Spectrophotometric determination of association constant

Computer program STEP

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225 PUBLICATIONS **1,983** CITATIONS

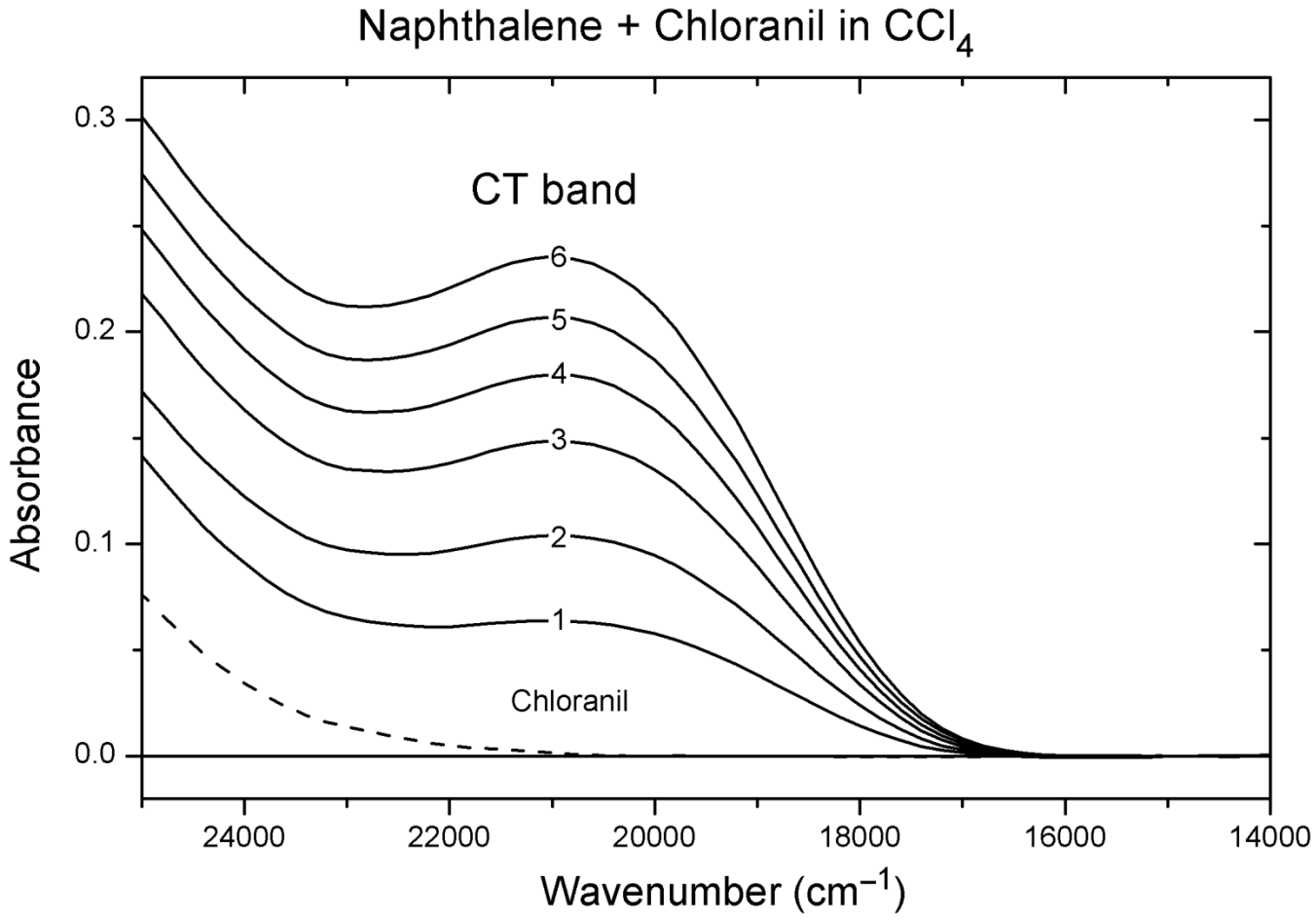
Computer Program STEP

Jens Spanget-Larsen, Roskilde University

Least-Squares “Systematic Trial-and-Error Procedure” for spectrophotometric evaluation of association constant *K* and molar absorption coefficient ε for a 1:1 molecular complex *C*,

$$A + B \leftrightarrows C,$$

with error analysis according to K. Conrow, G.D. Johnson, R.E. Bowen (1964). The present version of STEP treats data for up to 10 mixtures of *A* and *B*, for up to 20 different wavenumbers. An analysis of the Charge Transfer (CT) complex formation of naphthalene and chloranil is provided as an example.



STEP procedure:

Spectrophotometric determination of association constant (equilibrium constant) *K* for a 1:1 complex formation by a systematic trial-and-error procedure.

We consider the equilibrium

$$A + B \leftrightarrows C$$

$$K = \frac{[C]}{[A][B]} \quad \text{(neglecting activity effects)}$$

If A_0 and B_0 are the initial concentrations of *A* and *B*, and writing for simplicity *C* instead of $[C]$, we have

$$K = \frac{C}{(A_0 - C)(B_0 - C)}$$

$$C^2 - \left(A_0 + B_0 + K^{-1}\right)C + A_0 B_0 = 0$$

$$C = \frac{A_0 + B_0 + K^{-1}}{2} - \sqrt{\frac{\left(A_0 + B_0 + K^{-1}\right)^2}{4} - A_0 B_0} \quad \text{(discarding the other root)} \qquad (1)$$

We now assume the applicability of "Lambert-Beer's law":

$$E(\tilde{\nu}) = \varepsilon(\tilde{\nu}) \cdot d \cdot c$$

E is the measured absorbance, $\tilde{\nu}$ the wavenumber, ε the molar absorption coefficient, *d* the length of the light path through the sample, and *c* is the concentration (mol/L). In the present experiment we have

$$\begin{aligned} E &= E_A + E_B + E_C \\ &= \varepsilon_A d\,(A_0 - C) + \varepsilon_B d\,(B_0 - C) + \varepsilon_C d\,C \end{aligned} \qquad (2)$$

where the dependence on $\tilde{\nu}$ is implicit. In this equation, *E* can be measured and *d*, A_0, B_0, ε_A, and ε_B are assumed to be known. ε_C and *C* are so far unknown; ε_C can be expressed as a function of *C*:

$$\varepsilon_C = \frac{E - \varepsilon_A d\,(A_0 - C) - \varepsilon_B d\,(B_0 - C)}{d\,C} \qquad (3)$$

We now assume that absorbance measurements E for a particular wavenumber $\tilde{\nu}$ have been performed on a series of N mixtures of A and B with different concentrations, *i.e.*, different values of A_0 and B_0. The STEP procedure is carried out as follows (Conrow et al. 1964):

(i) Guess a value of the association constant K: $K = K'$.

