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APPENDIX I

Bairstow's method

Bairstow's method is an itrative method which involves the solutions of polynomial equation of the form

$$y^n + a_1 y^{n-1} + a_2 y^{n-2} + a_3 y^{n-3} + \ldots + a_n = 0 \qquad (1)$$

where a_1 , a_2 ,a_3 ,..., a_n are real coefficients.

This method are capable of finding both real and complex roots of polynomial. By dividing the left side of eq.(1) by a quardratic factor $(y^2 + uy + v)$ leads to the identity

$$(y^2 + uy + v)(b_0 y^{n-2} + b_1 y^{n-3} + b_2 y^{n-4} + \ldots + b_{n-3} y + b_{n-2}) + \text{remainder} = \text{eq(1)} \qquad (2)$$

Equating the coefficients and remainder, we get

$$\begin{aligned}
b_0 &= 1 \\
b_1 &= a_1 - u \\
b_2 &= a_2 - b_1 u - v \\
b_3 &= a_3 - b_2 u - b_1 v \\
b_4 &= a_4 - b_3 u - b_2 v \qquad (3) \\
&\vdots \\
b_k &= a_k - b_{k-1} u - b_{k-2} v \\
&\vdots
\end{aligned}$$

$$b_{n-1} = a_{n-1} - b_{n-2}u - b_{n-3}v$$

$$b_n = a_n - b_{n-1}u - b_{n-2}v$$

and

$$\text{remainder} = (y + u)b_{n-1} + b_n$$

Bairstow's method may be desired by the following step by step procedure

1) Select the initial values for u and v. Most frequently these are taken as $u_1 = v_1 = 0$

2) Calculate $b_1, b_2, \ldots, b_n$ from

$$b_k = a_k - b_{k-1}u - b_{k-2}v \qquad (k = 2,3,\ldots,n) \tag{4}$$

where $b_0 = 1$ and $b_1 = a_1 - u$ as shown in eq (3) and the synthetic procedure.

3) Calculate $C_1, C_2, C_3, \ldots, C_{n-1}$ from

$$C_k = b_k - C_{k-1}u - C_{k-2}v \qquad (k = 2,3,..,n-1) \tag{5}$$

where $C_0 = 1$ and $C_1 = b_1 - u$

4) Calculate u and v by

$$u = \frac{b_n C_{n-3} - b_{n-1} C_{n-2}}{C_{n-1} - C_{n-2}} \tag{6}$$

and

$$v = \frac{C_{n-1} b_{n-1} - C_{n-2} b_n}{C_{n-1} - C_{n-2}}$$

5) Increment u and v by Δu and Δv :

$$u_{i+1} = u_i + \Delta u_i$$
$$v_{i+1} = v_i + \Delta v_i$$

where i is the number of iterations.

6) Return to step 2 and repeat the procedure until u and v approach zero to within some preassigned value such that

$$[\ \Delta u_{i+1}\ ] + [\ \Delta v_{i+1}\ ] < \epsilon$$

(ϵ represents the desired accuracy of the result)

If convergence to the desired result does not occur after the specified number of iterations, then new starting values should be selected. Frequently, suitable starting values of u and v may be determined from

$$u_1 = a_{n-1} / a_{n-2} \quad \text{and} \quad v_1 = a_n / a_{n-2}$$

7) Calculate the two roots from the quardratic formula

$$r_{1,2} = \frac{-u + (u^2 - 4v)^{1/2}}{2}$$

8) Obtain additional roots by starting with step 1 and reduces polynomial which is formulated from the final values of the b's obtained at the end of step 6.

These following variable names and quantities which they

represented are used in the FORTRAN subprogramme,namely,root as shown in programme I.

Variable Name	Quantity Represented
A(I),B(I),C(I)	The a's, b's, and c's of Eqs.1,3,and 5, respectively.
EPSI	ϵ of Eq.9
N	The degree of the polynomial
UI and VI	Initial values of u and v
P and Q	The real and imaginary parts of a root, p+iq
U and V	The u and v of Eq.1
DELU and DELV	Increments of u and v, Δu and Δv, as given by Eq.6 and 7.
RAD	u^2-4v of Eq.10
W	$-u/2$ when u^2-4v is positive
Z	$u^2-4v/2$ when u^2-4v is positive
IT	The number of iterations
DENOM	The denominator of Eq.6 and 7
SUM	$\Delta u + \Delta v$
STORE	The first value of $\Delta u + \Delta v$

