BIBLIOGRAPHY

1. Beckmann, E. Z. Phys. Chem. 6(1890):444.
2. Taylor, M.D. "The Vapor Phase Dissociation of Some Carboxyric Acids. I. Acetic Acid" J. Amer. Chem. Soc. 73 (1951):315.
3. Harris, J.T. and Honbs, M.E., "A Study of the Association of Some Organic Acids by Infrared Absorption Measurements" J. Amer. Chem. Soc. 76(1954):1419.
4. Barrows, G.M. and Yerger, E.A., "The Dimerization of Acetic Acid in Carbontetrachloride and Chloroform" J. Amer. Chem. Soc. 76(1954):5248.
5. Wenograd, J. and Spurr, R.A., "Characteristic Integrated Intensities of Bands in the Infrared Spectra of Carboxylic Acids" J. Amer. Chem. Soc. 79(1957):5844.
6. Freedman, E. "On the Use of Ultrasonic Absorption for the Determination of Very Rapid Reaction Rates at Equilibrium: Application to the Liquid Phase Association of Carboxylic Acids" J. Chem. Phys. 21 (1953):1758.
7. Karle, J. and Brockway, L.O., "An Electron Diffraction Investigation of the Monomer and Dimers of Formic, Acetic and Trifluoroacetic Acids and the Dimer of Dueterium Acetate" J. Amer. Chem. Soc. 66(1944):574.

8. Huggins, C.M., Pimentel, G.C. and Shoolery, J.N., "Proton Magnetic Resonance Studies of the Hydrogen Bonding of Phenol, Substituted Phenols and Acetic Acid" J. Phys. Chem. 60(1956):1311.

9. Reeves, L.W. and Schneider, W.G., "Nuclear Magnetic Resonance Studies of Hydrogen Bonding in Acetic Acid" Trans. Faraday Soc. 54(1957):314.

10. Reeves, L.W. "Hydrogen Bonding in Carboxylic Acids" Trans. Faraday Soc. 55(1959):1684.

11. Maciel, G.E. and Traficante, D.D., "Carbon-13 Chemical Shifts of Carbonyl Group. IV. Dilution Curves for Acetic Acid in Representive Solvents" J. Amer. Chem. Soc. 88(1966):220.

12. Jones, R.E. and Templeton, D.H., "Crystal Structure of Acetic Acid" Acta Crystallogr. 11(1958):484.

13. Goldman, M.A. "Hydrogen-Bonded Species of Acetic Acid in Inert Solvents" J. Phys. Chem. 77(1973):2295.

14. Lascombe, J., Haurie, M. and Josien, M.,"Influence of Solvents on the Valence Vibration ν C=O of Some Monocarboxylic Acids Investigation by Infrared Spectroscopy" J. Chem. Phys. 59(1962):1233.

15. Bellamy, L.J., Lake, R. and Pace, R., "Hydrogen Bonding in Carboxylic Acids (II) Monocarboxylic Acids" Spectrochim. Acta. 19(1963):443.

16. Haurie, M. and Novak, A., "Oligomers in Pure Liquid Acetic Acid; Infrared and Raman Spectra" C.R. Acad. Sci. Paris, Ser. A,B 264B(9),(1967):694.

17. Servanton, M., Biais, J. and Lemanceau, B., "Self-Association of Acetic Acid in an Inert Solvent Solution Studied by Nuclear Magnetic Resonance" J. Chim. Phys. 67 (1970):800.

18. Panpa, S. "A Study of Acetic Acid at Various Concentrations by means of Certain Physical Properties" Master's Thesis, Department of Chemistry, Graduate School, Chulalongkorn University, 1977.

19. Gutowsky, H.S. and Saika, A., "Dissociation, Chemical Exchange, and Proton Magnetic Resonance in Some Aqueous Electrolytes" J. Chem. Phys. 21(1953):1688.

20. Sarolea-Mathot, L. "Thermodynamic and Spectroscopic Properties of Associated Solutions" Trans. Faraday Soc. 49(1953):8.

21. Coggeshall, N.D. and Saier, E.L., "Infrared Absorption Study of Hydrogen Bonding Equilibria" J. Amer. Chem. Soc. 73(1951):5414.