(ii) Using K', compute concentrations C' for each mixture from eqn. (1).

(iii) With the concentrations C', compute from eqn. (3) molar absorption coefficients ε'_C for each mixture.

(iv) Determine the mean value $\overline{\varepsilon'_C}$ for the N mixtures, $\overline{\varepsilon'_C} = \dfrac{\sum \varepsilon'_C}{N}$.

(v) Using $\overline{\varepsilon'_C}$, compute a value of E' for each mixture from eqn. (2).

(vi) Compare the E' values with the measured absorbances E. The overall deviation S is given by the least-squares standard error of estimate (RMS):

$$S = \sqrt{\frac{\sum (E - E')^2}{N}} \, .$$

(vii) Guess a new value of K and repeat the procedure.

By systematic variation of K, the program STEP determines the value which yields the smallest least-squares absorbance deviation S. In the vicinity of the minimum, a three-point parabolic interpolation procedure is applied. A range of K values, with corresponding values of ε_C, may be obtained by analyzing spectrophotometric data for a range of wavelengths $\tilde{\nu}$, thereby enabling a check of the consistency of the results. See program code and sample application below.

Error parameters, such as the *sharpness* (Conrow et al. 1964) of the individual and global determinations of K, are available. The results are very sensitive to the quality of the input data; see the discussions by Rose & Drago (1959) and by Conrow et al. (1964).

K. Conrow, G. D. Johnson, R. E Bowen, *J. Am. Chem. Soc*. **86**, 1025 (1964)

N. J. Rose, R. S. Drago, *J. Am. Chem. Soc.* **81**, 6138 (1959)

Student Projects at Roskilde University using program STEP:

J. S. Bennekou, P. Borling, M. B. W. Christensen, A. M. B. Giessing, S. R. Hansen, A. F. Jørgensen, D. Ohlrich, *Student Project Report* (in Danish), Roskilde University 1992.

