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APPENDIX A

RESULTS OF THE DENSITIES OF SOLUTIONS

Densities of aqueous $Zn(ClO_4)_2$, $ZnSO_4$, $ZnCl_2$ and $CdSO_4$ were measured at 25.00 $\pm$ 0.01 °C using 10-cm^3 pycnometer. Results of the densities as density curves are shown in Figs. 3.3, 3.4, 3.5 and 3.6.

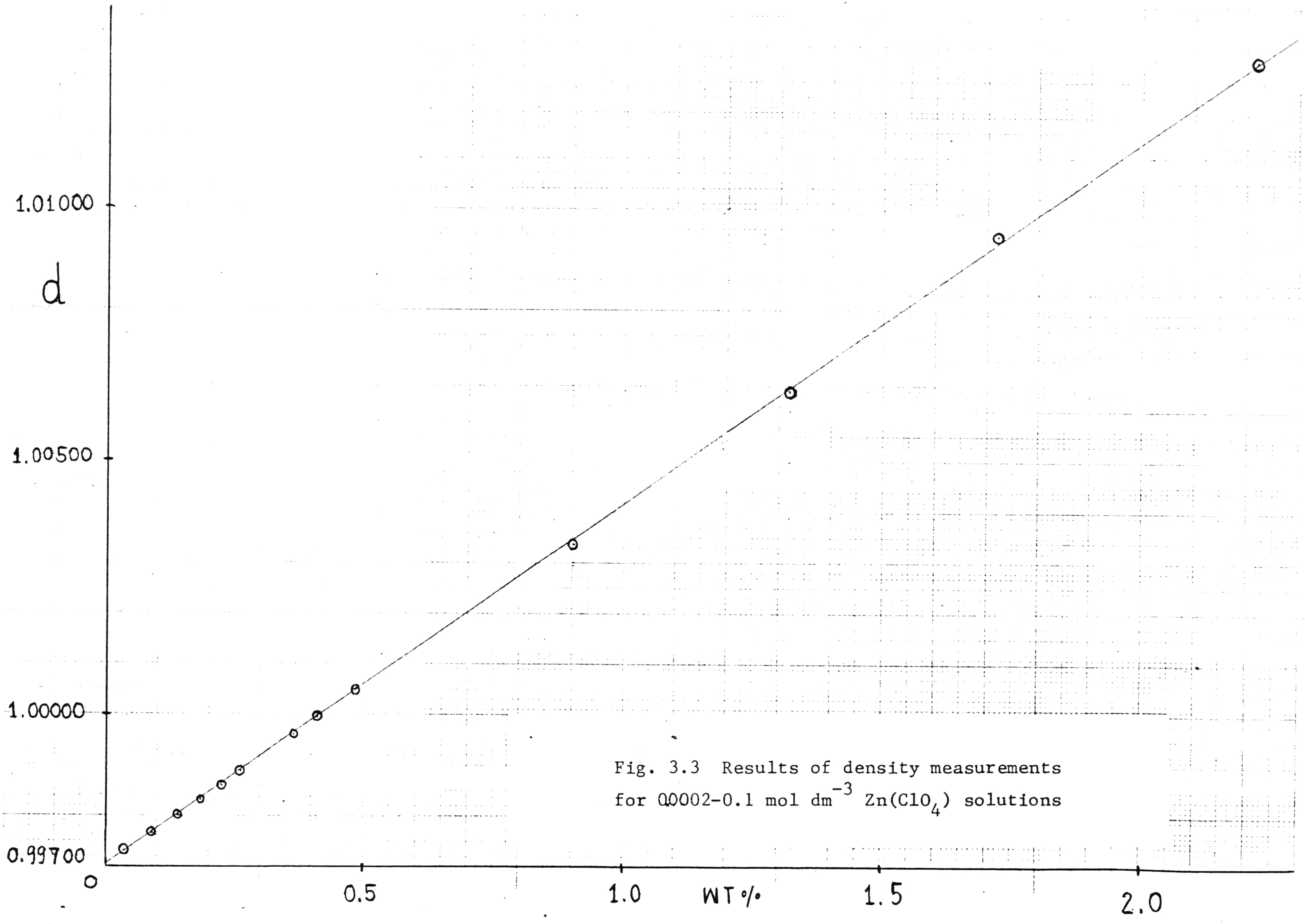

Fig. 3.3 Results of density measurements for 0.0002-0.1 mol dm^{-3} $Zn(ClO_4)$ solutions

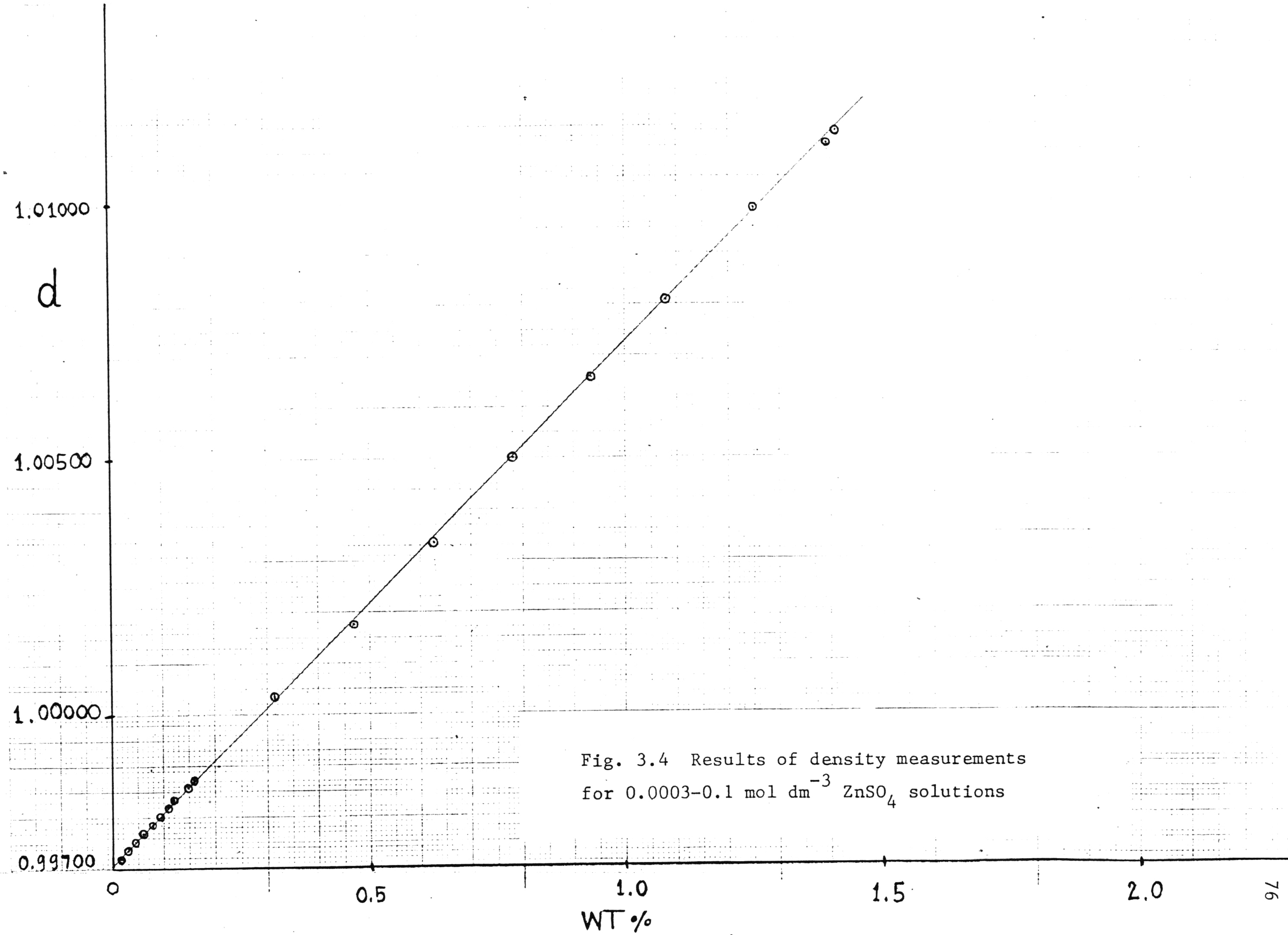

Fig. 3.4 Results of density measurements for 0.0003-0.1 mol dm^{-3} $ZnSO_4$ solutions