22. Goldman, M.A., Ph.D. Thesis, Florida State University, 1969.

23. Allen, G. and Caldin, E.F., "Association of Carboxylic Acids" Quart. Rev. 7(1953):255.

24. Arnold, J.T. and Packard, M.E., "Variations in Absolute Chemical Shift of Nuclear Induction Signals of Hydroxyl Groups of Methyl and Ethyl Alcohol" J. Chem. Phys. 19(1951):1608.

25. Davis, J.C. and Pitzer, K.S., "Nuclear Magnetic Resonance Studies of Hydrogen Bonding. I. Carboxylic Acids" J. Phys. Chem. 64(1960):886.

26. Capalbi, A., Franconi, C., Pisce, B. and Tosato, M.L., "Molecular Association of Carboxylic Acids Determinated by Nuclear Magnetic Resonance Spectroscopy" Sci. Tec. 5(1961):126.

27. Muller, N. and Rose, P., "Nuclear Magnetic Resonance Dilution Shifts for Carboxylic Acids in Rigorously Dried Solvents. I. Acetic Acid in Acetic Anhydride, Acetone, and 1,4-Dioxane" J. Phys Chem. 69(1965): 2564.

28. Muller, N. and Hughs, O.R., "Nuclear Magnetic Resonance Dilution Shifts for Carboxylic Acids in Rigorously Dried Solvents. II. Benzoic Acid in Benzene" J. Phys. Chem. 70(1966):3975.

29. Oliver, J.P. and De Roos, J.B., Private Communification, Wayne State University.

30. Goldman, M., Ph.D. Dissertation, Florida State University, 1969.

31. Muller, N. "Concerning Structural Models for Water and Chemical-Shift Data" J. Chem. Phys. 43(1965):2555.

32. Clark, J.H. and Emsley, J., "Proton Magnetic Resonance Studies of Fluoride and Acetate Solutions in Glacial Acetic Acid: The Shielding and Thermodinamics of Strong Hydrogen Bonds" J.C.S. Dalton (1973):2154.

33. Jones, G. and Bradshaw, B.C., "The Measurement of the Conductance of Electrolyses. V. A Redetermination of the Conductance of Standard Potassium Chloride Solutions in Absolute Units" J. Amer. Chem. Soc. 55 (1933):1780.

34. Daniels, F. and Albety, R. in Physical Chemistry pp. 169-174, Wiley, New York, 1956.

35. Harned, H.S, and Owen, B.B. in The Physical Chemistry of Electrolytic Solutions 3rd. ed.,pp. 228-231, American Chemical Society Reinhold Book Corporation, New York, 1985.

36. Salzberg, H.W., et al. in Physical Chemistry Laboratory pp. 29-33, Macmillan Publishing Co., Inc., New York, 1978.

37. Barrante, J.R. in Physical Chemistry for the Life Science pp. 249-254, Prentice-Hall Inc., Engle Wood Cliffs, New Jersey, U.S.A., 1977.

38. Levine, I.N. in Physical Chemistry pp. 152-157. MacGraw-Hill, 1978.

39. Vogel, A.I. in A Textbook of Quantitative Inorganic Analysis 3rd. ed.,pp. 48-50, Longman Ltd., London, England, 1961.

40. Stark, P.A. in Introduction to Numerical Methods pp. 103-115, Macmillan Publishing Co., Inc., New York, 1970.

41. Waldstein, P. and Blatz, L.A., "Low-frequency Raman Spectra and Molecular Assiciation in Liquid Formic and Acetic acids" J. Phys. Chem. 70(1966):2771.

42. Nakamoto, K. and Kishida, S., "Normal Coordinate Analysis of Hydrogen-Bonded Compounds. I. Monomeric Formic Acid and Acetic Acid" J. Chem. Phys. 41(1964):1554.

43. Nakamoto, K. and Kishida, S., "Normal Coordinate Analysis of Hydrogen-Bonded Compounds. II. Dimeric Formic and Acetic Acids" J. Chem. Phys. 41(1964):1558.

44. Sangsoontorn, T. "A Study of Ionic Interactions of Thallous-Thallic System in Glacial Acetic Acid" Master's Thesis, Department of Chemistry, Graduate School, Chulalongkorn University, 1975.

45. Davis, P.B. and Jones, H.C., "The Viscosities of Binary Mixtures of the Associated Liquids, Water, Formic Acid and Acetic Acid." J. Amer. Chem. Soc. 37(1915): 1194.