H. Steno, C. Overgaard, S. N. Olsen, *Student Project Report* (in Danish), Roskilde University 2000.

C. D. Christiansen, B. E. F. Ekbrant, L. A. Sørensen: *Student Project Report* (in Danish), Roskilde University 2012.

J. Spanget-Larsen
Roskilde University, February 2016

GWbasic program STEP-2

```
10 DEFINT I,N,P
20 ' DEFDBL A-H,J-M,O-Z
30 OPTION BASE 1
40 DIM A(10),B(10),C(10),D(10),F(10),L(10),G(10),H(10)
50 DIM M(20),O(20),U(20),J(20),T(20),V(20,10)
60 DIM R(20),S(20),W(20)
70 PRINT : PRINT "Program STEP-2 (JS-L, 2000, 2016)" : PRINT
80 LINE INPUT "Input File? ", E$
90 LINE INPUT "Output File? ", F$
100 OPEN "I",#1,E$
110 OPEN "O",#2,F$
120 X$=STRING$(78,95)
130 PRINT#2, "vs.2g"
140 PRINT#2, "                  *Program STEP*" : PRINT#2,
150 PRINT#2, "Least-Squares 'Systematic Trial-and-Error Procedure' for"
160 PRINT#2, "spectrophotometric evaluation of association constant K and"
170 PRINT#2, "molar absorption coefficient E for a 1:1 molecular complex,"
180 PRINT#2, "A + B = C, essentially according to  K Conrow, GD Johnson,
190 PRINT#2, "RE Bowen: J.Am.Chem.Soc. 86, 1025 (1964).  Present version"
200 PRINT#2, "treats data for up to 10 mixtures of A and B, for up to 20"
210 PRINT#2, "different wavenumbers."
220 PRINT#2, "                                        J Spanget-Larsen"
230 PRINT#2, "                                          RUC 2000, 2016"
240 PRINT#2, : PRINT#2,
250 '----read wavenumber-independent data----
260 LINE INPUT#1, T$ ' text heading
270 Y$=STRING$(LEN(T$),45)
280 PRINT : PRINT T$ : PRINT Y$ : PRINT
290 PRINT#2, Y$ : PRINT#2, T$ : PRINT#2, Y$ : PRINT#2,
300 INPUT#1, N ' No. of mixt. of A and B investigated
310 FOR I=1 TO N
320   INPUT#1, A(I) ' total conc. of A in I'th mixt.
330   INPUT#1, B(I) ' total conc. of B in I'th mixt.
340   INPUT#1, L(I) ' cell length for I'th mixt.
350   G(I)=A(I)+B(I) : H(I)=A(I)*B(I)
360 NEXT I
370 '----input search parameters----
380 P=0 : N1=0
390 PRINT : INPUT "Guess on Association Constant K";KSTART
400 PRINT#2, "Initial Value of Association Constant K    ";KSTART
410 INPUT "Initial Step Length";LSTART
420 PRINT#2, "Initial Value of Step Length               ";LSTART
430 INPUT "Lower Limit of Step Length";LIMIT
440 PRINT#2, "Lower Limit of Step Length                 ";LIMIT
450 INPUT "Maximal Number of Steps";MAX
460 PRINT#2, "Maximal Number of Steps                    ";MAX
470 ' PRINT#2, : PRINT#2, "[A] = Total Concentration of A"
480 ' PRINT#2, "[B] = Total Concentration of B"
490 ' PRINT#2, "Abs = Measured Absorbance"
500 ' PRINT#2, " d  = Length of Cell" : PRINT#2,
510 PRINT#2, : PRINT#2, X$
520 '----read abs. data for one wavenumber----
530 INPUT#1, W0 ' read wavenumber
540 IF W0=0 THEN 1860 ' (end of input file)
550 N1=N1+1
560 W(N1)=W0
570 INPUT#1, R(N1) ' read absorbancy of A
580 INPUT#1, S(N1) ' read absorbancy of B
590 E1=R(N1) : E2=S(N1)
600 FOR I=1 TO N
610   INPUT#1, F(I) ' read measured absorbances
620   D(I)=F(I)/L(I)
```

```
630   V(N1,I)=D(I)
640 NEXT I
650 '-------------------------------------
660 PRINT#2, : PRINT#2,
670 PRINT#2, "Wavenumber               ";W0;"cm-1"
680 PRINT#2, "Molar Absorbance of A    ";E1
690 PRINT#2, "Molar Absorbance of B    ";E2 : PRINT#2,
700 PRINT#2, "        [A]         [B]       Abs      d     Abs/d"
710 FOR I=1 TO N
720   PRINT#2, USING "###";I;
730   PRINT#2, USING " ##.####^^^^";A(I),B(I);
740   PRINT#2, USING " ##.####"  ;F(I),L(I),D(I)
750 NEXT I
760 PRINT
770 PRINT "Wavenumber   ";W0;"cm-1" : PRINT
780 PRINT "Molar Absorbance of A    ";E1
790 PRINT "Molar Absorbance of B    ";E2 : PRINT
800 PRINT "        [A]         [B]       Abs      d     Abs/d"
810 FOR I=1 TO N
820   PRINT USING "###";I;
830   PRINT USING " ##.####^^^^";A(I),B(I);
840   PRINT USING " ##.####"  ;F(I),L(I),D(I)
850 NEXT I
860 '=======================STEP=========================
870 PRINT : PRINT " K = Association Constant"
880 PRINT " E = Molar Absorbance of Complex C"
890 PRINT " S = RMS for Fit of Absorbances" : PRINT
900 PRINT "            K            E            S"
910 I0=0
920 '-----START
930 K=KSTART : L=LSTART : L0=LIMIT : I8=MAX
940 I0=I0+1
950 GOSUB 2940
960 IF I0>I8 THEN 1420 ' max no. of steps exceeded, exit
970 PRINT USING "######";I0;
980 PRINT USING "  ##.####^^^^";K,E;
990 PRINT USING "  ##.#######^^^^";S;
1000 PRINT CHR$(60) ' to indicate (re)start
1010 K1=K : S1=S
1020 '-----FIRST STEP
1030 K=K+L ' increase K by steplength
1040 GOSUB 2940
1050 I0=I0+1
1060 IF I0>I8 THEN 1420 ' max no. of steps exceeded, exit
1070 PRINT USING "######";I0;
1080 PRINT USING "  ##.####^^^^";K,E;
1090 PRINT USING "  ##.#######^^^^";S
1100 ' check direction
1110 IF S<S1 THEN 1170 ' RMS-error S decreases, continue
1120 K=K1-L ' reverse search direction
1130 L=-L
1140 S2=S
1150 GOTO 1210
1160 '-----INTERMEDIATE STEPS
1170 K1=K
1180 K=K+L ' increase K by steplength
1190 S2=S1
1200 S1=S
1210 IF K>0 THEN 1250
1220 L=L/4 ' reduce steplength to avoid K<=0
1230 K=K1+L ' increase old K by reduced steplength
1240 GOTO 940 ' restart from top
1250 GOSUB 2940
1260 I0=I0+1
1270 IF I0>I8 THEN 1420 ' max. no. of steps exceeded, exit
```

```
1280 PRINT USING "######";I0;
1290 PRINT USING "  ##.####^^^^";K,E;
1300 PRINT USING "  ##.#######^^^^";S
1310 ' check direction:
1320 IF S<S1 THEN 1170  ' S decreases, continue
1330 ' minimum was passed
1340 '-----FINAL INTERPOLATION STEP
1350 K=K1+L/2*(S2-S)/(S2-S1*2+S) ' 3-point parabolic interpolation
1360 L=ABS(L)/4 ' reduce steplength
1370 IF L<=L0 THEN 1420 ' min. steplength achieved, exit
1380 K=K-L
1390 '-----RESTART FROM TOP
1400 GOTO 940
1410 '============================================================
1420 M(N1)=K : O(N1)=E : J(N1)=S
1430 PRINT#2, : PRINT#2, "Results of Search Procedure:"
1440 PRINT#2, "(";I0;"Steps )" : PRINT#2,
1450 PRINT#2, "Best Fit for Association Constant K  ";K
1460 PRINT#2, "      -      Molar Absorbance of C   ";E : PRINT#2,
1470 PRINT#2, "Fit of Absorbances:" : PRINT#2,
1480 PRINT#2, "      Calc.   Exp.    Diff."
1490 PRINT
1500 PRINT "Best Fit for Association Constant K  ";K
1510 PRINT "Best Fit for Molar Absorbance of C   ";E
1520 PRINT "RMS Error of Absorbance Fit          ";S : PRINT
1530 PRINT "Fit of Absorbances:" : PRINT
1540 PRINT "      Calc.   Exp.    Diff."
1550 F1=0
1560 FOR I=1 TO N
1570   D1=E1*(A(I)-C(I))+E2*(B(I)-C(I))-D(I)
1580   D2=D1+E*C(I)
1590   F1=F1+(E+D1/C(I))^2
1600   D1=D2+D(I)
1610   PRINT#2, USING "###";I;
1620   PRINT#2, USING "###.####";D1,D(I),D2
1630   PRINT USING "###";I;
1640   PRINT USING "###.####";D1,D(I),D2
1650 NEXT I
1660 U(N1)=SQR(F1/N)
1670 PRINT#2, : PRINT#2, "RMS-Error of Absorbance Fit           ";S
1680 PRINT#2, "RMS-Error of Molar Absorbance of C    ";U(N1)
1690 X=K
1700 Y=S
1710 K=X-X/10
1720 GOSUB 2940
1730 Z1=10*(S-Y)/Y
1740 PRINT#2, "'Lower Sharpness of Fit' for K        ";Z1
1750 K=X+X/10
1760 GOSUB 2940
1770 Z2=10*(S-Y)/Y
1780 PRINT#2, "'Upper Sharpness of Fit' for K        ";Z2
1790 T(N1)=(Z1+Z2)/2
1800 PRINT#2, "'Average Sharpness of Fit' for K      ";T(N1)
1810 PRINT#2, : PRINT#2,
1820 PRINT : INPUT "Exit [1/0]";P
1830 IF P=1 THEN 1890
1840 PRINT#2, : PRINT#2, X$ : PRINT#2, : PRINT#2,
1850 GOTO 530
1860 P=1 ' end of input file
1870 PRINT#2, : PRINT#2,T$ : PRINT#2, Y$ : PRINT#2, : PRINT#2,
1880 PRINT#2, "Results of Individual Treatment of Data for Each Wavenumber:"
1890 PRINT : PRINT "Results of Individual Treatment of Data for Each Wavenumber:"
1900 PRINT#2, : PRINT
1910 PRINT#2, "  cm-1         K            E          RMS(E)      RMS(Abs)   Sharpness"
1920 PRINT "  cm-1         K            E          RMS(E)      RMS(Abs)   Sharpness"
```

```
1930 PRINT#2, STRING$(78,45)
1940 PRINT STRING$(78,45)
1950 K1=0 : T1=0 : J1=0 : K2=0 : J2=0
1960 FOR I=1 TO N1
1970   PRINT#2, USING "######";W(I);            ' Wavenumber
1980   PRINT#2, USING "#########.##";M(I);      ' K
1990   PRINT#2, USING "############";O(I),U(I); ' eps, RMS(eps)
2000   PRINT#2, USING "        ##.#^^^^";J(I);  ' RMS(Abs.Fit)
2010   PRINT#2, USING "  ####.####";T(I)        ' Sharpness
2020   PRINT USING "######";W(I);
2030   PRINT USING "#########.##";M(I);
2040   PRINT USING "############";O(I),U(I);
2050   PRINT USING "        ##.#^^^^";J(I);
2060   PRINT USING "  ####.####";T(I)
2070   K1=K1+M(I)*T(I) : T1=T1+T(I) : J1=J1+J(I)
2080 NEXT I
2090 K=K1/T1
2100 K1=0
2110 FOR I=1 TO N1
2120   K1=K1+T(I)*(K-M(I))^2
2130 NEXT I
2140 S=SQR(K1/T1)
2150 T1=T1/N1
2160 J1=J1/N1
2170 PRINT#2, STRING$(78,45)
2180 PRINT STRING$(78,45)
2190 PRINT#2, : PRINT#2, "Sharpness-Weighted Mean of K ";K
2200 PRINT#2,            "    -        -     SD of K   ";S
2210 PRINT : PRINT "Sharpness-Weighted Mean of K ";K
2220 PRINT "    -        -     RMS Dev.  ";S
2230 PRINT#2, "Mean RMS(abs)                ";J1
2240 PRINT#2, "Mean Sharpness               ";T1
2250 PRINT "Mean RMS(abs)                ";J1
2260 PRINT "Mean Sharpness               ";T1
2270 '---table with mean RMS(abs) for range of fixed K-values---
2280 PRINT : PRINT "Mean RMS(abs) for fixed K-values:"
2290 PRINT : INPUT "K-min,K-max,step [0's to exit]";Z0,Z1,Z2
2300 IF Z0=0 THEN 2490
2310 PRINT#2, : PRINT#2, "Mean RMS(abs) as a Function of K"
2320 PRINT#2, "       K     mean RMS(abs)"
2330 K=Z0 : Z1=Z1+Z2/10
2340 SS=0
2350 FOR I5=1 TO N1
2360   FOR I=1 TO N : D(I)=V(I5,I) : NEXT I
2370   E1=R(I5) : E2=S(I5)
2380   GOSUB 2940
2390   SS=SS+S
2400 NEXT I5
2410 SS=SS/N1
2420 PRINT USING "  ####.###";K;
2430 PRINT USING "  ###.#########";SS
2440 PRINT#2, USING "  ####.###";K;
2450 PRINT#2, USING "  ###.#########";SS
2460 K=K+Z2
2470 IF K>Z1 GOTO 2290
2480 GOTO 2340
2490 PRINT : INPUT "K-value for Calc. of Global Sharpness (0 to exit)";K0
2500 IF K0=0! GOTO 3080
2510 K=K0
2520 SS=0!
2530 FOR I5=1 TO N1
2540   FOR I=1 TO N : D(I)=V(I5,I) : NEXT I
2550   E1=R(I5) : E2=S(I5)
2560   GOSUB 2940
2570   SS=SS+S
```

```
2580 NEXT I5
2590 S0=SS/N1
2600 K=K0-K0/10
2610 SS=0!
2620 FOR I5=1 TO N1
2630   FOR I=1 TO N : D(I)=V(I5,I) : NEXT I
2640   E1=R(I5) : E2=S(I5)
2650   GOSUB 2940
2660   SS=SS+S
2670 NEXT I5
2680 SM=SS/N1
2690 SHL=10*(SM-S0)/S0
2700 K=K0+K0/10
2710 SS=0!
2720 FOR I5=1 TO N1
2730   FOR I=1 TO N : D(I)=V(I5,I) : NEXT I
2740   E1=R(I5) : E2=S(I5)
2750   GOSUB 2940
2760   SS=SS+S
2770 NEXT I5
2780 SP=SS/N1
2790 SHH=10*(SP-S0)/S0
2800 PRINT : PRINT "K =";K0"
2810 PRINT "'Lower Sharpness'   ";SHL
2820 PRINT "'Upper Sharpness'   ";SHH
2830 PRINT "'Average Sharpness' ";(SHL+SHH)/2
2840 PRINT#2, : PRINT#2, "K ="; : PRINT#2, USING "####.##";K0
2850 PRINT#2, "'Lower Sharpness'   ";SHL
2860 PRINT#2, "'Upper Sharpness'   ";SHH
2870 PRINT#2, "'Average Sharpness' ";(SHL+SHH)/2
2880 GOTO 2490
2890 '---------------SUBROUTINE------------------
2900 ' Compute E and S for Current Value of K
2910 '  E = Molar Absorbance of C
2920 '  S = RMS-error of Fit of Absorbances
2930 '  K = Association Constant
2940 E=0 : S=0
2950 FOR I=1 TO N
2960   X1=G(I)+1/K
2970   C(I)=X1/2-SQR(X1^2/4-H(I))
2980   E=E+(D(I)-E1*(A(I)-C(I))-E2*(B(I)-C(I)))/C(I)
2990 NEXT I
3000 E=E/N
3010 FOR I=1 TO N
3020   D1=E1*(A(I)-C(I))+E2*(B(I)-C(I))+E*C(I)
3030   S=S+(D1-D(I))^2
3040 NEXT I
3050 S=SQR(S/N)
3060 RETURN
3070 '----------------------------------------
3080 PRINT "END OF PROGRAM"
3090 PRINT : PRINT "Enter 'SYSTEM' to exit GwBasic"
3100 END
```