Programme I

```
 0171        SUBROUTINE ROOT
00172        IMPLICIT REAL*8(A-H,O-Z)
00173        DIMENSION B(5),C(5)
00174        COMMON/DD/A(5),FX,FY
00175        UI=0
00176        VI=0
00177        EPSI=0.00001
00178        N=5
00179    40  IF(N-1)100,5,7
00180     5  P=-A(1)
00181        Q=0
00182        FX(N)=P
00183        FY(N)=Q
00184        IT=1
00185        GO TO 100
00186     7  IF(N.EQ.2) GO TO 8
00187        GO TO 13
00188     8  U=A(1)
00189        V=A(2)
00190        IT=1
 0191     9  P=-U/2.
00192        RAD=U**2-4.*V
00193        IF(RAD.GT.0) GO TO 12
00194        RAD=-RAD
00195        Q=DSQRT(RAD)/2.
00196        FX(N)=P
00197        FY(N)=Q
00198        FYZ=-FY(N)
00199        FYW=FX(N)
00200        N=N-1
00201        FY(N)=FYZ
00202        FX(N)=FYW
00203    10  N=N-1
00204        IF(N.LE.0) GO TO 100
00205        DO 11I=1,N
00206    11  A(I)=B(I)
00207        GO TO 40
00208    12  Q=DSQRT(RAD)/2.
00209        W=P
00210        Z=Q
 0211        P=P+Q
00212        Q=0
00213        FX(N)=P
00214        FY(N)=Q
00215        N=N-1
00216        P=W-Z
00217        FX(N)=P
00218        FY(N)=0
00219        GO TO 10
00220    13  U=UI
00221        V=VI
00222        IT=1
00223    50  B(1)=A(1)-U
00224        B(2)=A(2)-B(1)*U-V
00225        DO 14K=3,N
00226    14  B(K)=A(K)-B(K-1)*U-B(K-2)*V
00227        C(1)=B(1)-U
00228        C(2)=B(2)-C(1)*U-V
00229        M=N-1
00230        DO 15K=3,N
```

```
 0231   15  C(K)=B(K)-C(K-1)*U-C(K-2)*V
00232        IF(N.GT.3) GO TO 17
00233        DENOM=C(N-1)-C(N-2)**2
00234        IF(DENOM.EQ.0) GO TO 100
00235        DELU=(B(N)-B(N-1)*C(N-2))/DENOM
00236   16   DELV=(C(N-1)*B(N-1)-C(N-2)*B(N))/DENOM
00237        GO TO 18
00238   17   DENOM=C(N-1)*C(N-3)-C(N-2)**2
00239        IF(DENOM.EQ.0) GO TO 100
00240        DELU=(B(N)*C(N-3)-B(N-1)*C(N-2))/DENOM
00241        GO TO 16
00242   18   U=U+DELU
00243        V=V+DELV
00244        SUM=DABS(DELU)+DABS(DELV)
00245        IF(IT.EQ.1) GO TO 19
00246        GO TO 20
00247   19   STORE=SUM
00248        GO TO 21
00249   20   IF(IT.EQ.50) GO TO 28
00250        IF(IT.GE.200) GO TO 100
 0251   21   IF(SUM.LE.EPSI) GO TO 9
00252        IF(IT.EQ.100) GO TO 22
00253   22   IT=IT+1
00254        GO TO 50
00255   28   IF(SUM.LT.STORE) GO TO 21
00256  100   RETURN
00257        END
00258 * * * End of File * * *
```

APPENDIX II

The Programme for the Determination the Value of the Standard Potential of Cell ($\overset{\circ}{E}$) and Complex Formation Constants