APPENDIX 1

DERIVATION OF X_i

Equilibrium processes of a linear dimer and a polymer are shown in eqs(A1.1) and (A1.2)-(A1.4) respectively.

$$X_1 + X_1 \xrightleftharpoons{K_1} X_2 \qquad (A1.1)$$

$$X_2 + X_1 \xrightleftharpoons{K} X_3 \qquad (A1.2)$$

$$X_3 + X_1 \xrightleftharpoons{K} X_4 \qquad (A1.3)$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$X_{i+1} + X_1 \xrightleftharpoons{K} X_i \qquad (A1.4)$$

The above equations can be alternatively expressed in terms of the equilibrium constants as follow.

$$X_2 = K_1X_1^2 \qquad (A1.5)$$

$$X_3 = KX_2X_1 = K_1KX_1^3 \qquad (A1.6)$$

$$X_4 = KX_3X_1 = K_1K^2X_1^4 \qquad (A1.7)$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$X_i = KX_{i-1}X_1 = K_1K^{i-2}X_1^i \qquad (A1.8)$$

or

$$X_i = (K_1/K^2)(KX_1)^i \qquad (A1.9)$$

APPENDIX 2

DERIVATION OF $\sum_{i=2}^{\infty} X_i$

Definition : $$\sum_{i=2}^{\infty} X_i = X_2 + X_3 + X_4 + \ldots\ldots\ldots \qquad \text{(A2.1)}$$

X_2, X_3, X_4, ...from appendix 1 were inserted into eq(A2.1).

$$\sum_{i=2}^{\infty} X_i = (K_1X_1^2)+(K_1KX_1^3)+(K_1K^2X_1^4)+\ldots\ldots$$

$$= \frac{K_1}{K^2}\left[K^2X_1^2+K^3X_1^3+K^4X_1^4+\ldots\right]$$

$$= \frac{K_1}{K^2}\left[Y^2 + Y^3 + Y^4 + \ldots\right] \qquad \text{(where } Y=KX_1\text{)}$$

$$= \frac{K_1}{K^2}Y^2\left[1 + Y + Y^2+\ldots\right]$$

(power series formular : $\sum_{i=0}^{\infty} Y^i = 1 + Y + Y^2+\ldots\ldots = 1/(1-Y)$)

Then $$\sum_{i=2}^{\infty} X_i = K_1Y^2/K^2(1-Y) \qquad \text{(A2.2)}$$

APPENDIX 3

DERIVATION OF $\sum_{i=2}^{\infty} (i)X_i$

Definition : $$\sum_{i=2}^{\infty} (i)X_i = 2X_2 + 3X_3 + 4X_4 + \ldots\ldots \qquad (A3.1)$$

From appendices 1 and 2

$$\sum_{i=2}^{\infty} (i)X_i = 2(K_1X_1^2)+3(K_1KX_1^3)+4(K_1K^2X_1^4)+\ldots\ldots$$

$$= \frac{K_1}{K^2}\left[2(K^2X_1^2)+3(K^3X_1^3)+4(K^4X_1^4)+\ldots\right]$$

$$= \frac{K_1}{K^2}\left[2Y^2 + 3Y^3 + 4Y^4 + \ldots\right]$$

$$= \frac{K_1}{K^2}\left[2\sum_{i=0}^{\infty} Y^i + \sum_{i=0}^{\infty} (i)Y^2\right]$$

(power series formular : $\sum_{i=0}^{\infty} (i)Y^i = Y/(1-Y)^2$)

Then

$$\sum_{i=2}^{\infty} (i)X_i = \frac{K_1Y^2}{K^2}\,\frac{(2-Y)}{(1-Y)^2} \qquad (A3.2)$$

APPENDIX 4

THE CONVERSION OF C_{H^+} TO X_{H^+}

The mole fraction of acetate ion can be evaluated by eq(A4.1).

$$X_{A^-} = \frac{C_{A^-}}{(1000D_{A,C}-60.05C_A)/18 + 2C_{H^+} + n_c + \sum_{i=1}^{\infty} n_i} \qquad (A4.1)$$

Assign $(1000D_{A,C}-60.05C_A)/18 + 2C_{H^+} = \beta$ (A4.2)

and $n_c + \sum_{i=1}^{\infty} n_i = \gamma$ (A4.3)

then $X_{A^-} = C_{A^-}/(B + \gamma) = C_{H^+}/(\beta + \gamma)$ (A4.4)