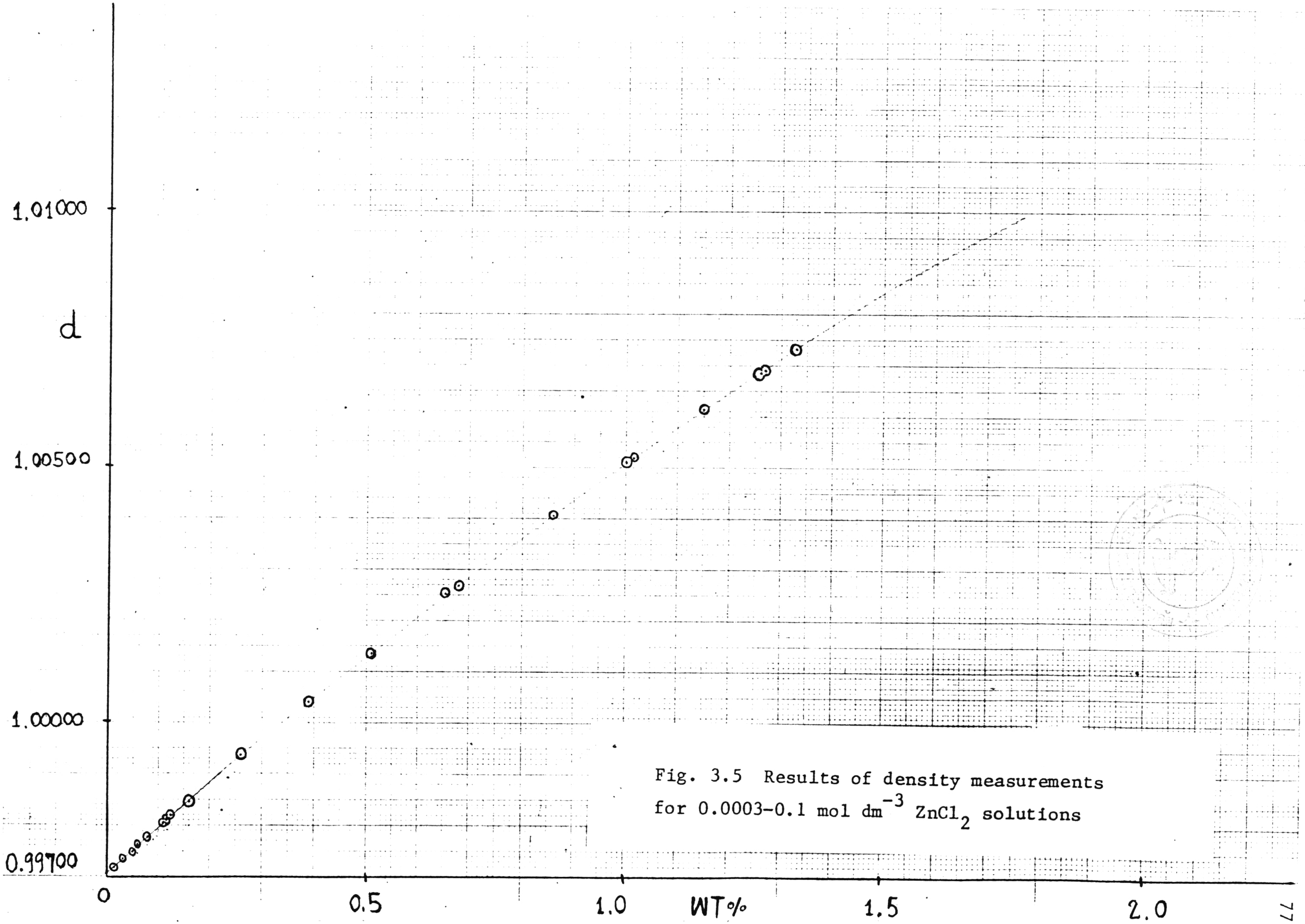

Fig. 3.5 Results of density measurements for 0.0003-0.1 mol dm^{-3} $ZnCl_2$ solutions

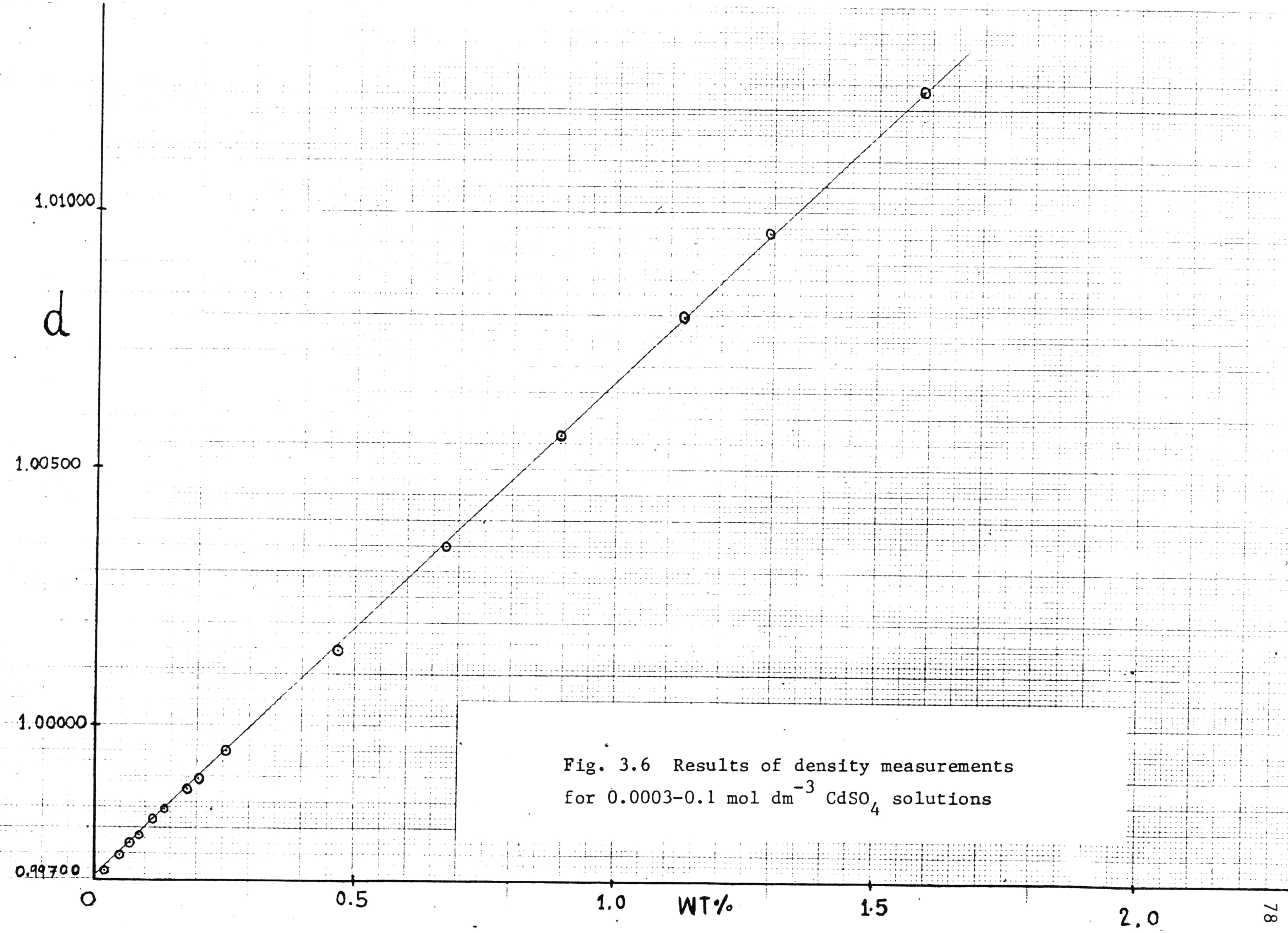

Fig. 3.6 Results of density measurements for 0.0003-0.1 mol dm^{-3} $CdSO_4$ solutions

APPENDIX B

CORRECTIONS TO THE LEE AND WHEATON EQUATIONS

Typing errors in references 5 and 6 have been corrected as follow:

Reference 5 (Part I)

Page 748: equation (5), $\beta = e^2/DkT$

(T is the absolute temperature used in the original text)

Page 760: equation (76), the denominator of the last term should read $(1 + q_p^{1/2}\kappa R + q_p\kappa^2R^2/2)$.

Page 763: equation (99), in the expression of $H_{2,p,1}(\kappa R)$, the last term on the third line should read

$(1 + q_p^{1/2}\kappa R)\ Tr\{\kappa R\}/q_p +$

Page 765: Appendix, in the expression of $\Delta X_j^{(0,3)}/X$, μ_i should read u_i, an ionic strength fraction used in the original text.

Page 766: Appendix, equation. (A2) for $J_2\ (\kappa R)$, a minus sign was missed out on the third paragraph.

Reference 6 (Part II)

Page 1462: equation (52), in the expression of $u_{je}^{(0)}$, μ_i should read u_i, an ionic strenght fraction.