GWbasic Program STEP-1 creates input data file for STEP-2

```
10 PRINT
20 PRINT "--------------------------"
30 PRINT "PROGRAM STEP-1 (10.02.1997)"
40 PRINT "--------------------------"
50 PRINT "Creates Input File for STEP-2"
60 PRINT
70 LINE INPUT "Name of File? ", E$
80 OPEN "O",#1,E$
90 LINE INPUT "Title? ",T$
100 PRINT#1, T$
110 PRINT
120 INPUT "Number of Mixtures of A and B Investigated";N
130 PRINT#1, N
140 PRINT
150 PRINT "Concentrations and Cell Lengths for the";N;"Mixtures:"
160 PRINT
170 FOR I=1 TO N
180 PRINT USING "#.";I;
190 INPUT " Total Concentration [A]";A
200 PRINT#1, A
210 PRINT USING "#.";I;
220 INPUT " Total Concentration [B]";B
230 PRINT#1, B
240 PRINT USING "#.";I;
250 INPUT " Cell Length";L
260 PRINT#1, L
270 PRINT
280 NEXT I
290 PRINT "ABSORBANCE DATA:"
300 PRINT
310 INPUT "Wavenumber [cm-1]";W0
320 PRINT#1, W0
330 IF W0=0 THEN 460
340 INPUT "   Molar Absorbance of A";E1
350 PRINT#1, E1
360 INPUT "   Molar Absorbance of B";E2
370 PRINT#1, E2
380 FOR I = 1 TO N
390 PRINT USING "#.";I;
400 INPUT " Measured Absorbance";F
410 PRINT#1, F
420 NEXT I
430 PRINT
440 INPUT "New Wavenumber (0 to quit)";W0
450 GOTO 320
460 PRINT
470 PRINT "Closing File [";E$;"]"
475 PRINT : PRINT "Type and enter 'SYSTEM' to exit from GWbasic ";
480 END
```

