5),Y(20,4),V1,N
>    40           INTEGER F3,F5,I,N1
>    41           DO 50 I=1,5
>    42      50   A(I)=0.0
>    43           N1=F3-F5+1
>    44           DO 51 I1=F5,F3
>    45           A(1)=A(1)+VV1(I1)
>    46           A(2)=A(2)+VV1(I1)*VV1(I1)
>    47           A(3)=A(3)+GG2(I1)
>    48           A(4)=A(4)+GG2(I1)*GG2(I1)
>    49           A(5)=A(5)+VV1(I1)*GG2(I1)
>    50      51   CONTINUE
>    51           M(1)=A(1)/N1
>    52           M(2)=(A(2)-A(1)*A(1)/N1)/(N1-1.0)
>    53           M(3)=A(3)/N1
>    54           M(4)=(A(4)-A(3)*A(3)/N1)/(N1-1.0)
>    55           M(5)=(A(5)-A(1)*A(3)/N1)/(A(2)-A(1)*A(1)/N1)
>    56           Y(F3,2)=M(3)-M(1)*M(5)
>    57           S=M(5)*(A(5)-A(1)*A(3)/N1)
>    58           Y(F3,1)=S/(A(4)-A(3)*A(3)/N1)
>    59           Y(F3,3)=M(5)
>    60           Y(F3,4)=ABS(Y(F3,2)/Y(F3,3)*N/V1)*1000000
>    61           RETURN
>    62           END
>    63
>    64     C
>    65     C*********************************************************************************
>    66     C
>    67     C  DOES COEFFICIENT DISPLAY
>    68     C  CALLED BY 'MAIN'. WRITES OMN *MSINK*
>    69     C
>    70     C*********************************************************************************
>    71     C
>    72           SUBROUTINE CODIS(Y,F2,F3,K1)
>    73           INTEGER F2,F3,K,K1
>    74           REAL Y(20,4),HOLD
>    75           WRITE(2,90)Y(1,1)
>    76      90   FORMAT(' R2(EXP) = ',F8.4)
>    77           K1=F2
>    78      51   CONTINUE
>    79           HOLD=-ALOG10(Y(K1,4)/1000000)
>    80           WRITE(2,91)K1,Y(K1,1),Y(K1,4),HOLD
*END OF FILE
*
```

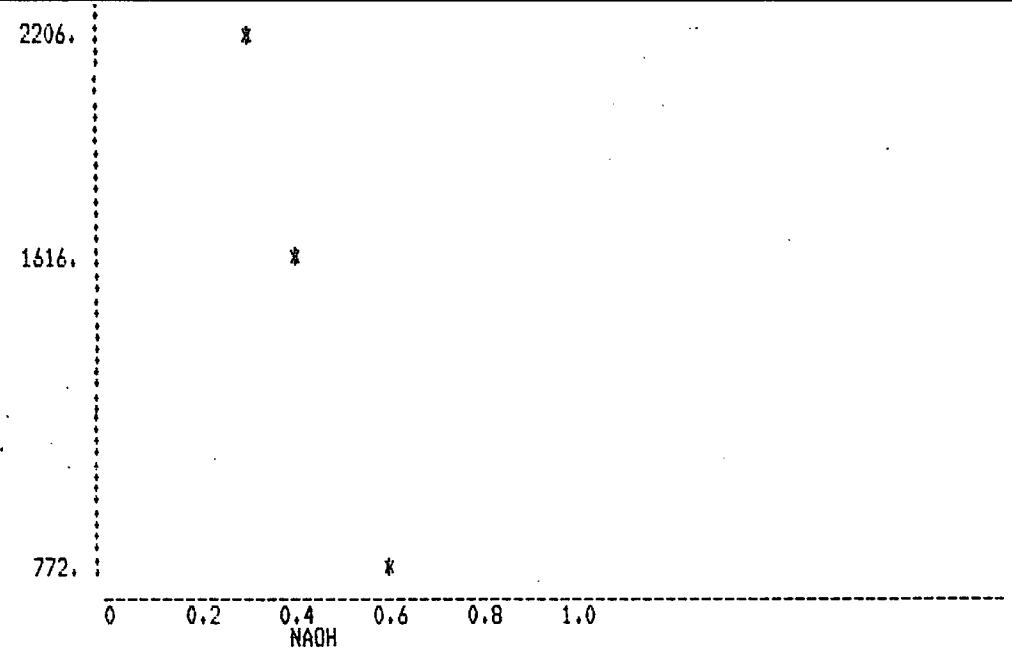
```
>   241          IF(N1.LT.5.0) GO TO 801
>   242          GO TO 802
>   243     801  CONTINUE
>   244          WRITE(2,953)
>   245     953  FORMAT('NOTE <4 PTS !',/)
>   246          F1=2.0
>   247     802  CONTINUE
>   248          WRITE(2,823)
>   249          F3=F3-1
>   250          CALL LIN(A,M,N1,F3,F5,GG2,VV1,Y,S,N,V1)
>   251          GO TO 850
>   252     980  CONTINUE
>   253          WRITE(2,700)
>   254     700  FORMAT(' DO YOU WISH TO VIEW GRAPHS ?',/)
>   255          CALL FREAD(3,'S:',CH,1)
>   256          IF(EQUC(CH,'N')) GO TO 701
>   257          CALL PLOT(VV1,VV2,GG1,I,MM,F,V2)
>   258     701  CONTINUE
>   259     3000 CONTINUE
>   260          F5=F2+1
>   261          P1=F2+1
>   262          Q4=F3
>   263          F3=I
>   264          P2=I
>   265          CALL LIN(A,M,N1,F3,F5,GG2,VV1,Y,S,N,V1)