Definition of the mole fraction.

$$n_c = X_c(\beta + \gamma) \qquad (A4.5)$$

$$n_1 = X_1(\beta + \gamma) \qquad (A4.6)$$

$$n_2 = X_2(\beta + \gamma) \qquad (A4.7)$$

$$\vdots \qquad \vdots$$

$$n_\infty = X_\infty(\beta + \gamma) \qquad (A4.8)$$

Substitution of n_c, n_1, n_2,...n_∞, in eq(A4.3) leads to

$$\gamma = (X_c + X_1 + \sum_{i=2}^{\infty} X_i)(\beta + \gamma)$$

$$= \frac{(X_c + X_1 + \sum_{i=2}^{\infty} X_i)\beta}{1 - (X_c + X_1 + \sum_{i=2}^{\infty} X_i)} \qquad (A4.9)$$

From $X_1 = Y/K$ and $X_c = K_c X_1^2$, then $X_c = K_c Y^2/K^2$, and eq(A2.2) of appendix 2, then eq(A4.9) can be written.

$$\gamma = \frac{(K_c Y^2(1-Y)+KY(1-Y)+K_1 Y^2)\beta}{K^2(1-Y)-(K_c Y^2(1-Y)+KY(1-Y)+K_1 Y^2)} \qquad (A4.10)$$

Then $$X_{A^-} = \frac{(K_c Y^3-(K_c+K_1)Y^2+(K-K^2)Y+K^2)C_{H^+}/\beta}{K^2(1-Y)} \qquad (A4.11)$$

or $$X_{H^+} = \frac{(K_c Y^3-(K_c+K_1)Y^2+(K-K^2)Y+K^2)C_{H^+}/\beta}{K^2(1-Y)} \qquad (A4.12)$$

APPENDIX 5

THE CONVERSION OF THE CONCENTRATION SCALES

$$X_{HCl} = \frac{1}{(1000D_{HCl,C}/C_{HCl}-36.46)/18 + 1} \quad (A5.1)$$

$$X_{AS} = \frac{1}{(100/(\%w/w)-1)60.05/18 + 1} \quad (A5.2)$$

$$C_{A} = \frac{(\%w/w)D_{A,C}}{6.005} \quad (A5.3)$$

$$X_{AS} = \frac{1}{(1000D_{A,C}/C_{A}-60.05)/18 + 1} \quad (A5.4)$$

APPENDIX 6

CALCULATION OF THE FRACTION OF PROTONS

$$f(1) = \frac{3X_{HCl}}{2 - X_{HCl}} \quad (A6.1)$$

$$f(H_2O) = \frac{2 - 2X_{AS}}{2 - X_{AS}} \quad (A6.2)$$

$$f(H^+) = \frac{X_{H^+S}}{2 - X_{AS}} \quad (A6.3)$$

APPENDIX 7

CONDUCTIVITY FORMULAES

$$K_{solution} = \text{cell constant}/R(\infty\,Hz) \quad (A7.1)$$

$$K_B = K_{solution} - K_{H_2O} \quad (A7.2)$$

$$\Lambda_B = \frac{1000K_B}{C_B} \quad (A7.3)$$

For aqueous acetic acid

$$\alpha_A = \Lambda_{HOAc}/\Lambda^o_{HOAc} \quad (A7.4)$$

$$C_{H^+} = \alpha_A C_A \quad (A7.5)$$

$$X_{H^+S} = \alpha_A X_{AS} \quad (A7.6)$$

Correction of the measured solution resistance

$$R(\infty\,Hz) = \frac{3R(3KHz)-R(1KHz)}{2} \quad (A7.7)$$

Kohlrausch's equation

$$\Lambda^o_{HOAc} = \Lambda^o_{HCl} + \Lambda^o_{NaOAc} - \Lambda^o_{NaCl} \quad (A7.8)$$

R(1KHz), R(3KHz) and R(∞ Hz) are the resistance of electrolytic solution at the frequency of 1KHz, 3KHz and ∞ Hz respectively.

APPENDIX 8

FORTRAN IV PROGRAM FOR CALCULATING THE EQUILIBRIUM CONSTANT SET BY THE LEAST SQUARES FIT METHOD OF THE PROTON NMR CHEMICAL SHIFTS

The variables used in the expressions for calculating the equilibrium constant set are denoted by the following symbols.