Page 1463: equation (64), the nominator of the first term of $u_{je}^{(1)}$ should read $e_j^2\kappa^2X$

Page 1463: equation (66), the denominator of the last term on the first line in the expression of $Q_p(\kappa R)$ should read $(1 + q_p^{1/2}\kappa R + q_p\kappa^2R^2/2)$.

Page 1468: equation (104), the denominator of the last term in the expression of $\Delta X_j^{(0,5)}/X$ should have the factor $(\omega_i + \omega_v)$.

Page 1473: equation (123), should read

$$\tau = F\xi e/6\pi\eta$$

Page 1475: equation (136), the first multiple term of the second term on the expression of $C_{8,p}(t)$ should read $(1 - q_p^2)/2q_p$.

APPENDIX C

THE CALCULATION OF THE SHEDLOVSKY EXTRAPOLATION FUNCTION

The Shedlovsky extrapolation function used for the plot of $\Lambda^{o'}$ vs. concentration for $Zn(ClO_4)_2$, $ZnSO_4$, $ZnCl_2$ and $CdSO_4$ solutions is

$$\Lambda^{o'} = \frac{\Lambda + B_2 M^{1/2}}{1 - B_1 M^{1/2}}$$

where Λ is the observed conductivity from a resistance measurement and B_1, B_2 are constants.

Assuming stoichiometric dissociation of these aqueous solutions are

$$Zn(ClO_4)_2 \longrightarrow Zn^{2+} + 2\ ClO_4^-$$

$$ZnSO_4 \longrightarrow Zn^{2+} + SO_4^{2-}$$

$$ZnCl_2 \longrightarrow Zn^{2+} + 2\ Cl^-$$

$$CdSO_4 \longrightarrow Cd^{2+} + SO_4^{2-}$$

thus at 25°C B_1 and B_2 can be calculated from the equations (24)

$$B_1 = 0.7852 |Z_A Z_B| \cdot \frac{q}{q^{1/2} + 1} \cdot \left(\frac{I}{M}\right)^{1/2}$$

$$B_2 = 30.32 \left(|Z_A| + |Z_B| \right) \cdot \left(\frac{I}{M}\right)^{1/2}$$

wher

$$q = \frac{|Z_A Z_B|}{|Z_A| + |Z_B|} \cdot \frac{\lambda_A^o + \lambda_B^o}{|Z_B| \lambda_A^o + |Z_A| \lambda_B^o}$$

for anion A and cation B.

Using $\lambda^{\circ}_{Zn^{2+}} = 53.0\ cm^2 \Omega^{-1}\ equiv.^{-1}$ (10), $\lambda^{\circ}_{Cd^{2+}} = 53.5\ cm^2 \Omega^{-1}\ equiv.^{-1}$ (14), $\lambda^{\circ}_{ClO_4^-} = 67.36\ cm^2 \Omega^{-1}\ equiv.^{-1}$ (29, 30), $\lambda^{\circ}_{Cl^-} = 76.35\ cm^2 \Omega^{-1}\ equiv.^{-1}$ (27, 28) and $\lambda^{\circ}_{SO_4^{2-}} = 80.02\ cm^2 \Omega^{-1}\ equiv.^{-1}$ (31) thus

for $Zn(ClO_4)_2$

$B_1 = 0.7030239\ mol^{-1/2}\ dm^{3/2}$

$B_2 = 1.57547 \times 10^2\ dm^{3/2}\ mol^{-1/2}\ cm^2 \Omega^{-1}\ equiv^{-1}$

and $q = 0.4274451$ where $(I/M)^{1/2} = \sqrt{3}$

for $ZnCl_2$

$B_1 = 0.6921399\ mol^{-1/2}\ dm^{3/2}$

$B_2 = 1.57547 \times 10^2\ dm^{3/2}\ mol^{-1/2}\ cm^2 \Omega^{-1}\ equiv^{-1}$

and $q = 0.4189781$ where $(I/M)^{1/2} = \sqrt{3}$

for $ZnSO_4$, $CdSO_4$

$B_1 = 1.8398381\ mol^{-1/2}\ dm^{3/2}$

$B_2 = 2.4256 \times 10^2\ dm^{3/2}\ mol^{-1/2}\ cm^2 \Omega^{-1}\ equiv^{-1}$

$q = 0.5$ where $(I/M)^{1/2} = 2$

Substituting B_1 and B_2 in the Shedlovsky equation, $\Lambda^{\circ\prime}$ can then be calculated for given values of concentration and the corresponding conductivity determined in the experiment.

APPENDIX D

THE CALCULATION OF IONIC SPECIES OF ZINC CHLORIDE SOLUTIONS

The effect of incomplete dissociation was studied by Paterson(13) using the method of Reilly and Stokes (15). If only the first complex is considered, then

$$Zn^{2+} + Cl^- \rightleftharpoons ZnCl^+ \; ; \; K_A = \frac{[ZnCl^+]}{[Zn^{2+}][Cl^-]} \cdot \frac{1}{\beta} \, , \; K_A = 4.5 \text{ kg mol}^{-1}$$

where $\beta = \dfrac{\gamma_{21}^3}{\gamma_{11}^2}$; γ's are activity coefficients in the extended Debye Hückel form.

From these values, the concentrations of the complexes were calculated at different ionic strengths, I by the following procedure.

Assuming the molality of Zn^{2+}, Cl^{-1} and $ZnCl^+$ are x, y and z respectively.

From the requirements of conservation of mass, electroneutrality and the definition of the ionic strength of the solution, the equation(1) was obtained, i.e.

$$(2K_A\beta)y^2 + (6-2IK_A\beta)y - 4I = 0 \qquad (1)$$

This equation was solved for a given value of ionic strength I. The solution of y therefore corresponds to the molality of Cl^-. The value of x is then calculated from

$$x = \frac{y}{(2 + y\,K_A\beta)}$$

which is the molality of Zn^{2+}. From the above equalities, the concentrations of complexes and the total stoichiometric concentration of $ZnCl_2$ can be determined.

APPENDIX E

PROGRAMME (1)