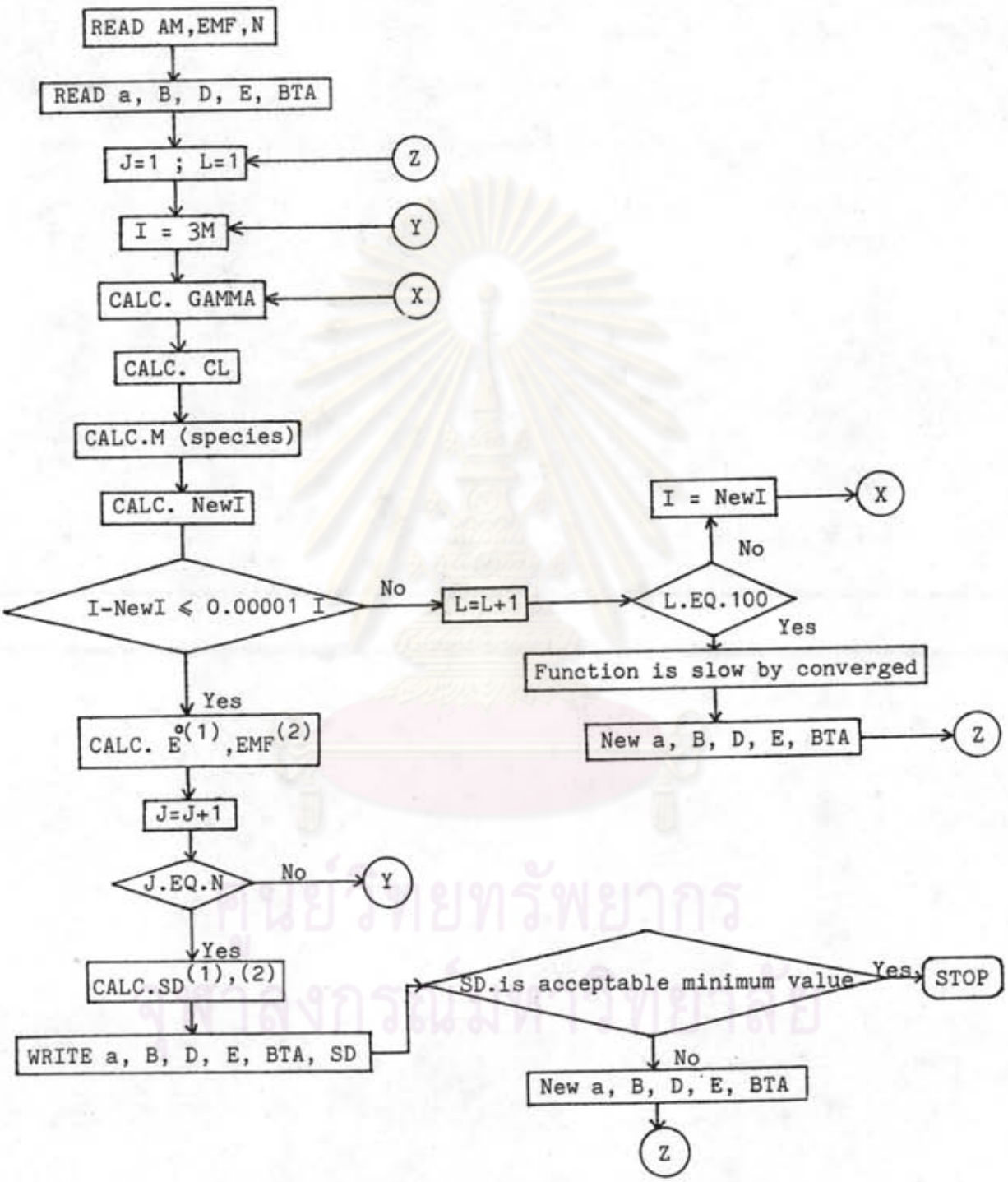
The programme II(a) and II(b) were used to determine the standard potential of cell studied (E°) and complex formation constants (β_n), respectively. The following variable names used in these programme are denoted as below.

Variable Name	Quantity Represented
SE	The standard potential of cell
BTA	The thermodynamic complex formation constants β_n
$(A,B,D,E)_{ik}$	The parameters as expressed in the Debye-Huckel of eq.(31)
AM , XM	The experimental and calculated total concentration of zinc
FX, TCL	The experimental and calculated total concentration of halide
EMF, CEMF	The experimental and calculated total concentration of emf
XI, NXI	The initial guess ionic strength and the new one's , respectively
GAMMA	The activity coefficients γ_{ik} of eq.(31)
A(I)	The coefficient constant's as expressed in the polynomial of eq.(29)
CL,ZN,ZNCL1,ZNCL2, ZNCL3,ZNCL4	The concentration of speciess Cl^-,Zn^{2+} $ZnCl^+$, $ZnCl_2$, $ZnCl_3^-$, and $ZnCl_4^{2-}$, respectively
SD	The standard deviation between the experimental and calculated values

ROOT — The name of subprogramme was called to determine CL by solving from polynomial equation.

The flowchart of these programme is shown as scheme I.

FLOW CHART OF THE PROGRAMME FOR THE DETERMINATION THE VALUE OF E° AND β



$$SD^{(1)} = = \sqrt{\sum (E^{\circ} - \bar{E})^2 / N-1} \quad ; \quad \bar{E} = \sum E^{\circ} / N$$

$$SD^{(2)} = = \sqrt{\sum (DIFF - \overline{DIFF})^2 / N-1} \quad ; \quad DIFF = E_{calcd.} - E_{measd.}$$