Variables	FORTRAN symbols
X_1	XL1
X_c	XC2
X_i	XL(I)
X_{A^-}	XAM
$\%X_1$	PXL1
$\%X_c$	PXC2
$\%X_i$	PXL(I)
$\%X_{GT4}$	PXGT4
$\%X_{A^-}$	PXAM
δ^{calcd}	CCAL
δ^{obsd}	COBS
$f(H^+)$	FH
$f(H_2O)$	FW
$f(E)$	FE
$f(I)$	FI
$f(C)$	FC
C_{H^+}/β	RATIO

(continued)

Variables	FORTRAN symbols
K	AK
K_1	AKL
K_c	AKC
X_{AS}	XAS
$\delta(E)$	CE
$\delta(I)$	CI
$\delta(C)$	CC
Y	Y
σ	SD

The computer programs used in the least squares fit for determining the equilibrium constants and the mole fractions of various species are next shown as programs I and II respectively.

PROGRAM I

```
C       MAIN PROGRAM
C       DETERMINATION OF THE EQUILIBRIUM CONSTANTS
        REAL*8 CCAL,COBS,FH,FW,FE,FI,FC,SUMSQ,Y,FUN,C,SD
        DIMENSION CCAL(10),COBS(10),FH(10),FW(10)
        COMMON /CONST/AK,AKL,AKC
        COMMON /RAXAM/RATIO(10),XAS(10),M
        COMMON /FUNCT/X(4),FX(4)
        DOUBLE PRECISION X,FX,RATIO,XAS,AK,AKL,AKC,CE,CI,CC
        DATA ICE,ICI,ICC/****,****,****/
        READ(1,10)(COBS(M1),M1=1,10)
     10 FORMAT(10D8.4)
        READ(1,20)(XAS(M2),M2=1,10)
     20 FORMAT(10D8.4)
        READ(1,30)(RATIO(M3),M3=1,8)
     30 FORMAT(8D10.4)
        READ(1,40)(RATIO(M4),M4=9,10)
     40 FORMAT(2D10.4)
        READ(1,50)(FW(M5),M5=1,10)
     50 FORMAT(10D8.4)
        READ(1,60)(FH(M6),M6=1,8)
     60 FORMAT(8D10.4)
        READ(1,70)(FH(M7),M7=9,10)
     70 FORMAT(2D10.4)
        READ(1,80) CW,CH
     80 FORMAT(2D8.4)
        DO  90 K =****,****,**
        DO 100 KL=****,****,**
        DO 110 KC=****,****,**
        AK =K *0.1
        AKL=KL*0.1
        AKC=KC*0.1
        CE=ICE*0.01
        CI=ICI*0.01
        CC=ICC*0.01
        SUMSQ=0
        DO 120 M=1,10
        CALL ROOT
        DO 130 L=1,4
        Y=X(L)
        FUN=FX(L)
        IF(Y.GE.AK.OR.Y.LE.0.OR.Y.EQ.1.) GOTO 130
        IF(FUN.GE.1.D-5.OR.FUN.LE.-1.D-5) GOTO 130
        C=2.*AKC*Y*Y+AK*Y+AKL*Y*Y(2.-Y)/(1.-Y)**2
       *+2.*AK*AK*(1.-XAS(M))+(AKC*Y*Y*Y-(AKC+AKL)*Y*Y
       *+(AK+AK*AK)*Y+AK*AK)/(1.-Y)*RATIO(M)