Data file created by STEP-1 for naphthalene + chloranil in CCl_4

Absorbance data for 6 mixtures and 16 wavenumbers in the range 19000–22000 cm^{-1} obtained by Henrik Steno, Christian Overgaard, Søren Nymand Olsen: *Student Project Report* (in Danish), Roskilde University 2000.

```
05/04-2000: A=Chloranil, B=Naphthalene (1-6)
 6
 .0006316
 .099974
 1
 .0006316
 .189948
 1
 .0006316
 .299922
 1
 .0006316
 .399896
 1
 .0006316
 .499870
 1
 .0006316
 .5999845
 1
19000
0
0
.0382
.0632
.0895
.108
.1231
.14
19200
0
0
.0432
.0712
.1007
.1213
.1389
.158
19400
0
0
.0475
.0779
.1108
.1336
.1522
.1732
19600
0
0
.0514
.0843
.1201
.1448
.1655
.1882
19800
0
```

0
.0549
.0901
.1285
.1547
.1768
.2015
20000
0
0
.0577
.0946
.135
.1633
.1868
.2124
20200
.1
0
.0597
.0981
.1403
.1694
.194
.2211
20400
.4
0
.0616
.1008
.1442
.1746
.2002
.2273
20600
.9
0
.0628
.1028
.1469
.1778
.2042
.2322
20800
1.6
0
.0634
.1038
.1482
.1795
.2064
.2346
21000
2.3
0
.0639
.104
.1486
.18
.2071
.2355
21200
3.5
0
.0637

.1034
.1478
.1789
.2062
.2345
21400
4.6
0
.0632
.1023
.146
.1771
.2043
.2323
21600
5.4
0
.0626
.1007
.1438
.1744
.2012
.2289
21800
6.4
0
.0616
.0986
.1407
.1709
.1975
.2247
22000
7.8
0
.0609
.0969
.1382
.1678
.1939
.2206
0

Output file for STEP-2 run on the above data

```
vs.2g
                    *Program STEP*

Least-Squares 'Systematic Trial-and-Error Procedure' for
spectrophotometric evaluation of association constant K and
molar absorption coefficient E for a 1:1 molecular complex,
A + B = C, essentially according to  K Conrow, GD Johnson,
RE Bowen: J.Am.Chem.Soc. 86, 1025 (1964).  Present version
treats data for up to 10 mixtures of A and B, for up to 20
different wavenumbers.
                                          J Spanget-Larsen
                                            RUC 2000, 2016


-----------------------------------------
05/04-2000: A=Chloranil, B=Naphthalene (1-6)
-----------------------------------------

Initial Value of Association Constant K     5
Initial Value of Step Length                1
Lower Limit of Step Length                  .0001
Maximal Number of Steps                     100
```

```
Wavenumber                19000 cm-1
Molar Absorbance of A     0
Molar Absorbance of B     0

        [A]         [B]       Abs      d     Abs/d
  1  6.3160E-04  9.9974E-02  0.0382  1.0000  0.0382
  2  6.3160E-04  1.8995E-01  0.0632  1.0000  0.0632
  3  6.3160E-04  2.9992E-01  0.0895  1.0000  0.0895
  4  6.3160E-04  3.9990E-01  0.1080  1.0000  0.1080
  5  6.3160E-04  4.9987E-01  0.1231  1.0000  0.1231
  6  6.3160E-04  5.9998E-01  0.1400  1.0000  0.1400

Results of Search Procedure:
( 27 Steps )

Best Fit for Association Constant K   1.40541
      -      Molar Absorbance of C    479.6143

Fit of Absorbances:

      Calc.   Exp.    Diff.
  1  0.0373  0.0382 -0.0009
  2  0.0638  0.0632  0.0006
  3  0.0898  0.0895  0.0003
  4  0.1089  0.1080  0.0009
  5  0.1250  0.1231  0.0019
  6  0.1385  0.1400 -0.0015

RMS-Error of Absorbance Fit            1.141938E-03
RMS-Error of Molar Absorbance of C     6.53837
'Lower Sharpness of Fit' for K         4.119671
'Upper Sharpness of Fit' for K         3.451221
'Average Sharpness of Fit' for K       3.785446
```

Wavenumber 19200 cm-1
Molar Absorbance of A 0
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0432	1.0000	0.0432
2	6.3160E-04	1.8995E-01	0.0712	1.0000	0.0712
3	6.3160E-04	2.9992E-01	0.1007	1.0000	0.1007
4	6.3160E-04	3.9990E-01	0.1213	1.0000	0.1213
5	6.3160E-04	4.9987E-01	0.1389	1.0000	0.1389
6	6.3160E-04	5.9998E-01	0.1580	1.0000	0.1580

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.403091
- Molar Absorbance of C 541.0912

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0420	0.0432	-0.0012
2	0.0719	0.0712	0.0007
3	0.1012	0.1007	0.0005
4	0.1228	0.1213	0.0015
5	0.1408	0.1389	0.0019
6	0.1562	0.1580	-0.0018

RMS-Error of Absorbance Fit 1.386934E-03
RMS-Error of Molar Absorbance of C 8.252928
'Lower Sharpness of Fit' for K 3.417498
'Upper Sharpness of Fit' for K 3.160125
'Average Sharpness of Fit' for K 3.288812

Wavenumber 19400 cm-1
Molar Absorbance of A 0
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0475	1.0000	0.0475
2	6.3160E-04	1.8995E-01	0.0779	1.0000	0.0779
3	6.3160E-04	2.9992E-01	0.1108	1.0000	0.1108
4	6.3160E-04	3.9990E-01	0.1336	1.0000	0.1336
5	6.3160E-04	4.9987E-01	0.1522	1.0000	0.1522
6	6.3160E-04	5.9998E-01	0.1732	1.0000	0.1732

Results of Search Procedure:
(29 Steps)

Best Fit for Association Constant K 1.402988
- Molar Absorbance of C 594.0836

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0461	0.0475	-0.0014
2	0.0789	0.0779	0.0010
3	0.1111	0.1108	0.0003
4	0.1348	0.1336	0.0012
5	0.1546	0.1522	0.0024
6	0.1715	0.1732	-0.0017

RMS-Error of Absorbance Fit 1.496326E-03
RMS-Error of Molar Absorbance of C 9.379225
'Lower Sharpness of Fit' for K 3.996974
'Upper Sharpness of Fit' for K 2.859056
'Average Sharpness of Fit' for K 3.428015