$$; \quad \overline{DIFF} = \sum DIFF / N$$

Programme II(a)

```
 0001      IMPLICIT REAL*8(A-H,S-Z)
00002       DIMENSION AN(50),EMF(50),DIFF(50),SE(50),FX(2)
00003       OPEN(5,FILE='DATA')
00004       READ(5,*) N
00005       READ(5,10) (AN(I),I=1,N)
00006    10 FORMAT(F10.5)
00007       READ(5,20) (EMF(J),J=1,N)
00008    20 FORMAT(F7.5)
00009 C ** READ PARAMETER  *****
00010       READ(5,30) BTA1,A21,A11,B21,B11
00011    20 FORMAT(5F10.5)
00012 C  ** INITIALLY TO CALCULATE THE STANDARD ELECTROMOTIVE FORCE IN EACH
00013 C  ** SET OF PARAMETER**************************************************
00014    15 SUM=0.0
00015       DO 100K=1,N
00016       SD=0.0
00017       SX=0.0
00018       SDX=0.0
00019       NET=0
00020       XI=3*AN(K)
 0021      5 SI=DSQRT(XI)
00022       GAM21=(-1.023*SI/(1.0+0.3291*A21*SI))+B21*XI
00023       IF(GAM21.GT.75.OR.GAM21.LT.-75) GO TO 116
00024       GAM11=(-0.5115*SI/(1.0+0.3291*A11*SI))+B11*XI
00025       IF(GAM11.GT.75.OR.GAM11.LT.-75) GO TO 116
00026       GAMA21=10.0D0**GAM21
00027       GAMA11=10.0D0**GAM11
00028       ZGAMA=GAMA21**3
00029       XGAMA=ZGAMA/GAMA11**2
00030       AA=BTA1*XGAMA
00031       BB=BTA1*XGAMA*AN(K)+1.0
00032       CC=-AN(K)
00033       FX(1)=(-BB+DSQRT(BB**2-(4*AA*CC)))/(2.*AA)
00034       FX(2)=(-BB-DSQRT(BB**2-(4*AA*CC)))/(2.*AA)
00035       DO 50M=1,2
00036       IF(FX(M).GT.0.0) THEN
00037       ZN=FX(M)
00038       CL=2*AN(K)/(1.+ZN*BTA1*XGAMA)
00039       ZNCL1=BTA1*ZN*CL*XGAMA
00040       XM=ZN+ZNCL1
 0041        ACCU=0.01/100*XI
00042       ZXI=0.5*(4*ZN+ZNCL1+CL)
00043       IF(ZXI.GT.0.0) GO TO 470
00044       ELSE
00045       END IF
00046    50 CONTINUE
00047       IF(FX(2).LT.0.) GO TO 116
00048   470 DELTI=XI-ZXI
00049       ADELTI=DABS(DELTI)
00050       IF(ADELTI.LE.ACCU) GO TO 45
00051       XI=ZXI
00052       NET=NET+1
00053       IF(NET.EQ.100) GO TO 116
00054       GO TO 5
00055    45 SE(K)=EMF(K)+0.02958*DLOG10(ZN*CL**2*ZGAMA)
00056       SUM=SUM+SE(K)
00057   100 CONTINUE
00058       AVSE=SUM/17
00059       DO 75L=1,17
00060       DIFF(L)=AVSE-SE(L)
```

```
 0061        SX=SX+DIFF(L)*DIFF(L)
00062    75  CONTINUE
00063        SD=DSQRT(SX/N-1)
00064   116  WRITE(6,117) SD,AVSE,BTA1,A21,A11,B21,B11
00065   117  FORMAT(7F10.5)
00066    55  STOP
00067        END
00068 * * * End of File * * *
```

```
 0001       IMPLICIT REAL*8(A-H,O-Z)
00002       DIMENSION CEMF(90),DIFF(90),AM(90),AMX(90),EMF(90)
00003       COMMON/DD/A(5),FX,FY
00004       SX=0.0
00005       SXX=0.0
00006 C ** READ INPUT DATA; EMF,CONC.,NO.OF DATA POINT**
00007       OPEN(5,FILE='DATA')
00008       READ(5,*)SE,N,NL,NX
00009       READ(5,10)(AM(I),I=1,N)
00010    10 FORMAT(F10.5)
00011       READ(5,20)(EMF(J),J=1,N)
00012    20 FORMAT(F9.4)
00013       IF(NL.LT.1) GOTO 1
00014       READ(5,30)(AMX(K),K=NX,N)
00015    30 FORMAT(F10.5)
00016 C ** READ PARAMETER ; BTA,A,B,D,E **
00017       READ(5,40)BTA1,BTA2,A21,B21,D21,E21
00018    40 FORMAT(6F10.5)
00019       SUM=0.0
00020       SX=0.0
 0021       SXX=0.0
00022       SD=0.0
00023 C  ** INITIALLY TO CALCULATE THE EMF.AND SD.IN EACH OF SET OF PARAMETER
00024       DO 100K=1,N
00025       NET=0.0
00026       IF(K.EQ.NX) GOTO 25
00027 C  ** ESTIMATE THE VALUE OF IONIC STRENGTH  **
00028       XI=3*AM(K)
00029       GOTO 2
00030     2 SI=DSQRT(XI)
00031       GAM21=(-1.023*SI/(1.0+0.3291*A21*SI))+B21*XI+D21*XI**2+E21*XI**3
00032       IF(GAM21.GT.75.OR.GAM21.LT.-75) GO TO 105
00033       GAM11=(-0.5115*SI/(1.0+0.3291*A11*SI))+B11*XI+D11*XI**2+E11*XI**3
00034       IF(GAM11.GT.75.OR.GAM11.LT.-75) GO TO 105
00035       GAM0=B0*XI+D0*XI**2-E0*XI**3
00036       IF(GAM0.GT.75.OR.GAM0.LT.-75) GO TO 105
00037       GAM12=(-1.023*SI/(1.0+0.3291*A12*SI))+B12*XI+D12*XI**2+E12*XI**3
00038       IF(GAM12.GT.75.OR.GAM12.LT.-75) GO TO 105
00039       GAMA21=10.0D0**GAM21
00040       GAMA11=10.0D0**GAM11
 0041       GAMA0=10.0D0**GAM0
00042       GAMA12=10.0D0**GAM12
00043       ZGAMA=GAMA21**3
00044       XGAMA=ZGAMA/GAMA11**2
00045       YGAMA=ZGAMA/GAMA0
00046       UGAMA=ZGAMA*GAMA11**4/GAMA12**3
00047       EE=BTA4*UGAMA
00048       A(1)=((BTA3*ZGAMA)+(BTA4*UGAMA*(2*AM(K))))/EE
00049       A(2)=((BTA2*YGAMA)+(BTA3*ZGAMA*(AM(K))))/EE
00050       A(3)=(BTA1*XGAMA)/EE
00051       A(4)=(1.-(BTA1*XGAMA*AM(K)))/EE
00052       A(5)=(-2.*AM(K))/EE
00053 C  ** DETERMINE THE HALIDE CONCENTRATION BY BAIRSTOW'S METHOID **
00054       CALL ROOT