        FE=(AK*Y+AKL*Y*Y/(1.-Y))/C
        FI=AKL*Y*Y/(1.-Y)**2)/C
        FC=2.*AKC*Y*Y/C
        CCAL(M)=FE*CE+FI*CI+FC*CC+FH(M)*CH+FE(M)*CW
        GOTO 140
    130 CONTINUE
```

```
      GOTO 110
  140 SUMSQ=SUMSQ+(COBS(M)-CCAL(M))**2
  120 CONTINUE
      SD=DSQRT(SUMSQ)/3.
      IF(SD.GT.******) GOTO 110
      WRITE(3,150) CE,CI,CC,AK,AKL,AKC,SD
  150 FORMAT(10X,'CE =',F5.2,5X,'CI =',F5.2,5X,'CC =',F6.2,
     *5X,'AK =',F6.1,5X,'AKL =',F7.1,5X,'AKC =',F7.1,
     *5X,'SD =',D17.10)
  110 CONTINUE
  100 CONTINUE
   90 CONTINUE
      STOP
      END
```

```
C     SUBPROGRAM
      SUBROUTINE ROOT
      DIMENSION COEFF(5),A(5),B(5)
      COMMON /CONST/AK,AKL,AKC
      COMMON /RAXAM/RATIO(10),XAS(10),M
      COMMON /FUNCT/X(4),FX(4)
      DOUBLE PRECISION COEFF,A,B,X,FX,RATIO,XAS
      DOUBLE PRECISION DFX,XNEW,D,AK,AKL,AKC
      D=(XAS(M)-2.+(XAS(M)+1.)*RATIO(M))*AKC
      COEFF(1)=1.
      COEFF(2)=((4.*AKC+AKL-AK)-2.*AKC*XAS(M)
      +((AK-2.*AKC-AKL)*XAS(M)
      +(AK-2.*AKC-AKL))*RATIO(M))/D
      COEFF(3)=(2.*(AK-AKC-AKL)+(AKC+AKL+AK*AK)*XAS(M)
      +((AKC+AKL-2.*AK-AK*AK)*XAS(M)
      +(AKC+AKL-2.*AK-AK*AK))*RATIO(M)/D
      COEFF(4)=-(2.*AK*AK*XAS(M)+AK-((2.*AK*AK+AK)*XAS(M)
      +(2.*AK*AK+AK)*RATIO(M))/D
      COEFF(5)=((XAS(M)-(XAS(M)+1.)*RATIO(M)*AK*AK)/D
      N=4
      DO 1000 J=1,3
      N1=N-1
      X(J)=0.
      DO 100 JJ=1,1000
      CALL SYDIV(COEFF,A,N,X(J))
      FX(J)=A(N+1)
      CALL SYDIV(A,B,N1,X(J))
      DFX=B(N1+1)
      IF(FX(J))10,300,10
   10 IF(DFX)20,200,20
   20 XNEW=X(J)-FX(J)/DFX
      IF(XNEW-X(J))100,300,100
  100 X(J)=XNEW
  200 X(J)=0.
  300 CALL SYDIV(COEFF,COEFF,N,X(J))
      N=N-1
 1000 CONTINUE
      X(4)=-COEFF(2)/COEFF(1)
      FX(4)COEFF(1)*X(4)+COEFF(2)
      RETURN
      END


C     SUBPROGRAM
      SUBROUTINE SYDIV(A,B,N,XX)
      DIMENSION A(5),B(5)
      DOUBLE PRECISION A,B,XX
      B(1)=A(1)
      DO 10 II=1,N
   10 B(II+1)=A(II+1)+B(II)*XX
      RETURN
      END
```