ANALYSIS BY THE LEE AND WHEATON EQUATIONS FOR $ZnCl_2$ SYSTEM

This programme was assembled according to the conductance equations given in Appendix (H). The numerical input data (e.g. D, η, Z_i, e_i, etc) may be altered depending on the system studies. In the programme, "x(1)" refers to R and "x(2)" refers to $\lambda^{\circ}_{ZnCl^+}$ if $\lambda^{\circ}_{Zn^{2+}}$ is fixed at "LAM 1", and vice versa. The list of programme (1) shown below was that used to process aqueous $ZnCl_2$ data at 25°C, optimising $\lambda^{\circ}_{Zn^{2+}}$ and R at fixed $\lambda^{\circ}_{ZnCl^+}$ value.

```
      DIMENSION UU(3),ZZ(3),EE(3),WW(3),X(2),ALAM(3),GAMCAL(50),
     *TT(3),ALPH(3),QQ(3),ENP(3),CHI(3,3),ZSUMP(3),FINALT(3)
      REAL K,LAM1,LAM2,KB,KR,MM(50),LL,NP(3)
      COMMON GAMEXP(50),CC(50,3),MM,IPOINT,X,N
      READ(1,5)N,IPOINT
    5 FORMAT(I1,I2)
      DO 10 IA =1,IPOINT
      READ(1,15)GAMEXP(IA),CC(IA,3),CC(IA,2),CC(IA,1),MM(IA)
   15 FORMAT(F7.3,4F10.5)
   10 CONTINUE
      R=0.1E-8
      X(1)=3.00E-8
      DO 31 IY=1,20
      Y=0.1
      X(2)=52.0
      DO 33 IX =1,30
      CALL CALCFX
      X(2)=X(2)+Y
   33 CONTINUE
      X(1)=X(1)+R
   31 CONTINUE
      STOP
      END
```

```
      SUBROUTINE CALCFX
      DIMENSION UU(3),ZZ(3),EE(3),WW(3),X(2),GAMCAL(50),
     *TT(3),ALPH(3),QQ(3),ENP(3),CHI(3,3),ZSUMP(3),FINALT(3),ALAM(3)
      REAL K,LAM1,LAM2,KB,KR,MM(50),LL,NP(3)
      COMMON GAMEXP(50),CC(50,3),MM,IPOINT,X,N
      TR(X)=EXP(X)*(-.57722-ALOG(X)+X-(X**2)/(2.*2.)+(X**3)/(3.*6.)-X**4
     */(4.*24.))
C     ZZ(1),ZZ(2),ZZ(3) ARE VALENCIES OF ION 1,2,3 RESPECTIVELY
C     EE(1),EE(2),EE(3) ARE CHARGES OF ION 1,2,3 RESPECTIVELY
C     D IS DIELECTRIC CONSTANT OF SOLVENT
C     KB IS BOLTZMANN CONSTANT
C     T IS ABSOLUTE TEMPERATURE
C     VIS IS VISCOSITY OF SOLVENT
      ZZ(1) =1
      ZZ(2) =-1
      ZZ(3) =2
      EE(1)=4.80325E-10
      EE(2) =-4.80325E-10
      EE(3)=2.*4.80325E-10
      D =78.30
      KB=1.380622E-16
      T=298.15
      VIS=8.903E-3
      LAM1=35.
      LAM2=76.35
      FF=96486.7
      BTA=2.307121E-19/(D*KB*T)
      TAU=FF*4.80325E-10/(6.*299.7925*3.1415926*VIS)
      WW(1)=6.468716E+6*LAM1/ABS(ZZ(1))
      WW(2)=6.468716E+6*LAM2/ABS(ZZ(2))
      DO 12 IC =1,IPOINT
      WW(3)=6.468716E+6*X(2)/ABS(ZZ(3))
C     CALCULATION OF MUI
      SUM1=0
      DO 30 IA=1,3
   30 SUM1=SUM1+6.0222*(4.80325*ABS(ZZ(IA)))**2*CC(IC,IA)
      DO 40 IA=1,3
   40 UU(IA)=6.0222*(4.80325*ABS(ZZ(IA)))**2*CC(IC,IA)/SUM1
C     CALCULATION OF KAPA
      SUM2=0
      DO 50 IA=1,3
   50 SUM2=SUM2+CC(IC,IA)*ZZ(IA)**2
      K=3.556143E+9*SQRT(SUM2)/SQRT(D*T)
C     CALCULATION OF THETA
      THETA=0
      DO 60 IA=1,3
   60 THETA=THETA+UU(IA)*ZZ(IA)**2
C     CALCULATION OF OMEGA
      OMEGA=0
      DO 70 IA=1,3
   70 OMEGA=OMEGA+UU(IA)*ZZ(IA)
C     CALCULATION OF KAPAR
      KR=K*X(1)
C     CALCULATION OF WBAR
```

```
      WBAR = 0
      DO 80 IA=1,3
   80 WBAR=WBAR+UU(IA)*WW(IA)
C     CALCULATION OF TEI
      DO 90 IA=1,3
   90 TT(IA) =UU(IA)*WW(IA)/WBAR
C     CALCULATION OF B
      BA=0
      DO 100 IA=1,3
  100 BA=BA+(1.-TT(IA))*WW(IA)**2
      B=BA/2.0
C     CALCULATION OF C
      CA=1.0
      DO 110 IA=1,3
  110 CA=CA*WW(IA)**2
      CB=0
      DO 120 IA=1,3
  120 CB=CB+TT(IA)/WW(IA)**2
      C=CA*CB
C     CALCULATION OF ALPHA1,ALPHA2,ALPHA3
      ALPH(1)=0
      G=SQRT(ABS(B**2-C))
      ALPH(2)=SQRT(ABS(B-G))
      ALPH(3)=SQRT(B+G)
C     CALCULATION OF ENP(IA)
      DO 125 IA =1,3
  125 NP(IA)=0
      DO 130 IA=1,3
      DO 130 IB=1,3
  130 NP(IA)=NP(IA)+(TT(IB)*WW(IB)**2)/((WW(IB)**2-(ALPH(IA)**2))**2)
      DO126 IA=1,3
  126 ENP(IA)=SQRT(ABS(1.0/NP(IA)))
C     CALCULATION OF CHI(IA,IB)
      DO 140 IA=1,3
      DO 140 IB=1,3
  140 CHI(IA,IB)=(ENP(IA)*WW(IB))/(WW(IB)**2-(ALPH(IA)**2))
C     CALCULATION OF QP
      DO 145 IA=1,3
  145 QQ(IA)=0
      DO 150 IA=1,3
      DO 150 IB=1,3
  150 QQ(IA)=QQ(IA)+(WBAR*TT(IB)*WW(IB))/(WW(IB)**2-(ALPH(IA)**2))
      DO 160 JM=1,3
      SUMP=0
      DO 170 IP=2,3
      SQP=SQRT(QQ(IP))
      XA=SQP*KR
      XB=(1.0+SQP)*KR
      XC=(2.0+SQP)*KR
      XD=(3.0+SQP)*KR
      XE=2.0*KR
      XF=3.0*KR
      TR1=TR(XA)
      TR2=TR(XB)
      TR3=TR(XC)
      TR4=TR(XD)
      TR5=TR(KR)
      TR6=TR(XE)
      TR7=TR(XF)
      C5P=-(((QQ(IP)-1.)-SQP/2.+SQP*(1.-SQP)*KR/2.)/SQP-(1.-QQ(IP)**2)*
     *TR2/QQ(IP)-QQ(IP)*(1.+KR+KR**2/2.)*TR1+(1.+SQP*KR)*TR5/QQ(IP))*
     *(1./((1.+KR)*(1.+SQP*KR+QQ(IP)*KR**2/2.)))*(1./12.)
      C3P=(-(1.-QQ(IP))*TR5/(2.*QQ(IP))+(1.-QQ(IP)**2)*
     *TR2/(2.*QQ(IP)*(1.+SQP*KR+QQ(IP)*KR**2/2.))+(3.+SQP)*(1.-QQ(IP))/
     *(6.*SQP)-(8.*(2.-QQ(IP))-5.*SQP-3.*SQP**3)*KR/24.)
      C1P=((1.+(1.+SQP)*KR/2.)/(1.+SQP*KR+QQ(IP)*KR**2/2.))*(1./((1.+SQP
     *)*(1.+KR)))*(1./3.)
      C2P=-((TR3+.5)/(1.+SQP*KR+QQ(IP)*KR**2/2.))*(1./((1.+
     *KR)**2))*(1./6.)
      C4P=-((4./(1.-QQ(IP)))*ALOG(3./(2.+SQP))+(2./3.)*((1.+SQP)/(2.+SQP
     *)))*(OMEGA**2)*(1./((1.+KR)**2*(1.+SQP*KR+QQ(IP)*KR**2/2.)))*
     *(1./24.)
      C3P=OMEGA*(ALOG(3./(2.+SQP))/(1.-QQ(IP)))*(1./((1.+KR)**2*
     *(1.+SQP*KR+QQ(IP)*KR**2/2.)))*(1./6.)
      C7P=-((3.+SQP)*TR4/((1.+KR)**3))*(1./(1.+SQP*KR+QQ(IP)*KR**2/2.))
     **(1./18.)
      SUMV=0
      DO 171 IV=1,3
C     CALCULATION OF AVP
      SUMPI1=0
      DO 190 I=1,3
  190 SUMPI1=SUMPI1   +UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))/(WW(I)+WW(IV)))
      AVP=SUMPI1*C1P
```

```
C      CALCULATION OF BVP
       BVP1=SUMPI1*C4P
       SUMPI2=0
       DO 200 I=1,3
 200   SUMPI2=SUMPI2  +ZZ(I)*ZZ(IV)*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))
      */(WW(I)+WW(IV))))
       BVP2=SUMPI2*(C2P+C5P)
       SUMPI3=0
       DO 210 I=1,3
 210   SUMPI3=SUMPI3  +(ZZ(I)+ZZ(IV))*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))
      */(WW(I)+WW(IV))))
       BVP3=SUMPI3*C3P
C      CALCULATION OF GVP
       SGVP1=0
       DO 220 I=1,3
       SGVP2=0
       DO 221 IL=2,3
       SQL=SQRT(QQ(IL))
       XG=(SQL+SQP)*KR
       TR8=TR(XG)
       C6PL1=((-(SQL+QQ(IP))*(1.-SQL)-(QQ(IP)*(1.-QQ(IL))-(1.-SQL)*(SQP*
      *SQL-1.)/2.)*KR)/(SQP*SQL)-(1.+SQL*KR+QQ(IL)*KR**2/2.)*(1.-QQ(IP)**
      *2)*TR2/QQ(IP)+(1.+SQL*KR+QQ(IL)*KR**2/2.)*(1.+SQP*KR)*TR5/QQ(IP)+
      *(QQ(IL)**2-QQ(IP)**2)*(1.+KR+KR**2/2.)*TR8/(QQ(IL)*QQ(IP))
      *+(1.+KR+KR**2/2.)*(QQ(IP)**2*(1.-QQ(IL))*(1.+SQL*KR+QQ(IL)*KR**
      *2/2.)-QQ(IL)**2*(1.+SQP*KR))*TR1/(QQ(IL)*QQ(IP)))
       C6PL2=(1./((1.+KR)*(1.+S
      *QP*KR+QQ(IP)*KR**2/2.)*(1.+SQL*KR+QQ(IL)*KR**2/2.)))
       C6PL=C6PL1*C6PL2
       SGVP3=0
       DO 230 IA=1,3
 230   SGVP3=SGVP3    +TT(IA)*CHI(IL,IA)*ZZ(IA)
       SGVP2=SGVP2+SGVP3       *(WW(I)*CHI(IL,IV)-WW(IV)*CHI(IL,I))*C6PL
 221   CONTINUE
       SGVP1=SGVP1+(UU(I)*ZZ(I)*ZZ(IV)*(SGVP2/(WW(I)+WW(IV))))
 220   CONTINUE
       GVP=(1./12.)*SGVP1
       BVP=BVP1+BVP2+BVP3+GVP
C      CALCULATION OF CVP
       SUMPI4=0
       DO 240 I=1,3
 240   SUMPI4=SUMPI4  +(ZZ(I)**2*ZZ(IV)**2)*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*
      *WW(IV))/(WW(I)+WW(IV))))
       CVP=0
       BTAK=AVP*(BTA*K)+BVP*((BTA*K)**2)+CVP*((BTA*K)**3)
       SUMV=SUMV+(TT(IV)*CHI(IP,IV))*BTAK
 171   CONTINUE
       SUMP=SUMP+CHI(IP,JM)*SUMV
 170   CONTINUE
       ZSUMP(JM)=ZZ(JM)*SUMP
C      CALCULATION OF VJ1 AND VJ2
       SUMP=0
       DO 250IP=2,3
       SUMV=0
       DO 251IV=1,3
       SUMPI6=0
       DO 260 I=1,3
 260   SUMPI6=SUMPI6  +UU(I)*(ZZ(I)-ZZ(IV))/(WW(I)+WW(IV))
       SUMV=SUMV+TT(IV)*CHI(IP,IV)*(ZZ(IV)*C8P/2.-WW(JM)*SUMPI6*C1P)
 251   CONTINUE
 250   SUMP=SUMP+CHI(IP,JM)*SUMV
       VJ1=-(ZZ(JM)*SUMP)-(1./2.)*(ZZ(JM)*OMEGA*
      *(TR6/((1.+KR)**2)+ALOG(2./3.))-OMEGA**2/6.)*(1.+KR)
       VJ2=0
       SUMPI5=0
       DO 270IV=1,3
 270   SUMPI5=SUMPI5  +(UU(IV)*((ZZ(IV)*WW(IV)-ZZ(JM)*WW(JM))
      */(WW(IV)+WW(J
      *M))))/ZZ(IV)
       FINALT(JM)=(ABS(ZZ(JM))*(K*TAJ)/(1.+KR))*(1.+VJ1*(BTA*K)+VJ2*
      *((BTA*K)**2)+SUMPI5*KR/6.)
 160   CONTINUE
       ALAM(1)=LAM1
       ALAM(3)=X(2)
       ALAM(2)=LAM2
       GAMCAL(IC) =0
       DO 280IA=1,3
       LL=ALAM(IA)*(1.+ZSUMP(IA))-FINALT(IA)
 280   GAMCAL(IC)=GAMCAL(IC)+ABS(ZZ(IA))*CC(IC,IA)*LL
       GAMCAL(IC)=GAMCAL(IC)/(2.*MM(IC))
 12    CONTINUE
       SUMSQ=0
       DO 13 IA =1,IPOINT
 13    SUMSQ = SUMSQ+((GAMCAL(IA)-GAMEXP(IA))**2)
       SUMSQ =SUMSQ/IPOINT
       F =SUMSQ*1.0E+3
       WRITE(3,18)(X(I),I=1,N),F,LAM1
 18    FORMAT(20X,E12.6,5X,E12.6,5X,E12.6,5X,F5.2)
       RETURN
       END
```