>   266          WRITE(2,990)Y(I,1),Y(I,4)
>   267     990  FORMAT(' R2(BASE PTS) =',F8.3,/,' CALC TOTAL ACID =',F8.3,' UEQ/L')
>   268          P3=P4
>   269          V2=VV1(I)
>   270          P4=VV1(I)
>   271          MM=GG2(I)
>   272          X2=VV1(I)-X2
>   273          X1=0.1
>   274          F=0
>   275          F4=0
>   276          F3=Q4
>   277          IF(F2.LT.4) GO TO 320
>   278          CALL CODIS(Y,F2,F3,K)
>   279          IF(C1.GT.15) GO TO 311
>   280          WRITE(2,991)
>   281     991  FORMAT(' STRONG ACID = <15 UEQ/L',/)
>   282          IF(IENTER.EQ.0) GO TO 360
>   283          CALL MOVEC(8,'L15     ',VALUE)
>   284          CALL INSPAR(ISAMP,'10260L',VALUE,'0',DATE,BOT,TEST)
>   285     360  CONTINUE
>   286          GO TO 320
>   287     311  CONTINUE
>   288          WRITE(2,992)C1
>   289     992  FORMAT(' STRONG ACID =',F8.4,' UEQ/L',/)
>   290          IF(IENTER.EQ.0) GO TO 361
>   291          CALL VALSTR(C1,STR)
>   292          CALL MOVEC(8,'        ',VALUE)
>   293          CALL MOVEC(6,STR,VALUE(3))
>   294          CALL INSPAR(ISAMP,'10260L',VALUE,'0',DATE,BOT,TEST)
>   295     361  CONTINUE
>   296     320  CONTINUE
>   297          WRITE(2,990)Y(I,1),Y(I,4)
>   298          IF(IENTER.EQ.0) GO TO 362
>   299          CALL VALSTR(Y(I,4),STR)
>   300          CALL MOVEC(8,'        ',VALUE)
>   301          CALL MOVEC(6,STR,VALUE(3))
>   302          CALL INSPAR(ISAMP,'10270L',VALUE,'0',DATE,BOT,TEST)
>   303     362  CONTINUE
>   304          WRITE(2,993)
>   305     993  FORMAT(/,/,/,/,/,/)
>   306          GO TO 250
>   307     999  CONTINUE
>   308          STOP
>   309          END
‡END OF FILE
‡
```

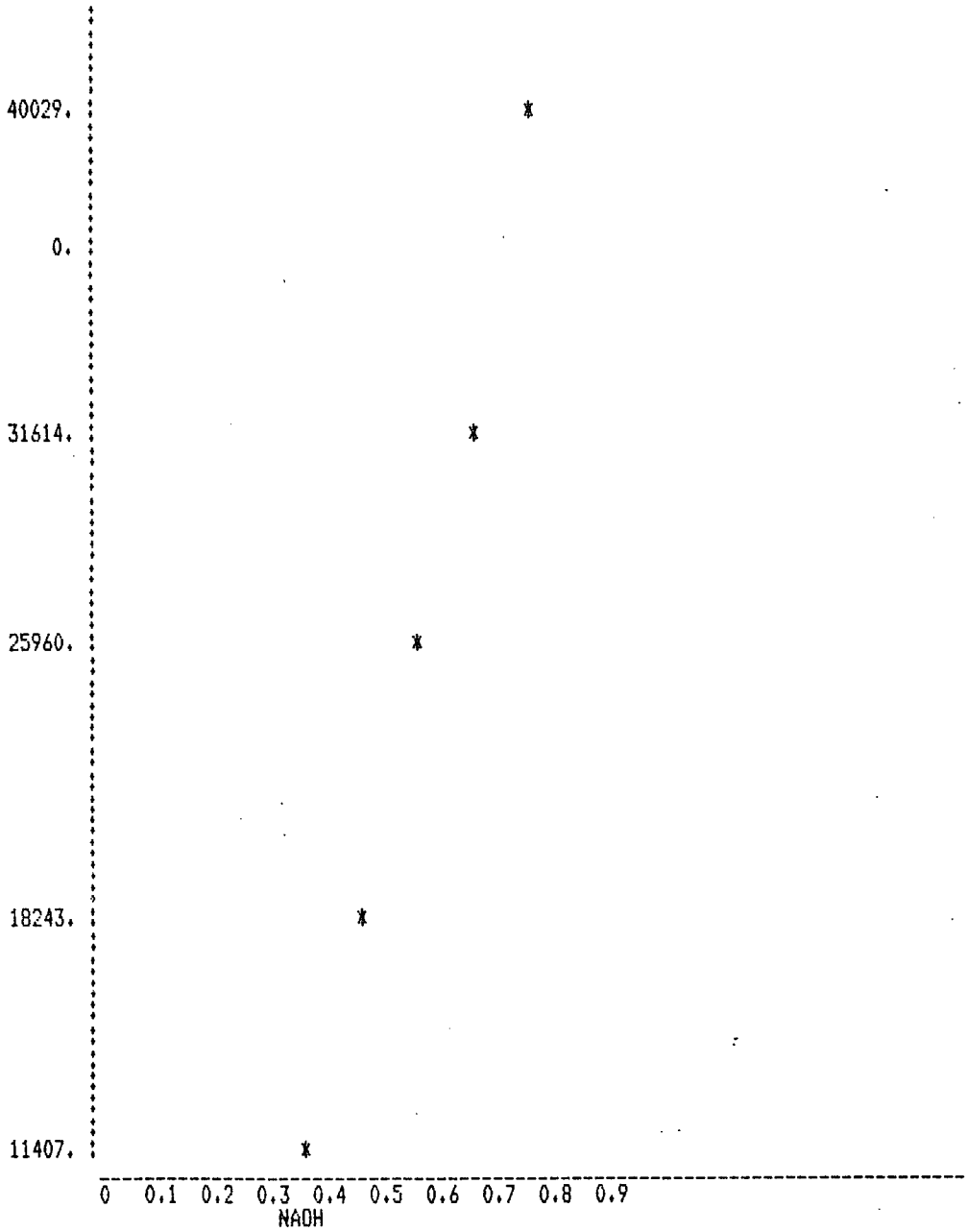
```
>   161          WRITE(2,500)NI
>   162      500 FORMAT(' SAMPLE IDENT',/,/,1X,15A1,/)
>   163          WRITE(2,501)PHVAL
>   164      501 FORMAT(' MEASURED PH',F8.3,/)
>   165          WRITE(2,502)
>   166      502 FORMAT(' #     ML      MV      GRAN''S FN',/)
>   167          DO 550 II=1,I
>   168          WRITE(2,503)II,VV1(II),VV2(II),GG1(II)
>   169      503 FORMAT(1X,I2,3X,F4.2,2X,F5.0,5X,2PE9.2)
>   170      550 CONTINUE
>   171          IF(F2.GT.3.0) GO TO 720
>   172          WRITE(2,551)
>   173      551 FORMAT('INSUFFICIENT ACID PTS',/,' <15 UEQ STRONG ACID',/)
>   174          F3=F2
>   175          C1=0.0
>   176          F4=0.0
>   177          X2=0.0
>   178          GO TO 3000
>   179      720 CONTINUE