00055       IF(FX(M).GT.0.0.AND.FY(M).EQ.0.) GOTO 3
00056       GOTO 105
00057    3  CL=FX(M)
00058 C  ** CALCULATE THE CONCENTRATION OF SPECIES **
00059       C11=BTA1*XGAMA*CL
00060       C12=BTA2*YGAMA*CL**2
```

```
 0061        C13=BTA3*ZGAMA*CL**3
00062        C14=BTA4*UGAMA*CL**4
00063        ZN=AM(K)/(1.+C11+C12+C13+C14)
00064        ZNCL1=C11*ZN
00065        ZNCL2=C12*ZN
00066        ZNCL3=C13*ZN
00067        ZNCL4=C14*ZN
00068        XM=ZN+ZNCL1+ZNCL2+ZNCL3+ZNCL4
00069        TCL=CL+ZNCL1+2*ZNCL2+3*ZNCL3+4*ZNCL4
00070        ACCU=0.01/100*XI
00071 C  ** CALCULATE THE NEW VALUE OF IONIC STRENGTH **
00072        ZXI=0.5*(4*ZN+ZNCL1+ZNCL3+4*ZNCL4+CL)
00073        IF(ZXI.GT.0.0) GO TO 4
00074   4    DELTI=XI-ZXI
00075        ADELTI=DABS(DELTI)
00076        IF(ADELTI.LE.ACCU) GO TO 35
00077        XI=ZXI
00078        NET=NET+1
00079        IF(NET.EQ.100) GO TO 105
00080        GO TO 2
 0081 C  ** ESTIMATE THE VALUE OF IONIC STRENGTH **
00082    25  XI=3.*AM(K)+(AMX(K)-2*AM(K))
00083     5  SI=DSQRT(XI)
00084        GAM21=(-1.023*SI/(1.0+0.3291*A21*SI))+B21*XI+D21*XI**2
00085       **+E21*XI**3
00086        IF(GAM21.GT.75.OR.GAM21.LT.-75) GO TO 105
00087        GAM11=(-0.5115*SI/(1.0+0.3291*A11*SI))+B11*XI+D11*XI**2
00088       **+E11*XI**3
00089        IF(GAM11.GT.75.OR.GAM11.LT.-75) GO TO 105
00090        GAM0=B0*XI+D0*XI**2-E0*XI**3
00091        IF(GAM0.GT.75.OR.GAM0.LT.-75) GO TO 105
00092        GAM12=(-1.023*SI/(1.0+0.3291*A12*SI))+B12*XI+D12*XI**2
00093       **+E12*XI**3
00094        IF(GAM12.GT.75.OR.GAM12.LT.-75) GO TO 105
00095 C ** CALCULATE THE ACTIVITY COEFFICIENT **
00096        GAMA21=10.0D0**GAM21
00097        GAMA11=10.0D0**GAM11
00098        GAMA0=10.0D0**GAM0
00099        GAMA12=10.0D0**GAM12
00100        ZGAMA=GAMA21**3
 0101        XGAMA=ZGAMA/GAMA11**2
00102        YGAMA=ZGAMA/GAMA0
00103        UGAMA=ZGAMA*GAMA11**4/GAMA12**3
00104        EE=BTA4*UGAMA
00105        A(1)=((BTA3*ZGAMA)+(BTA4*UGAMA*(4*AM(K)-AMX(K))))/EE
00106        A(2)=((BTA2*YGAMA)+(BTA3*ZGAMA*(3*AM(K)-AMX(K))))/EE
00107        A(3)=((BTA1*XGAMA)+(BTA2*YGAMA*(2*AM(K)-AMX(K))))/EE
00108        A(4)=(1.+(BTA1*XGAMA*(AM(K)-AMX(K))))/EE
00109        A(5)=(-AMX(K))/EE
00110 C  ** DETERMINE THE CONCENTRATION OF HALIDE BY BAIRSTOW'S METHOD *8
00111        CALL ROOT
00112        IF(FX.GT.0.0.AND.FY.EQ.0.0) GOTO 6
00113        GOTO 105
00114        CL=FX
00115        C11=BTA1*XGAMA*CL
00116        C12=BTA2*YGAMA*CL**2
00117        C13=BTA3*ZGAMA*CL**3
00118        C14=BTA4*UGAMA*CL**4
00119        ZN=AM(K)/(1.+C11+C12+C13+C14)
00120        ZNCL1=C11*ZN
```

```
 0121        ZNCL2=C12*ZN
00122        ZNCL3=C13*ZN
00123        ZNCL4=C14*ZN
00124        XM=ZN+ZNCL1+ZNCL2+ZNCL3+ZNCL4
00125        EM=CL+ZNCL3+2*ZNCL4-2*ZN-ZNCL1
00126        TCL=CL+ZNCL1+2*ZNCL2+3*ZNCL3+4*ZNCL4+EM
00127        ACCU=0.01/100*XI
00128 C  ** CALCULATE THE NEW VALUE OF IONIC STRENGTH **
00129        ZXI=0.5*(4.*ZN+ZNCL1+ZNCL3+4*ZNCL4+CL+EM)
00130        IF(ZXI.GT.0.0) GO TO 7
00131    7   DELTI=XI-ZXI
00132        ADELTI=DABS(DELTI)
00133        IF(ADELTI.LE.ACCU) GO TO 35
00134        XI=ZXI
00135        NET=NET+1
00136        IF(NET.EQ.100) GO TO 105
00137        GO TO 5
00138 C  ** CALCULATE THE EMF. VALUE *8
00139   35   CEMF(K)=SE-0.02958*DLOG10(ZN*CL**2*ZGAMA)
00140        DIFF(K)=CEMF(K)-EMF(K)
 0141        SXX=SXX+DIFF(K)
00142 C  ** CALCULATE PERCENTAGE DISTRIBUTION OF COMPLEX SPECIES **
00143 C      IF(K.GT.46) GOTO 46
00144 C      P1=ZN*100/AM(K)
00145 C      P2=CL*100/AM(K)
00146 C      P3=ZNCL1*100/AM(K)
00147 C      P4=ZNCL2*100/AM(K)
00148 C      P5=ZNCL3*100/AM(K)
00149 C      P6=ZNCL4*100/AM(K)
00150 C      WRITE(9,56)AM(K),AGAMA(K),HGAMA(K)
00151 C56    FORMAT(2X,3F10.5)
00152 C      WRITE(9,57)AM(K),GAMA21,GAMA11,GAMA0,GAMA12
00153 C57    FORMAT(2X,5F10.5)
00154 C      WRITE(9,59)AM(K),EMF(K),CEMF(K),DIFF(K),XI
00155 C59    FORMAT(2X,5F10.5)
00156 C      WRITE(9,89)ZN,CL,ZNCL1,ZNCL2,ZNCL3,ZNCL4
00157 C89    FORMAT(2X,6F10.5)
00158 C      WRITE(9,79)P1,P2,P3,P4,P5,P6
00159 C79    FORMAT(2X,6F10.5)
00160  100   CONTINUE
 0161 C ** CALCULATE THE STANDARD DEVIATION OF EMF.DATA **
00162        AVS=SXX/N.
00163        DO 101J=1,N
00164        SX=SX+(DIFF(J)-AVS)**2
00165  101   CONTINUE
00166  501   SD=DSQRT(SX/(N-1))
00167  102   WRITE(6,19)SD,BTA1,BTA2,A21,B21,D21,E21
00168   19   FORMAT(7F10.5)
00169  105   STOP
00170        END
00171 * * * End of File * * *
```