APPENDIX F

PROGRAMME (2)

ANALYSIS BY THE LEE AND WHEATON EQUATIONS FOR $ZnSO_4$ AND $CdSO_4$ SYSTEMS

This programme was assembled according to the conductance equations given in Appendix (H). The numerical input data (e.g. D, η, Z_i, e_i, etc) may be altered depending on the system studies. In the programme, "x(1)" refers to R and "x(2) refer to $\lambda^{o}_{M^{2+}}$ (M = Zn, Cd). The list of programme(2) shown below was that used to process aqueous $ZnSO_4$ and $CdSO_4$ data at 25°C, optimising $\lambda^{o}_{M^{2+}}$ and R value.

```
      DIMENSION GG(3),ZZ(3),EE(3),WW(3),X(2),
     *TT(3),ALPH(3),CO(3),ENP(3),CHI(3,3),ZSUMP(3),FINALT(3),
     *ALAM(3),XM(37),WT(30),GAMCAL(50)
      REAL KC,LAM1,LAM2,KB,KR,MM(50),LL,NP(3)
      COMMON GAMEXP(50),CC(50,3),MM,IPOINT,X,N
      DOUBLE PRECISION ACU(24),DIFXM,DELTAI,XML,DMREF,DIREF,AMEXPT(24),
     *FI,XI(37),XM,DELTA,YY1,XX1,ZZ1,SI,GAMMA2,GAMMA1,GAMA21,
     *GAMA11,ABETA,AAA,BBB,CCC,YYL,XXL,ZZL,AK,D,WT,YYR,XXR,ZZR,XMR
      READ(1,5) N,IPOINT
    5 FORMAT(I1,I2)
C     XI(J) IS IONIC STRENGTH
      READ(1,4) (XI(J),J=1,36)
    4 FORMAT(8E9.2)
C     AMEXPT(K) IS EXPERIMENTAL CONCENTRATION OF SOLUTION IN MOLE PER KG
C     WT(K) IS EXPERIMENTAL CONCENTRATION OF SOLUTION IN WEIGHT ,
      DO 10K=1,IPOINT
      READ(1,16)GAMEXP(K),AMEXPT(K),WT(K)
   16 FORMAT(F7.3,E9.4,F7.5)
   10 CONTINUE
C     AK IS ASSOCIATION CONSTANT
      AK=140.
      R=.05E-8
      X(1)=4.0E-8
      DO 31 IY=1,20
      DO 8J=1,36
      SI=DSQRT(XI(J))
      GAMMA2=(-0.5115*4.*SI)/(1.+0.3291*X(1)*SI)
      GAMA22=10.000**GAMMA2
      XX1=XI(J)/4.
      YY1=XI(J)/4.
      ZZ1=AK*XX1*YY1*GAMA22**2
C     XM(J) IS CONCENTRATION IN MOLE PER KG (CORRESPOND TO IONIC STRENGTH)
      XM(J)=XX1+ZZ1
    8 CONTINUE
      DO 7 K=1,IPOINT
C     ACU(K) IS THE ACCURACY OF CONCENTRATION
      ACU(K)=0.01/100.*AMEXPT(K)
      DO 12J=1,36
      L=J+1
      IF(AMEXPT(K).LT.XM(J).OR.AMEXPT(K).GT.XM(L)) GO TO 12
      DMREF=XM(L)-XM(J)
      DIREF=XI(L)-XI(J)
      DIFXM=AMEXPT(K)-XM(J)
      DELTAI=DIREF*DIFXM/DMREF
      FI=XI(J)+DELTAI
      GO TO 15
   12 CONTINUE
   15 SI=DSQRT(FI)
      GAMMA2=(-0.5115*4.*SI)/(1.+0.3291*X(1)*SI)
      GAMA22=10.000**GAMMA2
C     YYL,XXL,ZZL ARE CONCENTRATIONS OF IONIC SPECIES IN MOLE PER KG
      XXL=FI/4.
      YYL=FI/4.
      ZZL=AK*XXL*YYL*GAMA22**2
C     XML IS STOICHIOMETRIC CONCENTRATION OF ELECTROLYTE  IN MOLE PER KG
      XML=XXL+ZZL
      IF(XML.LT.AMEXPT(K)) DIFXM=AMEXPT(K)-XML
      IF(XML.GT.AMEXPT(K)) DIFXM=XML-AMEXPT(K)
      IF(DIFXM.LE.ACU(K)) GO TO 14
      DELTAI=DIREF*DIFXM/DMREF
      IF(XML.GT.AMEXPT(K))FI=FI-DELTAI
      IF(XML.LT.AMEXPT(K))FI=FI+DELTAI
      GO TO 15
C     D IS  THE DENSITY OF SOLUTION
   14 D=.997044+.0102283*WT(K)
      XXR=(XXL*D)/(1.+XXL*.1614316)
      YYR=(YYL*D)/(1.+YYL*.1614316)
      ZZR=(ZZL*D)/(1.+ZZL*.1614316)
      XMR=ZZR+XXR
      CC(K,1)=XXR
      CC(K,2)=YYR
      MM(K)=XMR
    7 CONTINUE
      Y=.02
      X(2)=52.0
      DO 33 IX=1,30
      CALL CALCFX
      X(2)=X(2)+Y
   33 CONTINUE
      X(1)=X(1)+R
   31 CONTINUE
      STOP
      END
```

```
      SUBROUTINE CALCFX
      DIMENSION LL(3),ZZ(3),EE(3),WW(3),X(2),ALAM(3),GAMCAL(50),
     *TT(3),ALPH(3),CQ(3),ENP(3),CHI(3,3),ZSUMF(3),FINALT(3)
      REAL KC,LAM1,LAM2,KB,KR,MM(50),LL,NP(3)
      COMMON GAMEXP(50),CC(50,3),MM,IPOINT,X,N
      TR(X)=EXP(X)*(-.57722-ALOG(X)+X-(X**2)/(2.*2.)+(X**3)/(3.*6.)-X**4
     */(4.*24.))
C     ZZ(1),ZZ(2),ZZ(3) ARE VALENCIES OF ION 1,2,3 RESPECTIVELY
C     EE(1),EE(2),EE(3) ARE CHARGES OF ION 1,2,3 RESPECTIVELY
C     D IS DIELECTRIC CONSTANT OF SOLVENT
C     KB IS BOLTZMANN CONSTANT
C     T IS ABSOLUTE TEMPERATURE
C     VIS IS VISCOSITY OF SOLVENT
      ZZ(1)=2
      ZZ(2)=-2
      EE(1)=2.*4.80325E-10
      EE(2)=-2.*4.80325E-10
      D =78.30
      KB=1.380622E-16
      T=298.15
      VIS=8.903E-3
      FF=96486.7
      LAM2=80.02
      BTA=2.307121E-19/(D*KB*T)
      TAU=FF*4.80325E-10/(6.*299.7925*3.141592*VIS)
      WW(2)=6.468716E+6*LAM2/ABS(ZZ(2))
      DO 12 IC =1,IPOINT
      WW(1)=6.468716E+6*X(2)/ABS(ZZ(1))
      SUM1=0
      DO 30IA=1,2
   30 SUM1=SUM1+6.0222*(4.80325*ABS(ZZ(IA)))**2*CC(IC,IA)
      DO 40IA=1,2
   40 LL(IA)=6.0222*(4.80325*ABS(ZZ(IA)))**2*CC(IC,IA)/SUM1
C     CALCULATION OF KAPA
      SUM2=0
      DO 50IA=1,2
   50 SUM2=SUM2+CC(IC,IA)*ZZ(IA)**2
      KC=3.556143E+9*SQRT(SUM2)/SQRT(D*T)
C     CALCULATION OF THETA
      THETA=0
      DO 60IA=1,2
   60 THETA=THETA+LL(IA)*ZZ(IA)**2
C     CALCULATION OF OMEGA
      OMEGA=0
      DO 70IA=1,2
   70 OMEGA=OMEGA+LL(IA)*ZZ(IA)
C     CALCULATION OF KAPAR
      KR=KC*X(1)
C     CALCULATION OF WBAR
      WBAR=0
      DO 80IA=1,2
   80 WBAR=WBAR+LL(IA)*WW(IA)
C     CALCULATION OF TEI
      DO 90IA=1,2
   90  TT(IA) =LL(IA)*WW(IA)/WBAR
       ALPH(1)=0
       ALPH(2)=SQRT(TT(2)*WW(1)**2+TT(1)*WW(2)**2)
C      CALCULATION OF ENP(IA)