PROGRAM II

```
C       MAIN PROGRAM
        REAL*8 XL1,XC2,XL,XAM,XMA,FH,FW,FE,FI,FC,Y,FUN,C
        REAL*8 PXL1,PXC2,PXL,PXAM,PXGT4
        REAL*8 CCAL,COBS,CE,CI,CC
        DIMENSION FH(10),FW(10),FE(10),FI(10),FC(10)
        DIMENSION XL1(10),XC2(10),XL(10,10),XAM(10),XMA(10)
        DIMENSION PXL1(10),PXC2(10),PXL(10,10),PXAM(10),PXGT4(10)
        DIMENSION CCAL(10),COBS(10)
        COMMON /CONST/AK,AKL,AKC
        COMMON /RAXAM/RATIO(10),XAS(10),M
        COMMON /FUNCT/X(4),FX(4)
        DOUBLE PRECISION X,FX,RATIO,XAS,AK,AKL,AKC,CE,CI,CC
        DATA CW,CH/4.70,408.02/
        DATA CE,CI,CC/5.02,7.17,14.77/
        READ(1,10)(COBS(M1),M1=1,10)
     10 FORMAT(10D8.4)
        READ(1,20)(XAS(M2),M2=1,10)
     20 FORMAT(10D8.4)
        READ(1,30)(RATIO(M3),M3=1,8)
     30 FORMAT(8D10.4)
        READ(1,40)(RATIO(M4),M4=9,10)
     40 FORMAT(2D10.4)
        READ(1,50)(FW(M5),M5=1,10)
     50 FORMAT(10D8.4)
        READ(1,60)(FH(M6),M6=1,8)
     60 FORMAT(8D10.4)
        READ(1,70)(FH(M7),M7=9,10)
     70 FORMAT(2D10.4)
        READ(1,80)AK,AKL,AKC
     80 FORMAT(3F10.1)
        DO  90 M=1,10
        CALL ROOT
        DO 100 L=1,4
        Y=X(L)
        FUN=FX(L)
        IF(Y.GE.AK.OR.Y.LE.0.OR.Y.EQ.1.) GOTO 100
        IF(FUN.GE.1.D-5.OR.FUN.LE.-1.D-5) GOTO 100
        C=2.*AKC*Y*Y+AK*Y+AKL*Y*Y*(2.-Y)/(1.-Y)**2
       *+2.AK*AK*(1.-XAS(M))+(AKC*Y*Y*Y-(AKC+AKL)*Y*Y
       *+(AK+AK*AK)*Y+AK*AK)/(1.-Y)*RATIO(M)
        FE(M)=(AK*Y+AKL*Y*Y/(1.-Y))/C
        FI(M)=(AKL*Y*Y/(1.-Y)**2)/C
        FC(M)=2.*AKC*Y*Y/C
        CCAL(M)=FE(M)*CE+FI(M)*CI+FC(M)*CC+FH(M)*CH+FW(M)*CW
        XL1(M)=Y/AK
        XC2(M)=AKC*XL1(M)**2
        XAM(M)=(AKC*Y*Y*Y-(AKC+AKL)*Y*Y+(AK-AK*AK)*Y+AK*AK)
       **RATIO(M)/(AK*AK*(1.-Y))
```

```
      XMA(M)=XL1(M)+XC2(M)+(AKL*Y*Y+(AKC*Y*Y*Y-(AKC+AKL)*Y*Y
     *+(AK-AK*AK)*Y+AK*AK)*RATIO(M))/(AK*AK*(1.-Y))
      PXL1(M)=XL1(M)*100./XMA(M)
      PXC2(M)=XC2(M)*100./XMA(M)
      PXAM(M)=XAM(M)*100./XMA(M)
      DO 110 N=2,10
      XL(N,M)=(AKL/AK**2)*(AK*XL1(M))**N
      PXL(N,M)=XL(N,M)*100./XMA(M)
  110 CONTINUE
      PXGT4(M)=100.-(PXL1(M)+PXC2(M)+PXL(2,M)+PXL(3,M)
     *+PXL(4,M)+PXAM(M))
      GOTO 90
  100 CONTINUE
   90 CONTINUE
      WRITE(3,120)(XC2(N2),N2=1,10),(XL1(N1),N1=1,10),
     *((XL(N3,N4),N4=1,10),N3=2,10),(XAM(NN),NN=1,10),
     *(XMA(N5),N5=1,10),(FH(N6),N6=1.10),(FW(N7),N7=1,10),
     *(FE(N8),N8=1,10),(FI(N9),N9=1,10),(FC(N10),N10=1,10),
     *(PXC2(N12),N12=1,10),(PXL1(N11),N11=1,10),
     *((PXL(N13,N14),N14=1,10),N13=2,10),(PXAM(N15),N15=1,10),
     *(PXGT4(N16),N16=1,10)
  120 FORMAT(27X,'XAS(1)',3X,'XAS(2)',3X,'XAS(3)',3X,'XAS(4)',
     *3X,'XAS(5)',3X,'XAS(6)',3X,'XAS(7)',3X,'XAS(8)','XAS(9)',
     *3X,'XAS(10)',///,15X,'XC2   =',3X,10F9.5,//,
     *15X,'XL1   =',3X,10F9.5,//,15X,'XL2   =',3X,10F9.5,//,