>   180          F=0
>   181          F1=0
>   182          CALL EDIT(VV1,VV2,F1,I)
>   183          IF(F1.NE.1) GO TO 630
>   184          WRITE(2,576)
>   185      576 FORMAT('CALCULATION NECESSARY - STANDBY',/)
>   186          GO TO 52
>   187      630 CONTINUE
>   188     C
>   189     C  ACID PLOT
>   190     C
>   191          MM=GG2(1)
>   192          X2=VV1(F2)*2
>   193          F4=VV1(F2)*2
>   194          V2=0.0
>   195          IF(X2.GT.0.2) GO TO 739
>   196          X1=0.02
>   197          GO TO 740
>   198      739 X1=0.1
>   199          IF(X2.LE.5.0) X1=0.05
>   200      740 CONTINUE
>   201          F2=F2
>   202          F3=F2
>   203          F1=0
>   204          F5=1
>   205          CALL LIN(A,M,N1,F3,F5,GG2,VV1,Y,S,N,V1)
>   206          CALL EXPREG(A,T2,M,Y,S,VV1,GG2,F3)
>   207      850 CONTINUE
>   208          CALL CODIS(Y,F2,F3,K1)
>   209          IF(Y(1,1).LT.Y(F3,1)) GO TO 910
>   210          F4=1.0
>   211          WRITE(2,950)
>   212      950 FORMAT('LESS THEN 15 UEQ/L STRONG ACID PRESENT!',/)
>   213          WRITE(2,951)
>   214      951 FORMAT('AGREED(Y/N)',/)
>   215          CALL FREAD(3,'S!',CH,1)
>   216          IF(EQUC(CH,'N')) GO TO 910
>   217      900 CONTINUE
>   218          IF(F4.EQ.1) KEEP=1
>   219          IF(F4.EQ.0) KEEP=0
>   220          WRITE(2,823)
>   221      823 FORMAT(/,/,/)
>   222          C1=0.0
>   223          GO TO 980
>   224      910 CONTINUE
>   225          F4=0.0
>   226          IF(F4.EQ.1) KEEP=1
>   227          IF(F4.EQ.0) KEEP=0
>   228          WRITE(2,823)
>   229          C1=Y(K1,4)
>   230          WRITE(2,961)
>   231      961 FORMAT('REMOVE POINTS (Y/N)',/)
>   232          CALL FREAD(3,'S!',CH,1)
>   233          IF(EQUC(CH,'N')) GO TO 980
>   234          IF(N1.GE.4.0) GO TO 800
>   235          WRITE(2,957)
>   236      957 FORMAT(' TOO FEW !',/)
>   237          WRITE(2,823)
>   238          F4=1.0
>   239          GO TO 900
>   240      800 CONTINUE
#END OF FILE
#
```

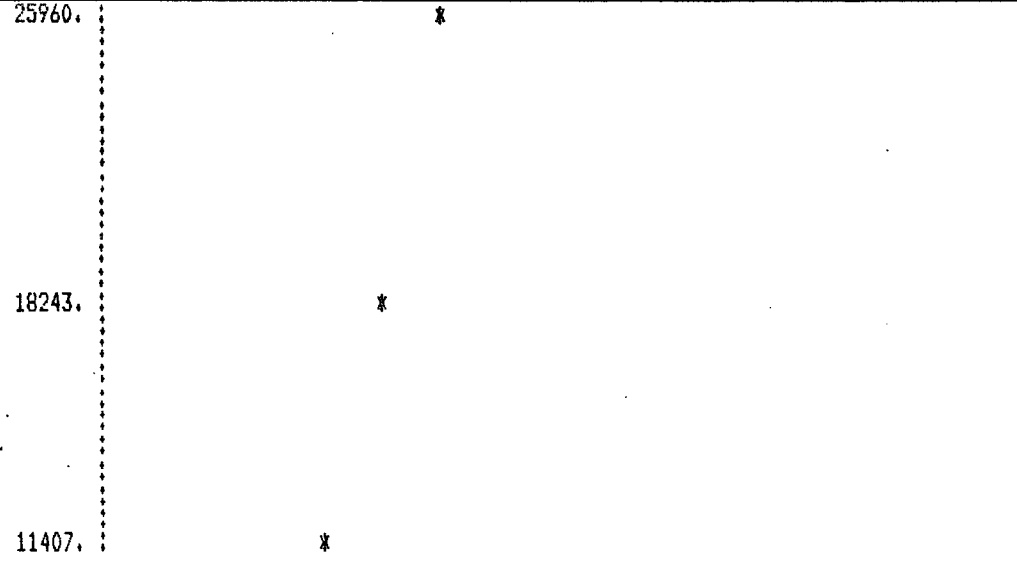
```
>    81          WRITE(2,402)
>    82      402 FORMAT('ENTER BOTTLE NUMBER')
>    83          CALL FREAD(3,'S:',BOT,10)
>    84      421 CONTINUE
>    85          WRITE(2,93)
>    86      93  FORMAT('ENTER MEASURED PH',/)
>    87          CALL FREAD(3,'R:',PHVAL)
>    88          IF(IENTER.EQ.0) GO TO 405
>    89          ICNT=6
>    90          CALL DTB(NI,ISAMP,ICNT,IKL,' ')
>    91          ISAMP=ISAMP*10000
>    92      C