Wavenumber 19600 cm-1
Molar Absorbance of A 0
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0514	1.0000	0.0514
2	6.3160E-04	1.8995E-01	0.0843	1.0000	0.0843
3	6.3160E-04	2.9992E-01	0.1201	1.0000	0.1201
4	6.3160E-04	3.9990E-01	0.1448	1.0000	0.1448
5	6.3160E-04	4.9987E-01	0.1655	1.0000	0.1655
6	6.3160E-04	5.9998E-01	0.1882	1.0000	0.1882

Results of Search Procedure:
(28 Steps)

Best Fit for Association Constant K 1.389104
- Molar Absorbance of C 648.7283

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0499	0.0514	-0.0015
2	0.0855	0.0843	0.0012
3	0.1204	0.1201	0.0003
4	0.1462	0.1448	0.0014
5	0.1679	0.1655	0.0024
6	0.1862	0.1882	-0.0020

RMS-Error of Absorbance Fit 1.600852E-03
RMS-Error of Molar Absorbance of C 10.21528
'Lower Sharpness of Fit' for K 3.675059
'Upper Sharpness of Fit' for K 3.265255
'Average Sharpness of Fit' for K 3.470157

Wavenumber 19800 cm-1
Molar Absorbance of A 0
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0549	1.0000	0.0549
2	6.3160E-04	1.8995E-01	0.0901	1.0000	0.0901
3	6.3160E-04	2.9992E-01	0.1285	1.0000	0.1285
4	6.3160E-04	3.9990E-01	0.1547	1.0000	0.1547
5	6.3160E-04	4.9987E-01	0.1768	1.0000	0.1768
6	6.3160E-04	5.9998E-01	0.2015	1.0000	0.2015

Results of Search Procedure:
(29 Steps)

Best Fit for Association Constant K 1.381512
- Molar Absorbance of C 696.2137

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0533	0.0549	-0.0016
2	0.0913	0.0901	0.0012
3	0.1287	0.1285	0.0002
4	0.1564	0.1547	0.0017
5	0.1796	0.1768	0.0028
6	0.1992	0.2015	-0.0023

RMS-Error of Absorbance Fit 1.82544E-03
RMS-Error of Molar Absorbance of C 11.27227
'Lower Sharpness of Fit' for K 3.338761
'Upper Sharpness of Fit' for K 2.843762
'Average Sharpness of Fit' for K 3.091262

Wavenumber 20000 cm-1
Molar Absorbance of A 0
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0577	1.0000	0.0577
2	6.3160E-04	1.8995E-01	0.0946	1.0000	0.0946
3	6.3160E-04	2.9992E-01	0.1350	1.0000	0.1350
4	6.3160E-04	3.9990E-01	0.1633	1.0000	0.1633
5	6.3160E-04	4.9987E-01	0.1868	1.0000	0.1868
6	6.3160E-04	5.9998E-01	0.2124	1.0000	0.2124

Results of Search Procedure:
(28 Steps)

Best Fit for Association Constant K 1.357548
- Molar Absorbance of C 741.8978

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0560	0.0577	-0.0017
2	0.0960	0.0946	0.0014
3	0.1355	0.1350	0.0005
4	0.1648	0.1633	0.0015
5	0.1894	0.1868	0.0026
6	0.2103	0.2124	-0.0021

RMS-Error of Absorbance Fit 1.761445E-03
RMS-Error of Molar Absorbance of C 11.97457
'Lower Sharpness of Fit' for K 3.925822
'Upper Sharpness of Fit' for K 3.327337
'Average Sharpness of Fit' for K 3.626579

Wavenumber 20200 cm-1
Molar Absorbance of A .1
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0597	1.0000	0.0597
2	6.3160E-04	1.8995E-01	0.0981	1.0000	0.0981
3	6.3160E-04	2.9992E-01	0.1403	1.0000	0.1403
4	6.3160E-04	3.9990E-01	0.1694	1.0000	0.1694
5	6.3160E-04	4.9987E-01	0.1940	1.0000	0.1940
6	6.3160E-04	5.9998E-01	0.2211	1.0000	0.2211

Results of Search Procedure:
(31 Steps)

Best Fit for Association Constant K 1.336165
- Molar Absorbance of C 778.2265

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0579	0.0597	-0.0018
2	0.0995	0.0981	0.0014
3	0.1406	0.1403	0.0003
4	0.1712	0.1694	0.0018
5	0.1969	0.1940	0.0029
6	0.2187	0.2211	-0.0024

RMS-Error of Absorbance Fit 1.921932E-03
RMS-Error of Molar Absorbance of C 12.54743
'Lower Sharpness of Fit' for K 3.406904
'Upper Sharpness of Fit' for K 3.050022
'Average Sharpness of Fit' for K 3.228463

Wavenumber 20400 cm-1
Molar Absorbance of A .4
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0616	1.0000	0.0616
2	6.3160E-04	1.8995E-01	0.1008	1.0000	0.1008
3	6.3160E-04	2.9992E-01	0.1442	1.0000	0.1442
4	6.3160E-04	3.9990E-01	0.1746	1.0000	0.1746
5	6.3160E-04	4.9987E-01	0.2002	1.0000	0.2002

6	6.3160E-04	5.9998E-01	0.2273	1.0000	0.2273

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.327642
- Molar Absorbance of C 804.0053

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0597	0.0616	-0.0019
2	0.1024	0.1008	0.0016
3	0.1448	0.1442	0.0006
4	0.1762	0.1746	0.0016
5	0.2027	0.2002	0.0025
6	0.2252	0.2273	-0.0021

RMS-Error of Absorbance Fit 1.808425E-03
RMS-Error of Molar Absorbance of C 13.1785
'Lower Sharpness of Fit' for K 4.084016
'Upper Sharpness of Fit' for K 3.506764
'Average Sharpness of Fit' for K 3.79539

Wavenumber 20600 cm-1
Molar Absorbance of A .9
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0628	1.0000	0.0628
2	6.3160E-04	1.8995E-01	0.1028	1.0000	0.1028
3	6.3160E-04	2.9992E-01	0.1469	1.0000	0.1469
4	6.3160E-04	3.9990E-01	0.1778	1.0000	0.1778
5	6.3160E-04	4.9987E-01	0.2042	1.0000	0.2042
6	6.3160E-04	5.9998E-01	0.2322	1.0000	0.2322

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.301899
- Molar Absorbance of C 829.8494

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0608	0.0628	-0.0020
2	0.1043	0.1028	0.0015
3	0.1475	0.1469	0.0006
4	0.1797	0.1778	0.0019
5	0.2069	0.2042	0.0027
6	0.2301	0.2322	-0.0021

RMS-Error of Absorbance Fit 1.922109E-03
RMS-Error of Molar Absorbance of C 13.9722
'Lower Sharpness of Fit' for K 3.876022
'Upper Sharpness of Fit' for K 2.969719
'Average Sharpness of Fit' for K 3.422871