     *15X,'XL3   =',3X,10F9.5,//,15X,'XL4   =',3X,10F9.5,//,
     *15X,'XL5   =',3X,10F9.5,//,15X,'XL6   =',3X,10F9.5,//,
     *15X,'XL7   =',3X,10F9.5,//,15X,'XL8   =',3X,10F9.5,//,
     *15X,'XL9   =',3X,10F9.5,//,15X,'XL10  =',3X,10F9.5,//,
     *15X,'XAM   =',3X,10F9.5,//,15X,'XMA   =',3X,10F9.5,///,
     *15X,'FH    =',3X,10F9.5,//,15X,'FW    =',3X,10F9.5,//,
     *15X,'FE    =',3X,10F9.5,//,15X,'FI    =',3X,10F9.5,//,
     *15X,'FC    =',3X,10F9.5,///,
     *15X,'PXC2  =',3X,10F9.5,//,15X,'PXL1  =',3X,10F9.5,//,
     *15X,'PXL2  =',3X,10F9.5,//,15X,'PXL3  =',3X,10F9.5,//,
     *15X,'PXL4  =',3X,10F9.5,//,15X,'PXL5  =',3X,10F9.5,//,
     *15X,'PXL6  =',3X,10F9.5,//,15X,'PXL7  =',3X,10F9.5,//,
     *15X,'PXL8  =',3X,10F9.5,//,15X,'PXL9  =',3X,10F9.5,//,
     *15X,'PXL10 =',3X,10F9.5,//,15X,'PXAM  =',3X,10F9.5,//,
     *15X,'PXGT4 =',3X,10F9.5)
      WRITE(3,130)(COBS(N100),N100=1,10),(CCAL(N200),N200=1,10)
  130 FORMAT(///,15X,'COBS  =',3X,10F9.5,//,
     *15X,'CCAL  =',3X,10F9.5)
      STOP
      END
```

```
C      SUBPROGRAM
       SUBROUTINE ROOT
       DIMENSION COEFF(5),A(5),B(5)
       COMMON /CONST/AK,AKL,AKC
       COMMON /RAXAM/RATIO(10),XAS(10),M
       COMMON /FUNCT/X(4),FX(4)
       DOUBLE PRECISION COEFF,A,B,X,FX,RATIO,XAS
       DOUBLE PRECISION DFX,XNEW,D,AK,AKL,AKC
       D=(XAS(M)-2.+(XAS(M)+1.)*RATIO(M))*AKC
       COEFF(1)=1.
       COEFF(2)=((4.*AKC+AKL-AK)-2.*AKC*XAS(M)
       +((AK-2.*AKC-AKL)*XAS(M)
       +(AK-2.*AKC-AKL))*RATIO(M))/D
       COEFF(3)=(2.*(AK-AKC-AKL)+(AKC+AKL+AK*AK)*XAS(M)
       +((AKC+AKL-2.*AK-AK*AK)*XAS(M)
       +(AKC+AKL-2.*AK-AK*AK))*RATIO(M)/D
       COEFF(4)=-(2.*AK*AK*XAS(M)+AK-((2.*AK*AK+AK)*XAS(M)
       +(2.*AK*AK+AK)*RATIO(M))/D
       COEFF(5)=((XAS(M)-(XAS(M)+1.)*RATIO(M)*AK*AK)/D
       N=4
       DO 1000 J=1,3
       N1=N-1
       X(J)=0.
       DO 100 JJ=1,1000
       CALL SYDIV(COEFF,A,N,X(J))
       FX(J)=A(N+1)
       CALL SYDIV(A,B,N1,X(J))
       DFX=B(N1+1)
       IF(FX(J))10,300,10
    10 IF(DFX)20,200,20
    20 XNEW=X(J)-FX(J)/DFX
       IF(XNEW-X(J))100,300,100
   100 X(J)=XNEW
   200 X(J)=0.
   300 CALL SYDIV(COEFF,COEFF,N,X(J))
       N=N-1
  1000 CONTINUE
       X(4)=-COEFF(2)/COEFF(1)
       FX(4)COEFF(1)*X(4)+COEFF(2)
       RETURN
       END


C      SUBPROGRAM
       SUBROUTINE SYDIV(A,B,N,XX)
       DIMENSION A(5),B(5)
       DOUBLE PRECISION A,B,XX
       B(1)=A(1)
       DO 10 II=1,N
    10 B(II+1)=A(II+1)+B(II)*XX
       RETURN
       END
```

VITA

Mr.Vitaya Ruangpornvisuti was born on October 23, 1957 in Phichit, Thailand. He recieved his B.Sc. in Chemistry from Faculty of Science, Chiangmai University in 1980. Since 1981 he has been a graduate student in Physical Chemistry, Graduate School, Chulalongkorn University.