>    93      C STORE THE PH VALUE
>    94      C
>    95          XPH=PHVAL
>    96          CALL VALSTR(XPH,STR)
>    97          CALL MOVEC(8,'        ',VALUE)
>    98          CALL MOVEC(6,STR,VALUE(3))
>    99          CALL INSPAR(ISAMP,'1030-L',VALUE,'1',DATE,BOT,TEST)
>   100          IF(TEST.EQ.1.OR.TEST.EQ.2) GO TO 250
>   101          WRITE(2,363)
>   102      363 FORMAT('ENTER TEMPERATURE',/)
>   103          CALL FREAD(3,'R:',TEMP)
>   104          CALL VALSTR(TEMP,STR)
>   105          CALL MOVEC(8,'        ',VALUE)
>   106          CALL MOVEC(6,STR,VALUE(3))
>   107          CALL INSPAR(ISAMP,'0206-L',VALUE,'1',DATE,BOT,TEST)
>   108          WRITE(2,364)
>   109      364 FORMAT('ENTER SPECIFIC CONDUCTANCE',/)
>   110          CALL FREAD(3,'R:',SP)
>   111          CALL VALSTR(SP,STR)
>   112          CALL MOVEC(8,'        ',VALUE)
>   113          CALL MOVEC(6,STR,VALUE(3))
>   114          CALL INSPAR(ISAMP,'0204-L',VALUE,'1',DATE,BOT,TEST)
>   115      405 CONTINUE
>   116          WRITE(2,94)
>   117      94  FORMAT('ENTER ML,MV IN ORDER - MAX 20',/)
>   118          WRITE(2,95)
>   119      95  FORMAT('DATA PTS 0,0 TO END',/)
>   120          DO 50 I=1,20
>   121          CALL FREAD(3,'R,R:',VV1(I),VV2(I))
>   122          IF(VV2(I).EQ.0.0.AND.VV1(I).EQ.0.0) GO TO 40
>   123          GO TO 41
>   124      40  I=I-1
>   125          GO TO 52
>   126      41  CONTINUE
>   127      50  CONTINUE
>   128      52  CONTINUE
>   129      C
>   130      C   CALCULATES GRAN'S FN.
>   131      C
>   132          DO 55 J=1,I
>   133          IF(VV1(J).EQ.0.0) VV1(J)=0.0001
>   134          GG1(J)=FND(J,VV1,VV2,V1)
>   135          IF(VV2(J).GT.0.0) MM=GG1(1)
>   136          IF(VV2(J).LT.0.0.AND.F.NE.1) GO TO 59
>   137          GO TO 60
>   138      59  MM=FND(I,VV1,VV2,V1)
>   139          F=1
>   140          F2=J-1
>   141      60  CONTINUE
>   142          GG2(J)=GG1(J)/(10.0**INT(ALOG10(MM)))
>   143      55  CONTINUE
>   144          MM=GG2(1)
>   145          P1=1
>   146          P2=I
>   147          V2=0.0
>   148          P3=0.0
>   149          X1=0.1
>   150          X2=VV1(I)
>   151          P4=VV1(I)
>   152          WRITE(2,515)
>   153      515 FORMAT(' DO YOU WANT TO VIEW GRAPHS?',/)
>   154          CALL FREAD(3,'S:',CH,1)
>   155          IF(EQUC(CH,'N')) GO TO 516
>   156          CALL PLOT(VV1,VV2,GG1,I,MM,F,V2)
>   157      516 CONTINUE
>   158      C
>   159      C   PRINT DATA
>   160      C
$END OF FILE
$
```