APPENDIX III

The Rosenbrock Minimizing Programme

The programme namely, Rosenbrock, which used to adjust parameters in order to minimize the value of standard deviation of the emf is shown in Programme III.

The minimising programme may be describing by the following step by step procedure.

1) The initial estimated parameters and theirs jumping step are selected.

2) The vector matrix of A,E and V used for developing the minimisation process, are an index matrix, developing factor and unit matrix respectively.

3) Firstly, an error function (which expressed in form of the standard deviation) will be calculated from the first set of initial parameters.

4) Secondly, the expected parameters are roughly computed through the simple first equation namely

$$X_i' = X_i + E_i V_{ij}$$

and the parameters will be kept if its error function is less than the previous value. Unless the new error is smaller than the old one, new parameter will be computed from equation

$$X_i' = X_i - E_i V_{ij}$$

The set of parameter of the smaller error compare to the previous value will be kept. For the bigger error function, the new parameter will be expected to obtain their values by the equation

$$X_i'' = X_i' + E_i V_{ij} \quad \text{or also} \quad X_i'' = X_i' - E_i V_{ij} ,$$

respectively.

If its error, indicated by A_i index vector vector is not much decreasingly, the new V_{ij} vector will be calculated through the Gram-Schmidt process (28).

5) Step (4) will be iteratively repeated until the error function is statistically accepted.