Wavenumber 20800 cm-1
Molar Absorbance of A 1.6
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0634	1.0000	0.0634
2	6.3160E-04	1.8995E-01	0.1038	1.0000	0.1038
3	6.3160E-04	2.9992E-01	0.1482	1.0000	0.1482
4	6.3160E-04	3.9990E-01	0.1795	1.0000	0.1795
5	6.3160E-04	4.9987E-01	0.2064	1.0000	0.2064
6	6.3160E-04	5.9998E-01	0.2346	1.0000	0.2346

Results of Search Procedure:
(30 Steps)

Best Fit for Association Constant K 1.286537
- Molar Absorbance of C 842.7705

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0615	0.0634	-0.0019
2	0.1053	0.1038	0.0015
3	0.1489	0.1482	0.0007
4	0.1814	0.1795	0.0019
5	0.2089	0.2064	0.0025
6	0.2323	0.2346	-0.0023

RMS-Error of Absorbance Fit 1.874622E-03
RMS-Error of Molar Absorbance of C 13.53524
'Lower Sharpness of Fit' for K 3.803871
'Upper Sharpness of Fit' for K 3.472872
'Average Sharpness of Fit' for K 3.638371

Wavenumber 21000 cm-1
Molar Absorbance of A 2.3
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0639	1.0000	0.0639
2	6.3160E-04	1.8995E-01	0.1040	1.0000	0.1040
3	6.3160E-04	2.9992E-01	0.1486	1.0000	0.1486
4	6.3160E-04	3.9990E-01	0.1800	1.0000	0.1800
5	6.3160E-04	4.9987E-01	0.2071	1.0000	0.2071
6	6.3160E-04	5.9998E-01	0.2355	1.0000	0.2355

Results of Search Procedure:
(26 Steps)

Best Fit for Association Constant K 1.270381
- Molar Absorbance of C 851.1369

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0618	0.0639	-0.0021
2	0.1056	0.1040	0.0016
3	0.1493	0.1486	0.0007
4	0.1820	0.1800	0.0020
5	0.2096	0.2071	0.0025
6	0.2333	0.2355	-0.0022

RMS-Error of Absorbance Fit	1.954436E-03
RMS-Error of Molar Absorbance of C	14.7029
'Lower Sharpness of Fit' for K	3.560078
'Upper Sharpness of Fit' for K	3.132296
'Average Sharpness of Fit' for K	3.346187

Wavenumber	21200 cm-1
Molar Absorbance of A	3.5
Molar Absorbance of B	0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0637	1.0000	0.0637
2	6.3160E-04	1.8995E-01	0.1034	1.0000	0.1034
3	6.3160E-04	2.9992E-01	0.1478	1.0000	0.1478
4	6.3160E-04	3.9990E-01	0.1789	1.0000	0.1789
5	6.3160E-04	4.9987E-01	0.2062	1.0000	0.2062
6	6.3160E-04	5.9998E-01	0.2345	1.0000	0.2345

Results of Search Procedure:
(29 Steps)

Best Fit for Association Constant K		1.241571
-	Molar Absorbance of C	856.8926

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0617	0.0637	-0.0020
2	0.1050	0.1034	0.0016
3	0.1484	0.1478	0.0006
4	0.1810	0.1789	0.0021
5	0.2086	0.2062	0.0024
6	0.2323	0.2345	-0.0022

RMS-Error of Absorbance Fit	1.91706E-03
RMS-Error of Molar Absorbance of C	14.6425
'Lower Sharpness of Fit' for K	3.486342
'Upper Sharpness of Fit' for K	3.270104
'Average Sharpness of Fit' for K	3.378223

Wavenumber 21400 cm-1
Molar Absorbance of A 4.6
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0632	1.0000	0.0632
2	6.3160E-04	1.8995E-01	0.1023	1.0000	0.1023
3	6.3160E-04	2.9992E-01	0.1460	1.0000	0.1460
4	6.3160E-04	3.9990E-01	0.1771	1.0000	0.1771
5	6.3160E-04	4.9987E-01	0.2043	1.0000	0.2043
6	6.3160E-04	5.9998E-01	0.2323	1.0000	0.2323

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.203988
- Molar Absorbance of C 863.5906

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0611	0.0632	-0.0021
2	0.1038	0.1023	0.0015
3	0.1468	0.1460	0.0008
4	0.1791	0.1771	0.0020
5	0.2067	0.2043	0.0024
6	0.2304	0.2323	-0.0019

RMS-Error of Absorbance Fit 1.853333E-03
RMS-Error of Molar Absorbance of C 15.04894
'Lower Sharpness of Fit' for K 3.890289
'Upper Sharpness of Fit' for K 2.990496
'Average Sharpness of Fit' for K 3.440392

Wavenumber 21600 cm-1
Molar Absorbance of A 5.4
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0626	1.0000	0.0626
2	6.3160E-04	1.8995E-01	0.1007	1.0000	0.1007
3	6.3160E-04	2.9992E-01	0.1438	1.0000	0.1438
4	6.3160E-04	3.9990E-01	0.1744	1.0000	0.1744
5	6.3160E-04	4.9987E-01	0.2012	1.0000	0.2012
6	6.3160E-04	5.9998E-01	0.2289	1.0000	0.2289

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.191211
- Molar Absorbance of C 854.5854

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0605	0.0626	-0.0021
2	0.1024	0.1007	0.0017
3	0.1446	0.1438	0.0008

4	0.1765	0.1744	0.0021
5	0.2036	0.2012	0.0024
6	0.2270	0.2289	-0.0019

RMS-Error of Absorbance Fit 1.900166E-03
RMS-Error of Molar Absorbance of C 15.83869
'Lower Sharpness of Fit' for K 3.581328
'Upper Sharpness of Fit' for K 2.687795
'Average Sharpness of Fit' for K 3.134562

Wavenumber 21800 cm-1
Molar Absorbance of A 6.4
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0616	1.0000	0.0616
2	6.3160E-04	1.8995E-01	0.0986	1.0000	0.0986
3	6.3160E-04	2.9992E-01	0.1407	1.0000	0.1407
4	6.3160E-04	3.9990E-01	0.1709	1.0000	0.1709
5	6.3160E-04	4.9987E-01	0.1975	1.0000	0.1975
6	6.3160E-04	5.9998E-01	0.2247	1.0000	0.2247

Results of Search Procedure:
(27 Steps)

Best Fit for Association Constant K 1.157405
- Molar Absorbance of C 852.2187

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0594	0.0616	-0.0022
2	0.1003	0.0986	0.0017
3	0.1416	0.1407	0.0009
4	0.1730	0.1709	0.0021
5	0.1998	0.1975	0.0023
6	0.2229	0.2247	-0.0018