```
>     1     C
>     2     C*****************************************************************************************
>     3     C
>     4     C THIS INTERACTIVE PROGRAM DOES ANALYSIS OF GRAN'S PLOT ACIDITY DATA.
>     5     C IT REQUIRES AS INPUT THE NORMALITY OF NAOH,SAMPLE VOLUME,SAMPLE NAME,
>     6     C MEASURED PH,VOLUME AND METER READINGS FOR EACH POINT IN THTE TITRATION(MAX 20 POINTS).
>     7     C
>     8     C*****************************************************************************************
>     9     C
>    10           LOGICAL*1 STR(6),VALUE(8),NI(15),CH,BOT(10),DAT(8),DATE(6),YR(2),STRIN(22),NI2(15)
>    11           REAL V2,GG2(20),VV2(20),VV1(20),V1,PHVAL,N,GG1(20),M(5),MM,M1,X,P3,P4
>    12           REAL Y(20,4),T2,A(5),S,X1,X2,C1,F4
>    13           LOGICAL EQUC,EQCMP
>    14           INTEGER F,F2,B,F3,F5,P2,F1,K,I,KEEP,P1,Q4,TIM(2),TEST
>    15           CALL FTNCMD('ASSIGN 2=*MSINK*',16)
>    16           CALL FTNCMD('ASSIGN 3=*MSOURCE*',18)
>    17     C
>    18     C GET DATE
>    19     C
>    20           EQUIVALENCE (DAT(1),TIM(1))
>    21           CALL TIME(10,0,TIM)
>    22           CALL MOVEC(6,DAT,DATE)
>    23           CALL MOVEC(15,'               ',NI2)
>    24           CALL MOVEC(15,'               ',NI)
>    25           IENTER=0
>    26           ITIME=0
>    27           WRITE(2,400)
>    28       400 FORMAT('ARE THESE TO BE ENTERED INTO WQB6 DATA FILE ? (Y/N)',/)
>    29           CALL FREAD(3,'S:',CH,1)
>    30           IF(EQUC(CH,'Y')) GO TO 450
>    31           GO TO 451
>    32       450 CONTINUE
>    33           IENTER=1
>    34           WRITE(2,401)
>    35       401 FORMAT('ENTER FISCAL YEAR.  EG: 81',/)
>    36           CALL FREAD(3,'S:',YR,2)
>    37           CALL MOVEC(22,'ASSIGN 4=WQB6:TABLE.YR',STRIN)
>    38           CALL MOVEC(2,YR,STRIN(21))
>    39           CALL FTNCMD(STRIN,22)
>    40       451 CONTINUE
>    41     C
>    42     C
>    43     C ENTER DATA
>    44     C
>    45           F=0
>    46           F1=0
>    47     C
>    48     C  INPUT DATA
>    49     C
>    50           WRITE(2,90)
>    51        90 FORMAT('ENTER NORMALITY OF NAOH',/)
>    52           CALL FREAD(3,'R:',N)
>    53           WRITE(2,91)
>    54        91 FORMAT('ENTER SAMPLE VOLUME(ML)',/)
>    55           CALL FREAD(3,'R:',V1)
>    56       250 CONTINUE
>    57           IF(ITIME.EQ.0.OR.IENTER.EQ.1) GO TO 404
>    58           ITIME=1
>    59           WRITE(2,400)
>    60           CALL FREAD(3,'S:',CH,1)
>    61           IF(EQUC(CH,'Y')) GO TO 403
>    62           GO TO 404
>    63       403 CONTINUE
>    64           IENTER=1
>    65           WRITE(2,401)
>    66           CALL FREAD(3,'S:',YR,2)
>    67           CALL MOVEC(22,'ASSIGN 4=WQB6:TABLE.YR',STRIN)
>    68           CALL MOVEC(2,YR,STRIN(21))
>    69           CALL FTNCMD(STRIN,22)
>    70       404 CONTINUE
>    71           WRITE(2,552)
>    72       552 FORMAT('ENTER SAMPLE NAME OR ''STOP''',/)
>    73           CALL FREAD(3,'S:',NI,15)
>    74           IF(EQCMP(4,'STOP',NI(1))) GO TO 999
>    75           CALL MOVEC(15,NI,NI2)
>    76           CALL MOVEC(15,NI2,NI)
>    77           IF(IENTER.EQ.0) GO TO 421
>    78     C
>    79     C GET BOTTLE NUMBER
>    80     C
$END OF FILE
$
```

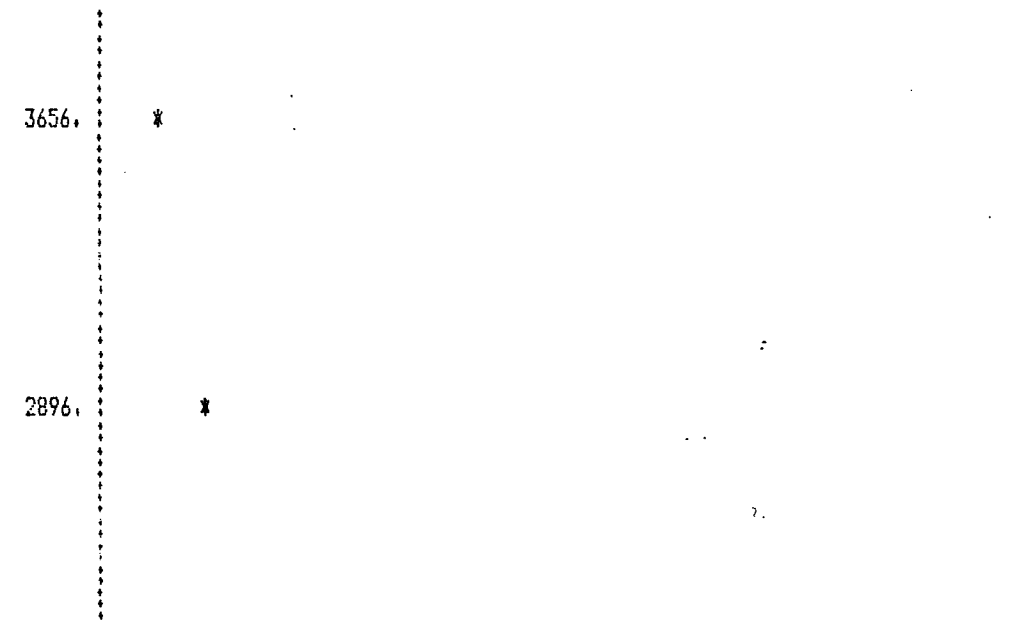
```
R2(BASE PTS) =   0.951
CALC TOTAL ACID =  14.501 UEQ/L
R2(EXP) =   0.9905
R2 (   5 PT. LIN ) =  0.9814 CALC  16.0513 UEQ/L - PH =  4.7945
R2 (   4 PT. LIN ) =  0.9968 CALC  14.3031 UEQ/L - PH =  4.8446
STRONG ACID = <15 UEQ/L