       DO 125IA=1,2
  125  NP(IA)=0
       DO 130IA=1,2
       DO 130IB=1,2
  130  NP(IA)=NP(IA)+(TT(IB)*WW(IB)**2)/((WW(IB)**2-(ALPH(IA)**2))**2)
       DO 126IA=1,2
  126  ENP(IA)=SQRT(ABS(1.0/NP(IA)))
C      CALCULATION OF CHI(IA,IB)
       DO 140IA=1,2
       DO 140IB=1,2
  140  CHI(IA,IB)=(ENP(IA)*WW(IB))/(WW(IB)**2-(ALPH(IA)**2))
C      CALCULATION OF QP
       DO 145IA=1,2
  145  CQ(IA)=0
       DO 150IA=1,2
       DO 150IB=1,2
  150  CQ(IA)=CQ(IA)+(WBAR*TT(IB)*WW(IB))/(WW(IB)**2-(ALPH(IA)**2))
       DO 160JM=1,2
       SUMF=0
       DO 170IP=2,2
       SQP=SQRT(CQ(IP))
       XA=SQP*KR
       XB=(1.0+SQP)*KR
       XC=(2.0+SQP)*KR
       XD=(3.0+SQP)*KR
```

```
      XE=2.0*KR
      XF=3.0*KR
      TR1=TR(XA)
      TR2=TR(XB)
      TR3=TR(XC)
      TR4=TR(XD)
      TR5=TR(KR)
      TR6=TR(XE)
      TR7=TR(XF)
      C5P=-(((CC(IP)-1.)-SCP/2.+SCP*(1.-SCP)*KR/2.)/SCP-(1.-CC(IP))**2)*
     *TR2/CC(IP)-CC(IP)*(1.+KR+KR**2/2.)*TR1+(1.+SCP*KR)*TR5/CC(IP))*
     *(1./((1.+KR)*(1.+SCP*KR+CC(IP)*KR**2/2.)))*(1./12.)
      C8P=(-(1.-CC(IP))*TR5/(2.*CC(IP))+(1.-CC(IP)**2)*
     *TR2/(2.*CC(IP)*(1.+SCP*KR+CC(IP)*KR**2/2.))+(3.+SCP)*(1.-CC(IP))/
     *(6.*SCP)-(8.*(2.-CC(IP))-5.*SCP-3.*SCP**3)*KR/24.)
      C1P=((1.+(1.+SCP)*KR/2.)/(1.+SQP*KR+CQ(IP)*KR**2/2.))*(1./((1.+SQP
     *)*(1.+KR)))*(1./3.)
      C2P=-((TR3+.5)/(1.+SQP*KR+CC(IP)*KR**2/2.))*(1./((1.+
     *KR)**2))*(1./6.)
      C4P=-((4./(1.-CC(IP)))*ALOG(3./(2.+SCP))+(2./3.)*((1.+SQP)/(2.+SQP
     *)))*(OMEGA**2)*(1./((1.+KR)**2*(1.+SCP*KR+CC(IP)*KR**2/2.)))*
     *(1./24.)
      C3P=OMEGA*(ALOG(3./(2.+SCP))/(1.-CC(IP)))*(1./((1.+KR)**2*
     *(1.+SCP*KR+CC(IP)*KR**2/2.)))*(1./6.)
      C7P=-((3.+SCP)*TR4/((1.+KR)**3))*(1./(1.+SCP*KR+CC(IP)*KR**2/2.))
     **(1./18.)
      SUMV=0
      DO 171IV=1,2
C     CALCULATION OF AVP
      SUMPI1=0
      DO 190I=1,2
  190 SUMPI1=SUMPI1   +UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))/(WW(I)+WW(IV)))
      AVP=SUMPI1*C1P
C     CALCULATION OF BVP
      BVP1=SUMPI1*C4P
      SUMPI2=0
      DO 200I=1,2
  200 SUMPI2=SUMPI2   +ZZ(I)*ZZ(IV)*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))
     */(WW(I)+WW(IV))))
      BVP2=SUMPI2*(C2P+C5P)
      SUMPI3=0
      DO 210I=1,2
  210 SUMPI3=SUMPI3   +(ZZ(I)+ZZ(IV))*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*WW(IV))
     */(WW(I)+WW(IV))))
      BVP3=SUMPI3*C3P
C     CALCULATION OF GVP
      SGVP1=0
      DO 220I=1,2
      SGVP2=0
      DO 221IL=2,2
      SQL=SQRT(CC(IL))
      XG=(SQL+SQP)*KR
      TR8=TR(XG)
      C6PL1=((-(SQL+CC(IP))*(1.-SQL)-(CC(IP)*(1.-CC(IL))-(1.-SQL)*(SCP*
     *SQL-1.)/2.)*KR)/(SQP*SQL)-(1.+SQL*KR+CC(IL)*KR**2/2.)*(1.-CC(IP)**
     *2)*TR2/CQ(IP)+(1.+SQL*KR+CC(IL)*KR**2/2.)*(1.+SCP*KR)*TR5/CC(IP)+
     *(CQ(IL)**2-CC(IP)**2)*(1.+KR+KR**2/2.)*TR8/(CC(IL)*CC(IP))
     *+(1.+KR+KR**2/2.)*(CC(IP)**2*(1.-CC(IL))*(1.+SQL*KR+CC(IL)*KR**
     *2/2.)-CQ(IL)**2*(1.+SCP*KR))*TR1/(CC(IL)*CC(IP)))
      C6PL2=(1./((1.+KR)*(1.+S
     *QP*KR+CC(IP)*KR**2/2.)*(1.+SQL*KR+CC(IL)*KR**2/2.)))
      C6PL=C6PL1*C6PL2
      SGVP3=0
      DO 230IA=1,2
  230 SGVP3=SGVP3     +TT(IA)*CHI(IL,IA)*ZZ(IA)
      SGVP2=SGVP2+SGVP3        *(WW(I)*CHI(IL,IV)-WW(IV)*CHI(IL,I))*C6PL
  221 CONTINUE
      SGVP1=SGVP1+(UU(I)*ZZ(I)*ZZ(IV)*(SGVP2/(WW(I)+WW(IV))))
  220 CONTINUE
      GVP=(1./12.)*SGVP1
      BVP=BVP1+BVP2+BVP3+GVP
C     CALCULATION OF CVP
      SUMPI4=0
      DO 240I=1,2
  240 SUMPI4=SUMPI4   +(ZZ(I)**2*ZZ(IV)**2)*(UU(I)*((ZZ(I)*WW(I)-ZZ(IV)*
     *WW(IV))/(WW(I)+WW(IV))))
      CVP=0
      QTAK=AVP*(BTA*KQ)+BVP*((BTA*KQ)**2)+CVP*((BTA*KQ)**3)
      SUMV=SUMV+(TT(IV)*CHI(IP,IV))*QTAK
  171 CONTINUE
      SUMP=SUMP+CHI(IP,IM)*SUMV
  170 CONTINUE
```

```
      ZSUMP(JM)=ZZ(JM)*SUMP
C     CALCULATION OF VJ1 AND VJ2
      SUMP=0
      DO 250IP=2,2
      SUMV=0
      DO 251IV=1,2
      SUMPI6=0
      DO 260I=1,2
  260 SUMPI6=SUMPI6   +UU(I)*(ZZ(I)-ZZ(IV))/(WW(I)+WW(IV))
      SUMV=SUMV+TT(IV)*CHI(IP,IV)*(ZZ(IV)*C8F/2.-WW(JM)*SUMPI6*C1P)
  251 CONTINUE
  250 SUMP=SUMP+CHI(IP,JM)*SUMV
      VJ1=-(ZZ(JM)*SUMP)-(1./2.)*(ZZ(JM)*OMEGA*
     *(TR6/((1.+KR)**2)+ALOG(2./3.))-OMEGA**2/6.)*(1.+KR)
      VJ2=0
      SUMPI5=0
      DO 270IV=1,2
  270 SUMPI5=SUMPI5   +(UU(IV)*((ZZ(IV)*WW(IV)-ZZ(JM)*WW(JM))
     */(WW(IV)+WW(JM))))/ZZ(IV)
      FINALT(JM)=(ABS(ZZ(JM))*(KQ*TAU)/(1.+KR))*(1.+VJ1*(BTA*KC)+VJ2*
      ((BTA*KC)**2)+SUMPI5*KR/6.)
  160 CONTINUE
      ALAM(2)=LAM2
      ALAM(1)=X(2)
      GAMCAL(IC) =0
      DO 280IA=1,2
      LL=ALAM(IA)*(1.+ZSUMP(IA))-FINALT(IA)
  280 GAMCAL(IC)=GAMCAL(IC)+ABS(ZZ(IA))*CC(IC,IA)*LL
      GAMCAL(IC)=GAMCAL(IC)/(2.*MM(IC))
  12  CONTINUE
      SUMSQ=0
      DO 13 IA =1,IFCINT
   13 SUMSQ = SUMSQ+((GAMCAL(IA)-GAMEXP(IA))**2)
      SUMSQ=SUMSQ/IFCINT
      F =SUMSQ*1.0E+3
      WRITE(3,18)(X(I),I=1,N),F
  18  FORMAT(20X,E12.6,5X,E12.6,5X,E12.6)
      RETURN
      END
```