RMS-Error of Absorbance Fit 1.880337E-03
RMS-Error of Molar Absorbance of C 16.51237
'Lower Sharpness of Fit' for K 3.429185
'Upper Sharpness of Fit' for K 2.639244
'Average Sharpness of Fit' for K 3.034214

Wavenumber 22000 cm-1
Molar Absorbance of A 7.8
Molar Absorbance of B 0

	[A]	[B]	Abs	d	Abs/d
1	6.3160E-04	9.9974E-02	0.0609	1.0000	0.0609
2	6.3160E-04	1.8995E-01	0.0969	1.0000	0.0969

3	6.3160E-04	2.9992E-01	0.1382	1.0000	0.1382
4	6.3160E-04	3.9990E-01	0.1678	1.0000	0.1678
5	6.3160E-04	4.9987E-01	0.1939	1.0000	0.1939
6	6.3160E-04	5.9998E-01	0.2206	1.0000	0.2206

Results of Search Procedure:
(28 Steps)

Best Fit for Association Constant K 1.142882
- Molar Absorbance of C 840.2615

Fit of Absorbances:

	Calc.	Exp.	Diff.
1	0.0588	0.0609	-0.0021
2	0.0987	0.0969	0.0018
3	0.1390	0.1382	0.0008
4	0.1698	0.1678	0.0020
5	0.1960	0.1939	0.0021
6	0.2187	0.2206	-0.0019

RMS-Error of Absorbance Fit 1.827032E-03
RMS-Error of Molar Absorbance of C 16.18611
'Lower Sharpness of Fit' for K 3.081424
'Upper Sharpness of Fit' for K 2.861856
'Average Sharpness of Fit' for K 2.97164

05/04-2000: A=Chloranil, B=Naphthalene (1-6)

Results of Individual Treatment of Data for Each Wavenumber:

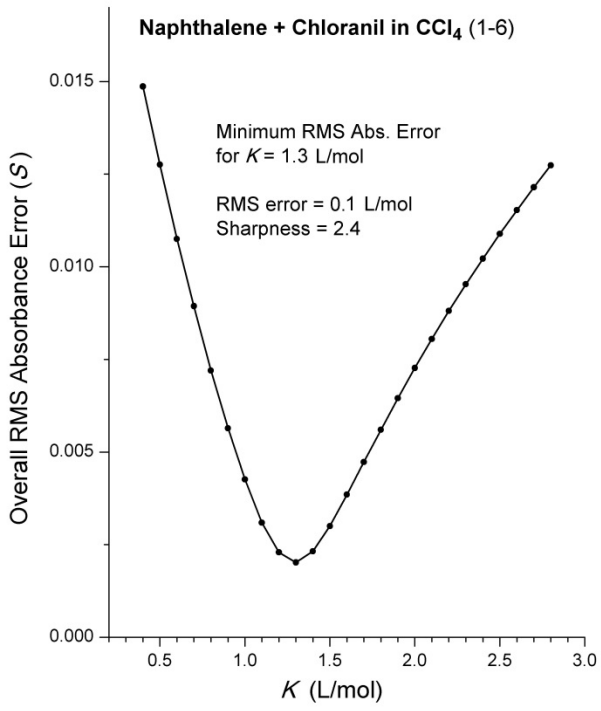
cm-1	K	E	RMS(E)	RMS(Abs)	Sharpness
19000	1.41	480	7	1.1E-03	3.7854
19200	1.40	541	8	1.4E-03	3.2888
19400	1.40	594	9	1.5E-03	3.4280
19600	1.39	649	10	1.6E-03	3.4702
19800	1.38	696	11	1.8E-03	3.0913
20000	1.36	742	12	1.8E-03	3.6266
20200	1.34	778	13	1.9E-03	3.2285
20400	1.33	804	13	1.8E-03	3.7954
20600	1.30	830	14	1.9E-03	3.4229
20800	1.29	843	14	1.9E-03	3.6384
21000	1.27	851	15	2.0E-03	3.3462
21200	1.24	857	15	1.9E-03	3.3782
21400	1.20	864	15	1.9E-03	3.4404
21600	1.19	855	16	1.9E-03	3.1346
21800	1.16	852	17	1.9E-03	3.0342
22000	1.14	840	16	1.8E-03	2.9716

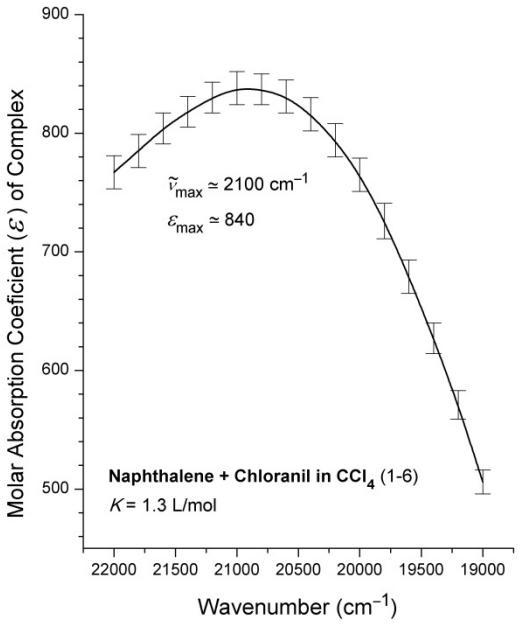
Sharpness-Weighted Mean of K 1.303195
- - SD of K 8.590018E-02
Mean RMS(abs) 1.754524E-03
Mean Sharpness 3.380037

```
Mean RMS(abs) as a Function of K
       K     mean RMS(abs)
     0.400    0.014865960
     0.500    0.012755720
     0.600    0.010750230
     0.700    0.008936689
     0.800    0.007200669
     0.900    0.005638171
     1.000    0.004260350
     1.100    0.003092693
     1.200    0.002286736
     1.300    0.002023212
     1.400    0.002316501
     1.500    0.002999234
     1.600    0.003851042
     1.700    0.004732078
     1.800    0.005603755
     1.900    0.006454099
     2.000    0.007268483
     2.100    0.008050848
     2.200    0.008810796
     2.300    0.009527423
     2.400    0.010219190
     2.500    0.010890680
     2.600    0.011529410
     2.700    0.012147210
     2.800    0.012743490

K =   1.30
'Lower Sharpness'    2.333469
'Upper Sharpness'    2.391323
'Average Sharpness'  2.362396
```

The final results of this run:
$K = 1.3 \pm 0.1$ L/mol, $\varepsilon_{max} = 840 \pm 14$ for $\tilde{\nu}_{max} \approx 2100$ cm^{-1}





This diagram refers to the results of a run with fixed association constant $K = 1.3$ L/mol for all wavenumbers.