R2(BASE PTS) =   0.951
CALC TOTAL ACID =  14.501 UEQ/L



ENTER SAMPLE NAME OR 'STOP'

.?STOP
#Execution Terminated   10:52:39  T=2.402
$
```


2206.
1616.
772.
0
0.2
0.4
0.6
0.8
1.0
NAOH


40029.
0.
31614.
25960.
18243.
11407.
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
NAOH




```
R2(EXP) =   0.9905
R2 (   5 PT. LIN ) =  0.9814 CALC  16.0513 UEQ/L - PH =  4.7945
LESS THEN 15 UEQ/L STRONG ACID PRESENT!

AGREED(Y/N)

?N


REMOVE POINTS (Y/N)

?Y


R2(EXP) =   0.9905
R2 (   5 PT. LIN ) =  0.9814 CALC  16.0513 UEQ/L - PH =  4.7945
R2 (   4 PT. LIN ) =  0.9968 CALC  14.3031 UEQ/L - PH =  4.8446


REMOVE POINTS (Y/N)

?N
```



```
>  321      63   CONTINUE
>  322           IF(ARRH1(J).NE.0.0) GO TO 914
>  323           WRITE(2,995)STR
>  324      995  FORMAT('        :',50A1)
>  325           GO TO 915
>  326      914  CONTINUE
>  327           WRITE(2,926)ARRH1(J),STR
>  328      926  FORMAT(1X,F6.0,' :',50A1)
>  329      915  CONTINUE
>  330      69   CONTINUE
>  331      55   CONTINUE
>  332           WRITE(2,863)
>  333      863  FORMAT(9X,'--------------------------------------------------------------------------------')
>  334           WRITE(2,997)
>  335      997  FORMAT(9X,'0',6X,'0.2',5X,'0.4',5X,'0.6',5X,'0.8',5X,'1.0')
>  336           WRITE(2,996)
>  337      996  FORMAT(25X,'NAOH',/,/,/,/)
>  338     C
>  339     C  PLOT SECOND PLOT
>  340     C
>  341           DO 665 JJ=1,50
>  342           J=50-JJ+1
>  343           CALL MOVEC(50,'                                                    ',STR)
>  344           IF(ARR2(J).EQ.0) GO TO 330
>  345           CALL TRNST(STR,50,' ','*',1,ARR2(J),K)
>  346      330  CONTINUE
>  347           IF(ARRH2(J).NE.0.0) GO TO 917
>  348           WRITE(2,995)STR
>  349           GO TO 918
>  350      917  CONTINUE
>  351           WRITE(2,926)ARRH2(J),STR
>  352      918  CONTINUE
>  353      665  CONTINUE
>  354           WRITE(2,863)
>  355           WRITE(2,987)
>  356      987  FORMAT(9X,'0',3X,'0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9')
>  357           WRITE(2,996)
>  358           GO TO 999
>  359      998  CONTINUE
>  360           WRITE(2,960)X,Y
>  361      960  FORMAT(' INDEX OUT OF RANGE ',2I6)
>  362      999  CONTINUE
>  363           RETURN
>  364           END
$END OF FILE
$
```