The variable names used in the programme are denoted by the following symbols.

Variable Name	Quantity Represented
N or NVAR	the number of independent variables
X(N)	an estimate of the solution : on entry, an initial estimate : on exit, the best estimate of the solution found
STEP(N)	an initial step length for all coordinate directions at the start of the process.
R	the actual number of function evaluation (for the initial estimate R = 0)

MAXR	the maximum number of times the function is to be evaluated
B	the value of the euclidian norm of the vector representing the total progress made since the axes were last rotated.
TOL	is used for convergence criteria.
NR	is the monitor index
CON	is a logical variable. At the start of subroutine romin, CON is set to .FALSE. If the convergence criteria (B.LE.TOL.) of the routine monitor are satisfied, CON must be set .TRUE. to stop the process.
TRACE	is a logical variable. If .TRUE. then the monitor will print, If .FALSE. the values are passed back to the calling programme without being printed.
E(I)	is a set of steps to be taken in the corresponding coordinate directions.
V(I,J)	is an matrix defining a set of N mutually orthogonal coordinate directions. V(I,J) is the unit matrix at the start.
FUNCT	the name of subprogramme which used to calculate the emf and standard deviation of emf.

```
0001 C****** READ AND WRITE PARAMETERS AND CRITICAL VALUE******
00002       IMPLICIT REAL*8(A-H,O-Z)
00003       LOGICAL TRACE
00004       COMMON/A1/NVAR,MAXR,TOL,STEP(19)
00005       COMMON/A2/TRACE
00006       COMMON/AA/F,X(19)
00007 C     OPEN(5,FILE='DATACHU')
00008       READ(5,1000)TRACE
00009  1000 FORMAT(L10)
00010       READ(5,2000)NVAR
00011  2000 FORMAT(I10)
00012       READ(5,3000)MAXR
00013  3000 FORMAT(I10)
00014       READ(5,4000)TOL
00015  4000 FORMAT(D10.4)
00016       DO 11I=1,NVAR
00017    11 READ(5,5000)X(I),STEP(I)
00018  5000 FORMAT(F10.5,F10.5)
00019       WRITE(6,99)TOL,(STEP(I),I=1,NVAR)
00020       CALL ROMIN
0021     99 FORMAT('1',5X,'TOLERANCE=',D15.7,/,5X,'STEP=',19F10.4)
00022       STOP
00023       END
00024 C ****** SUBROUTINE MINIMIZES A FUNCTION OF N VARIABLES *******
00025       SUBROUTINE ROMIN
00026       IMPLICIT REAL*8(A-H,S-Z)
00027       LOGICAL TRACE,CON
00028       INTEGER P,R
00029       DIMENSION A(19),D(19),V(19,19),ALPHA(19,19),
00030      *BETA(19),E(19),AV(19)
00031       COMMON/A1/N,MAXR,TOL,STEP(19)
00032       COMMON/A2/TRACE
00033       COMMON/A3/R,NR
00034       COMMON/A4/B
00035       COMMON/A5/CON
00036       COMMON/AA/F,X(19)
00037 C ****** INITIALIZE CON,E(I),R,B ******
00038       CON=.FALSE.
00039       B=1.00
00040       DO 10I=1,N
0041       E(I)=STEP(I)
00042    10 CONTINUE
00043       R=0
00044       DO 30I=1,N
00045       DO 20J=1,N
00046        V(I,J)=0.0
00047        IF(I.EQ.J) V(I,J)=1.0
00048    20 CONTINUE
00049    30 CONTINUE
00050       CALL FUNCT
00051       F0=F
00052       NR=1
00053       CALL MONITR
00054 C ******* START OF THE INITIAL LOOP ******
00055    40 DO 50I=1,N
00056         A(I)=2.0
00057         D(I)=0.0
00058    50 CONTINUE
00059 C ******* EVALUATE F AT THE NEW POINT X ******
00060    60 DO 130I=1,N
```

```
 0061        DO 70J=1,N
00062        X(J)=X(J)+E(I)*V(I,J)
00063     70 CONTINUE
00064        R=R+1
00065        CALL FUNCT
00066        F1=F
00067        NR=2
00068        CALL MONITR
00069        IF(CON) GO TO 290
00070        IF(F1-F0)80,90,90
00071 C ****** THE NEW VALUE OF THE FUNCTION IS LESS THAN THE OLD ONE ******
00072     80 D(I)=D(I)+E(I)
00073        E(I)=3.0*E(I)
00074        F0=F1
00075        IF(A(I).GT.1.5) A(I)=1.0