APPENDIX G

PROGRAMME FOR CALCULATING THE IONIC SPECIES OF ZINC CHLORIDE SOLUTIONS

```
      DIMENSION XM(37),WT(37)
      DOUBLE PRECISION ACU(24),DIFXM,DELTAI,XML,DMREF,DIREF,AMEXPT(24),
     *FI,XI(37),XM,DELTA,YY,XX,ZZ,SI,GAMMA2,GAMMA1,GAMA21,
     *GAMA11,ABETA,AAA,BBB,CCC,YYL,XXL,ZZL,AK,D,WT,YYR,XXR,ZZR,XMR
C     XI(J) IS IONIC STRENGTH
      READ(1,4) (XI(J),J=1,36)
    4 FORMAT(6E9.2)
C     AMEXPT(K) IS EXPERIMENTAL CONCENTRATION OF SOLUTION IN MOLE PER KG
      READ(1,6) (AMEXPT(K),K=1,24)
    6 FORMAT(6E1).4)
C     WT(K) IS EXPERIMENTAL CONCENTRATION OF SOLUTION IN WEIGHT ,
      READ(1,2)(WT(K),K=1,24)
    2 FORMAT(6F7.5)
C     AK IS ASSOCIATION CONSTANT
      AK=4.5
      DO 8J=1,36
      SI=DSQRT(XI(J))
      GAMMA2=(-1.0230*SI/(1.0+1.48095*SI))+0.30*XI(J)
      GAMMA1=( 0.5115*SI/(1.0+1.3164*SI))-0.055*XI(J)
      GAMA21=10.000**GAMMA2
      GAMA11=10.000**GAMMA1
      ABETA=(GAMA21**3)/(GAMA11**2)
      AAA=2.*AK*ABETA
      BBB=6.-(2.*XI(J)*AK*ABETA)
      CCC=4.*XI(J)
      DELTA=BBB**2+4.*AAA*CCC
      YY=(-BBB+DSQRT(DELTA))/(2.*AAA)
      XX =YY/(2.+(YY*AK*ABETA))
      ZZ =YY-(2.*XX)
C     XM(J) IS CONCENTRATION IN MOLE PER KG (CORRESPOND TO IONIC STRENGTH)
      XM(J)=XX+ZZ
    8 CONTINUE
      DO 7 K=1,24
C     ACU(K) IS THE ACCURACY OF CONCENTRATION
      ACU(K)=0.01/100.*AMEXPT(K)
      DO 12J=1,36
      L=J+1
      IF(AMEXPT(K).LT.XM(J).OR.AMEXPT(K).GT.XM(L)) GO TO 12
      DMREF=XM(L)-XM(J)
      DIREF=XI(L)-XI(J)
      DIFXM=AMEXPT(K)-XM(J)
      DELTAI=DIREF*DIFXM/DMREF
      FI=XI(J)+DELTAI
      GO TO 15
   12 CONTINUE
   15 SI=DSQRT(FI)
      GAMMA2=(-1.0230*SI/(1.0+1.48095*SI))+0.30*FI
      GAMMA1=( 0.5115*SI/(1.0+1.3164*SI))-0.055*FI
      GAMA21=10.000**GAMMA2
      GAMA11=10.000**GAMMA1
      ABETA=(GAMA21**3)/(GAMA11**2)
      AAA=2.*AK*ABETA
      BBB=6.-(2.*FI*AK*ABETA)
      CCC=4.*FI
C     YYL,XXL,ZZL ARE CONCENTRATIONS OF IONIC SPECIES IN MOLE PER KG
      YYL=(-BBB+DSQRT(BBB**2+(4.*AAA*CCC)))/(2.*AAA)
      XXL=YYL/(2.+(YYL*AK*ABETA))
      ZZL=YYL-(2.*XXL)
C     XML IS STOICHIOMETRIC CONCENTRATION OF ZINC CHLORIDE IN MOLE PER KG
      XML=XXL+ZZL
      IF(XML.LT.AMEXPT(K)) DIFXM=AMEXPT(K)-XML
      IF(XML.GT.AMEXPT(K)) DIFXM=XML-AMEXPT(K)
      IF(DIFXM.LE.ACU(K)) GO TO 14
      DELTAI=DIREF*DIFXM/DMREF
      IF(XML.GT.AMEXPT(K))FI=FI-DELTAI
      IF(XML.LT.AMEXPT(K))FI=FI+DELTAI
      GO TO 15
C     D IS THE DENSITY OF SOLUTION
   14 D=.997044+.00923076*WT(K)
      YYR=(YYL*D)/(1.+YYL*0.13628)
      XXR=(XXL*D)/(1.+XXL*0.13628)
      ZZR=(ZZL*D)/(1.+ZZL*0.13628)
      XMR=ZZR+XXR
      WRITE(3,17)YYR,XXR,ZZR,XMR
   17 FORMAT(20X,4(5X,D16.8))
    7 CONTINUE
      STOP
      END
```

APPENDIX H

THE FINAL CONDUCTANCE EQUATION BY LEE AND WHEATON

A detailed equations used in programme (1) and (2) for calculations in the analysis by the Lee and Wheaton equation are givne here. Some corrections have been made as outlined in Appendix (B). These are equations (120) - (137) in the reference 6.