```
>  241          RETURN
>  242          END
>  243     C
>  244     C*****************************************************************************
>  245     C
>  246     C PLOTS THE NAOH'S VS GRAN'S FUNCTION(PLOT2 2 GRAPHS)
>  247     C  CALLED BY MAIN. ALL PLOTS ARE 50 BY 50 LINED AND USE DATA FOR
>  248     C  SCALING.
>  249     C
>  250     C*****************************************************************************
>  251     C
>  252          SUBROUTINE PLOT(VV1,VV2,GG2,I,MM,F,V2)
>  253          REAL VV1(20),VV2(20),GG2(20),MIN1,MIN2,ARRH1(50),ARRH2(50),MAX1,MAX2,V2,MM
>  254          INTEGER I,J,ARR(50),ARR2(50),X,Y,F
>  255          LOGICAL*1 STR(50)
>  256          DO 50 J=1,50
>  257          ARRH1(J)=0.0
>  258          ARRH2(J)=0.0
>  259          ARR(J)=0
>  260     50   ARR2(J)=0
>  261          MAX1=0.0
>  262          MAX2=0.0
>  263          MIN1=9999999999.9
>  264          MIN2=9999999999.9
>  265     C
>  266     C GET MAX AND MIN OF GRAN'S FN. FOR POSITIVE METER READINGS
>  267     C
>  268          DO 35 J=1,20
>  269          IF(VV2(J).LT.0.0) GO TO 31
>  270          IF(GG2(J).GT.MAX1) MAX1=GG2(J)
>  271          IF(GG2(J).LT.MIN1) MIN1=GG2(J)
>  272     35   CONTINUE
>  273     31   CONTINUE
>  274     C
>  275     C GET MAX AND MIN OF GRAN'S FN. FOR NEG. METER READINGS
>  276     C
>  277          DO 32 JJ=J,I
>  278          IF(VV2(JJ).EQ.0.0) GO TO 33
>  279          IF(GG2(JJ).GT.MAX2) MAX2=GG2(JJ)
>  280          IF(GG2(JJ).LT.MIN2) MIN2=GG2(JJ)
>  281     32   CONTINUE
>  282     33   CONTINUE
>  283     C
>  284     C CALCULATES SCALE FACTOR
>  285     C
>  286          SCALE1=(MAX1-MIN1)/45.0
>  287          SCALE2=(MAX2-MIN2)/45.0
>  288          DO 53 J=1,I
>  289          IF(VV2(J).LT.0.0) GO TO 54
>  290          XX=VV1(J)*400.0+1.1
>  291          YY=(GG2(J)-MIN1)/SCALE1+1.0
>  292          X=XX
>  293          Y=YY
>  294          IF(X.GT.50.OR.Y.GT.50) GO TO 998
>  295          ARRH1(Y)=GG2(J)
>  296          ARR(Y)=X
>  297          GO TO 53
>  298     54   CONTINUE
>  299          XX=VV1(J)*50.0+1.1
>  300          YY=(GG2(J)-MIN2)/SCALE2+1.1
>  301          X=XX
>  302          Y=YY
>  303     C
>  304     C  SCALE VALUES INTO ARRAYS
>  305     C
>  306          IF(X.GT.50.OR.Y.GT.50) GO TO 998
>  307          ARRH2(Y)=GG2(J)
>  308          ARR2(Y)=X
>  309     53   CONTINUE
>  310          WRITE(2,90)
>  311     90   FORMAT(/,/,/)
>  312     C
>  313     C  PLOT FIRST PLOT
>  314     C
>  315          DO 55 JJ=1,50
>  316          J=50-JJ+1
>  317          CALL MOVEC(50,'                                                  ',STR)
>  318          IF(ARR(J).EQ.0) GO TO 30
>  319          CALL TRNST(STR,50,' ','*',1,ARR(J),K)
>  320     30   CONTINUE
#END OF FILE
#
```

```
>  161      90   FORMAT('INDEX OF PAIR TO CORRECT',/)
>  162           CALL FREAD(3,'I:',I1)
>  163           IF(I1.LT.1) GO TO 999
>  164           IF(I1.GT.1) GO TO 120
>  165           WRITE(2,91)VV1(I1),VV2(I1)
>  166      91   FORMAT('OLD ML=',F8.4,/,'OLD MV=',F8.4)
>  167           WRITE(2,92)
>  168      92   FORMAT('ENTER NEW ML,MV',/)
>  169           CALL FREAD(3,'R,R:',VV1(I1),VV2(I1))
>  170           F1=1
>  171           GO TO 120
>  172      999  CONTINUE
>  173           RETURN
>  174           END
>  175      C
>  176      C*********************************************************************
>  177      C
>  178      C  DOES DELETING OF INPUT VOLUMES AND METER READINGS. CALLED BY EDIT
>  179      C  SETS FLAG,F1, IF ANY DELETING IS DONE
>  180      C
>  181      C*********************************************************************
>  182      C
>  183           SUBROUTINE DELETE(VV1,VV2,F1,I)
>  184           REAL VV1(20),VV2(20)
>  185           INTEGER F1,I
>  186      140  CONTINUE
>  187           WRITE(2,90)
>  188      90   FORMAT('INDEX OF PAIR TO DELETE',/)
>  189           CALL FREAD(3,'I:',I1)
>  190           IF(I1.LT.1) GO TO 999
>  191           IF(I1.GT.I) GO TO 140
>  192           WRITE(2,91)VV1(I1),VV2(I1)
>  193      91   FORMAT('DELETE ',F8.4,1X,F8.4)
>  194           JJ=I1+1
>  195           DO 50 J=JJ,I
>  196           IJ=J-1
>  197           VV1(IJ)=VV1(J)
>  198           VV2(IJ)=VV2(J)
>  199      50   CONTINUE
>  200           I=I-1
>  201           F1=1
>  202           GO TO 140
>  203      999  CONTINUE
>  204           RETURN
>  205           END
>  206      C
>  207      C*********************************************************************
>  208      C
>  209      C  DOES INSERTING OF INPUT VOLUMES AND METER READINGS. CALLED BY EDIT
>  210      C  SETS FLAG,F1, IF ANY INSERTING IS DONE
>  211      C
>  212      C*********************************************************************
>  213      C
>  214           SUBROUTINE INSERT(VV1,VV2,F1,I)
>  215           REAL VV1(20),VV2(20)
>  216           INTEGER F1,I
>  217      130  CONTINUE
>  218           WRITE(2,90)
>  219      90   FORMAT('INDEX OF PAIR TO INSERT',/)
>  220           CALL FREAD(3,'I:',I1)
>  221           IF(I1.LT.1) GO TO 999
>  222           II=I+1
>  223           IF(I1.GT.II) GO TO 130
>  224           I=I+1
>  225           IF(I1.EQ.1) GO TO 137
>  226           II=I1+1
>  227           J=I
>  228      50   CONTINUE
>  229           JJ=J-1
>  230           VV1(J)=VV1(JJ)
>  231           VV2(J)=VV2(JJ)
>  232           J=J-1
>  233           IF(J.GE.II) GO TO 50
>  234      137  CONTINUE
>  235           WRITE(2,91)
>  236      91   FORMAT('ENTER NEW ML,MV',/)
>  237           CALL FREAD(3,'R,R:',VV1(I1),VV2(I1))
>  238           F1=1
>  239           GO TO 130
>  240      999  CONTINUE
#END OF FILE
#
```