00076        GO TO 110
00077 C ****** THE NEW VALUE OF THE FUNCTION IS.GT.OR.EQ. THE OLD FUNCTION ***
00078     90 DO 100J=1,N
00079        X(J)=X(J)-E(I)*V(I,J)
00080    100 CONTINUE
 0081        E(I)=-0.5*E(I)
00082        IF(A(I).LT.1.5) A(I)=0.0
00083    110 DO 120J=1,N
00084        IF(A(J).GE.0.5) GO TO 130
00085    120 CONTINUE
00086        GO TO 140
00087    130 CONTINUE
00088        GO TO 60
00089 C ****** GRAM - SCHMIDT PROCESS ******
00090    140 DO 160K=1,N
00091        DO 150L=1,N
00092        ALPHA(K,L)=0.0
00093    150 CONTINUE
00094    160 CONTINUE
00095        DO 190I=1,N
00096         DO 180J=1,N
00097          DO 170L=1,N
00098        ALPHA(I,J)=ALPHA(I,J)+D(L)*V(L,J)
00099    170 CONTINUE
00100    180 CONTINUE
 0101    190 CONTINUE
00102        B=0.0
00103        DO 200J=1,N
00104         B=B+ALPHA(1,J)**2
00105    200 CONTINUE
00106        B=DSQRT(B)
00107        DO 210J=1,N
00108        V(1,J)=ALPHA(1,J)/B
00109    210 CONTINUE
00110        DO 280P=2,N
00111        BETY=0.0
00112        IP=P-1
00113        DO 220M=1,N
00114        BETA(M)=0.0
00115    220 CONTINUE
00116        DO 240K=1,IP
00117        AV(K)=0.0
00118         DO 230L=1,N
00119          AV(K)=AV(K)+ALPHA(P,L)*V(K,L)
00120    230 CONTINUE
```

```
 0121   240 CONTINUE
00122       DO 260J=1,N
00123       DO 250K=1,IP
00124       BETA(J)=BETA(J)-AV(K)*V(K,J)
00125   250 CONTINUE
00126       BETA(J)=BETA(J)+ALPHA(P,J)
00127       BETY=BETY+BETA(J)**2
00128   260 CONTINUE
00129       IF(BETY.LT.1.0D-30) GO TO 280
00130       BETY=DSQRT(BETY)
00131       DO 270J=1,N
00132       V(P,J)=BETA(J)/BETY
00133   270 CONTINUE
00134   280 CONTINUE
00135 C ****** END OF GRAM-SCHMIDT ******
00136       NR=3
00137       CALL MONITR
00138       IF(CON) GO TO 290
00139       GO TO 40
00140   290 RETURN
 0141       END
00142       SUBROUTINE MONITR
00143       IMPLICIT REAL*8(A-H,S-Z)
00144       CHARACTER*6 STRNG(19)
00145       LOGICAL TRACE,CON
00146       INTEGER R
00147       COMMON/A1/N,MAXR,TOL,STEP(19)
00148       COMMON/A2/TRACE
00149       COMMON/A3/R,NR
00150       COMMON/A4/B
00151       COMMON/A5/CON
00152       COMMON/AA/F,X(19)
00153       DATA STRNG/'X(1)','X(2)','X(3)','X(4)','X(5)','X(6)','X(7)',
00154      *'X(8)','X(9)','X(10)','X(11)','X(12)','X(13)','X(14)','X(15)',
00155      *'X(16)','X(17)','X(18)','X(19)'/
00156       IF(TRACE) GO TO 5
00157       IF(B.LE.TOL) CON=.TRUE.
00158       IF(R.GE.MAXR) CON=.TRUE.
00159       GO TO 20
00160     5 GO TO (1,2,3),NR
 0161     1 IF(N.GT.5) GO TO 4
00162       WRITE(6,100)(STRNG(I),I=1,N)
00163       WRITE(6,103)
00164       WRITE(6,99)R,F,(X(I),I=1,N)
00165       GO TO 20
00166     2 IF(R.LE.MAXR) GO TO 20
00167       WRITE(6,98)
00168       CON=.TRUE.
00169       GO TO 20
00170     4 WRITE(6,101)(STRNG(I),I=1,N)
00171       WRITE(6,103)
00172       WRITE(6,102)R,F,(X(I),I=1,N)
00173       WRITE(6,104)
00174       GO TO 20
00175     3 WRITE(6,102)R,F,(X(I),I=1,N)
00176       IF(N.GT.5) WRITE(6,104)
00177       IF(B.LE.TOL) CON=.TRUE.
00178    98 FORMAT(5X,'R EXCEEDS FNC EVALUATION LIMIT')
00179    99 FORMAT(3X,'(',I3,')',D16.7,5D18.7)
00180   100 FORMAT(//,5X,'(R)  F VALUE',7X,5(5X,A4,9X))
```

```
 0181  101  FORMAT(//,5X,'(R)  F VALUE',7X,5(5X,A4,9X),/,25X,5(5X,A4,9X),
00182       */,25X,5(5X,A4,9X),/,25X,5(5X,A4,9X))
00183  102  FORMAT(3X,'(',I3,')',D16.7,5D18.7,/,25X,5D18.7,/,25X,5D18.7,
00184       */,25X,5D18.7)
00185  103  FORMAT(2X,120('-')/)
00186  104  FORMAT(/)
00187   20  RETURN
00188       END
00189 * * * End of File * * *
```

VITA

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