At this stage it is useful to define some new functions; let

$$\xi_{ji} = \frac{u_i(z_i\omega_i - z_j\omega_j)}{(\omega_i + \omega_j)} \qquad (120)$$

and let

$$\Pi_j^{(1)} = \sum_{i=1}^{s} \xi_{ji} \qquad \Pi_j^{(2)} = z_j \sum_{i=1}^{s} \xi_{ji} z_i$$

$$\Pi_j^{(3)} = \sum_{i=1}^{s} \xi_{ji}(z_i + z_j) \qquad \Pi_j^{(4)} = z_j^2 \sum_{i=1}^{s} \xi_{ji} z_i^2$$

$$\Pi_j^{(5)} = \sum_{i=1}^{s} \xi_{ji}/z_i \qquad \Pi_j^{(6)} = \sum_{i=1}^{s} \frac{u_i(z_i - z_j)}{(\omega_i + \omega_j)} \qquad (121)$$

also let

$$\Omega = \sum_{i=1}^{s} u_i z_i \quad \text{and} \quad \theta = \sum_{i=1}^{s} u_i z_i^2 \qquad (122)$$

$$\tau = F\zeta e/6\pi\eta. \qquad (123)$$

Assembling and rearranging all of the relaxation and electrophoretic terms we finally obtain *for the New model*

$$\lambda_j = \lambda_j^{\circ}\left\{1 + z_j \sum_{p=2}^{s} \chi_j^p \sum_{\upsilon=1}^{s} t_\upsilon \chi_\upsilon^p [A_\upsilon^p(t)(\beta\kappa) + B_\upsilon^p(t)(\beta\kappa)^2 + C_\upsilon^p(t)(\beta\kappa)^3]\right\} -$$

$$\frac{|z_j|(\kappa\tau)}{(1+t)}\{1 + V_j^{(1)}(t)(\beta\kappa) + V_j^{(2)}(t)(\beta\kappa)^2 + \Pi_j^{(5)} t/6\} \qquad (124)$$

where $t = \kappa R$ and

$$A_\upsilon^p(t) = \Pi_\upsilon^{(1)} C_{1,p}(t) \qquad C_\upsilon^p(t) = \Pi_\upsilon^{(4)} C_{7,p}(t) \qquad (125)$$

$$B_\upsilon^p(t) = \{\Pi_\upsilon^{(1)} C_{4,p}(t) + \Pi_\upsilon^{(2)}[C_{2,p}(t) + C_{5,p}(t)] + \Pi_\upsilon^{(3)} C_{3,p}(t) + G_\upsilon^p(t)\} \qquad (126)$$

For the New model;

$$C_{1,p}(t) = \frac{(1+(1+q_p^{1/2})t/2)}{3(1+q_p^{1/2})(1+t)(1+q_p^{1/2}t+q_p t^2/2)} \qquad (127)$$

$$C_{2,p}(t) = -\frac{(\mathrm{Tr}\,\{(2+q_p^{1/2})t\}+\tfrac{1}{2})}{6(1+t)^2(1+q_p^{1/2}t+q_p t^2/2)} \qquad (128)$$

$$C_{3,p}(t) = \frac{\Omega \ln(3/(2+q_p^{1/2}))}{6(1+t)^2(1-q_p)(1+q_p^{1/2}t+q_p t^2/2)} \qquad (129)$$

$$C_{4,p}(t) = -\frac{\Omega^2}{24(1+t)^2(1+q_p^{1/2}t+q_p t^2/2)}\left\{\frac{4}{(1-q_p)}\ln(3/(2+q_p^{1/2})) + \frac{2}{3}\frac{(1+q_p^{1/2})}{(2+q_p^{1/2})}\right\} \qquad (130)$$

$$C_{5,p}(t) = -\frac{1}{12(1+t)(1+q_p^{1/2}t+q_p t^2/2)}[\{(q_p-1)-q_p^{1/2}/2+q_p^{1/2}(1-q_p^{1/2})t/2\}/q_p^{1/2} -$$

$$(1-q_p^2)\,\mathrm{Tr}\,\{(1+q_p^{1/2})t\}/q_p - q_p(1+t+t^2/2)\,\mathrm{Tr}\,\{q_p^{1/2}t\} +$$

$$(1+q_p^{1/2}t)\,\mathrm{Tr}\,\{t\}/q_p] \qquad (131)$$

$$C_{7,p}(t) = -\frac{(3+q_p^{1/2})\,\mathrm{Tr}\,\{(3+q_p^{1/2})t\}}{18(1+t)^3(1+q_p^{1/2}t+q_p t^2/2)} \qquad (132)$$

$$G_\upsilon^p(t) = (1/12)\sum_{l=1}^{s}\frac{u_l z_l z_\upsilon}{(\omega_l+\omega_\upsilon)}\sum_{l=2}^{s}(t_\sigma \chi_\sigma^l z_\sigma)(\omega_i \chi_\upsilon^l - \omega_\upsilon \chi_i^l) C_{6,p,l}(t) \qquad (133)$$

[see below, eqn (I.72)]

$$C_{6,p,l}(t) = \frac{1}{\{(1+t)(1+q_p^{1/2}t+q_p t^2/2)(1+q_l^{1/2}t+q_l t^2/2)\}}[\{-(q_l^{1/2}+q_p)(1-q_l^{1/2}) -$$

$$[q_p(1-q_l)-(1-q_l^{1/2})(q_p^{1/2}q_l^{1/2}-1)/2]t\}/q_p^{1/2}q_l^{1/2} - (1+q_l^{1/2}t+q_l t^2/2)(1-q_p^2)\times$$

$$\mathrm{Tr}\,\{(1+q_p^{1/2})t\}/q_p + (1+q_l^{1/2}t+q_l t^2/2)(1+q_p^{1/2}t)\,\mathrm{Tr}\,\{t\}/q_p +$$

$$(q_l^2-q_p^2)(1+t+t^2/2)\,\mathrm{Tr}\,\{(q_l^{1/2}+q_p^{1/2})t\}/q_l q_p +$$

$$(1+t+t^2/2)\{q_p^2(1-q_l)(1+q_l^{1/2}t+q_l t^2/2) -$$

$$q_l^2(1+q_p^{1/2}t)\}\,\mathrm{Tr}\,\{q_p^{1/2}t\}/q_l q_p] \qquad (134)$$

$$V_j^{(1)} = -z_j\sum_{p=2}^{s}\chi_j^p\sum_{\upsilon=1}^{s} t_\upsilon \chi_\upsilon^p\{z_\upsilon C_{8,p}(t)/2 - \omega_j \Pi_\upsilon^{(6)} C_{1,p}(t)\} -$$

$$\tfrac{1}{2}\left[z_j\Omega\left\{\frac{\mathrm{Tr}\,\{2t\}}{(1+t)^2} + \ln(2/3)\right\} - \Omega^2/6\right](1+t) \qquad (135)$$

where

$$C_{8,p}(t) = \left\{-\frac{(1-q_p)}{2q_p}\mathrm{Tr}\,\{t\} + \frac{(1-q_p^2)}{2q_p}\frac{\mathrm{Tr}\,\{(1+q_p^{1/2})t\}}{(1+q_p^{1/2}t+q_p t^2/2)} + \frac{(3+q_p^{1/2})(1-q_p)}{6q_p^{1/2}} -\right.$$

$$\left.[8(2-q_p)-5q_p^{1/2}-3q_p^{3/2}]t/24\right\} \qquad (136)$$

$$V_j^{(2)} = -\frac{z_j^2\theta\,\mathrm{Tr}\,\{3t\}}{2(1+t)^2}. \qquad (137)$$

As mentioned in Section 4.2.2, Chapter 4, the programme was written in the way the terms were grouped and combined as outlined above. The λ_j term was was expressed in ($\rho\kappa$) series as shown in equation (124). The advantage of such expression is to minimise the "rounding off" of the numerical value involved in the calculations. The omitted terms suggested by Wheaton (3) correspond to c_v^p (t)and $V_j^{(2)}$(t) terms in equation (124) given by equations (125), (132) and (137).

VITA

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