```
>    81      91   FORMAT(' R2 (',I4,' PT. LIN ) =',F8.4,' CALC ',F8.4,' UEQ/L - PH =',F8.4)
>    82           K1=K1-1
>    83           IF(K1.GE.F3) GO TO 51
>    84           K1=K1+1
>    85           RETURN
>    86           END
>    87
>    88      C
>    89      C*****************************************************************
>    90      C
>    91      C  EXPONENTIAL REGRESSION CALCULATIONS
>    92      C  CALLED BY MAIN
>    93      C
>    94      C*****************************************************************
>    95      C
>    96           SUBROUTINE EXPREG(A,T2,M,Y,S,VV1,GG2,F3)
>    97           REAL GG2(20),VV1(20),Y(20,4),A(5),T2,M(5),S
>    98           INTEGER J,F3
>    99           A(3)=0.0
>   100           A(4)=0.0
>   101           A(5)=0.0
>   102           DO 50 J=1,F3
>   103           T2=ALOG(GG2(J))
>   104           A(3)=A(3)+T2
>   105           A(4)=A(4)+T2*T2
>   106           A(5)=A(5)+VV1(J)*T2
>   107      50   CONTINUE
>   108           M(3)=A(3)/F3
>   109           M(4)=(A(4)-A(3)**2/F3)/(F3-1)
>   110           M(5)=(A(5)-A(1)*A(3)/F3)/(A(2)-A(1)*A(1)/F3)
>   111           Y(1,2)=M(3)-M(1)*M(5)
>   112           S=M(5)*(A(5)-A(1)*A(3)/F3)
>   113           Y(1,1)=S/(A(4)-A(3)*A(3)/F3)
>   114           Y(1,3)=M(5)
>   115           RETURN
>   116           END
>   117      C
>   118      C*************************************************************
>   119      C
>   120      C  DOES EDITING ON INPUT VOLUMES AND METER READINGS
>   121      C  CALLED BY 'MAIN',AND CALLS CORREC,DELETE AND INSERT
>   122      C
>   123      C*************************************************************
>   124      C
>   125           SUBROUTINE EDIT(VV1,VV2,F1,I)
>   126           REAL VV1(20),VV2(20)
>   127           INTEGER F1,I,I1
>   128           LOGICAL*1 CH
>   129           LOGICAL EQUC
>   130           WRITE(2,90)
>   131      90   FORMAT(' DO YOU WISH TO EDIT? (Y/N)',/)
>   132           CALL FREAD(3,'S:',CH,1)
>   133           IF(EQUC(CH,'N')) GO TO 999
>   134      80   CONTINUE
>   135           WRITE(2,91)
>   136      91   FORMAT('ENTER ONE OF ''CORRECT'',''INSERT'',''DELETE'' ',/)
>   137           CALL FREAD(3,'S:',CH,1)
>   138           IF(EQUC(CH,'C')) CALL CORREC(VV1,VV2,F1,I)
>   139           IF(EQUC(CH,'I')) CALL INSERT(VV1,VV2,F1,I)
>   140           IF(EQUC(CH,'D')) CALL DELETE(VV1,VV2,F1,I)
>   141           WRITE(2,92)
>   142      92   FORMAT('MORE EDITING? (Y/N)')
>   143           CALL FREAD(3,'S:',CH,1)
>   144           IF(EQUC(CH,'Y')) GO TO 80
>   145      999  CONTINUE
>   146           RETURN
>   147           END
>   148      C
>   149      C*****************************************************************
>   150      C
>   151      C DOES CORRECTING OF INPUT VOLUMES AND METER READINGS. CALLED BY EDIT
>   152      C SETS FLAG (F1) IF ANY CORRECTING IS DONE
>   153      C
>   154      C*****************************************************************
>   155      C
>   156           SUBROUTINE CORREC(VV1,VV2,F1,I)
>   157           REAL VV1(20),VV2(20)
>   158           INTEGER F1,I
>   159      120  CONTINUE
>   160           WRITE(2,90)
#END OF FILE
#
```