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APPENDIX

1.) Fortran program to calculate cartesian coordinates of Zn(II) ion in different direction from water.

```
C   This program calculate the coordinate of Zn(II)
C   12345678901234567890123456789012345678901234567890123456789012345678901234567890
C   ************* Y O N G Y O S  Y O N G Y A I *********
        real fact,phi,zet
        real d(40),x(40),y(40),z(40)
        fact=2.*3.1415927/360
        num=5
        print*,'Pls enter Zeta  Phi '
        read*, zet,phi
        zeta=30.

10      format(2f4.1)
        open(6,file='zn.cor')
        open(7,file='znwa.co')
        open(8,file='znwa.l')
        open(9,file='znwa.run')
        do 50 i=1,num
        d(i)=1.0+(i*.2)
        x(i)=d(i)*cos(zet*fact)*sin(phi*fact)
        y(i)=d(i)*sin(zet*fact)*sin(phi*fact)
        z(i)=d(i)*cos(phi*fact)
50      continue
        write(6,60)
60      format(/'     Dist      X      Y      Z '/)
        do 80 i=1,num
        write(6,70) d(i),x(i),y(i),z(i)
70  format(4f15.5)
        write(7,75) x(i),y(i),z(i)
75  format('ZN',10x,'30.',6x,f10.6,10x,f10.6,10x,f10.6)
        write(8,85) d(i)
85  format('*** ZN - H2O ***   distance O-Zn =',2x,f4.1)
        write(9,90) d(i),d(i)
90  format('znwa.jj "',f4.1,'" "',f8.5,'"')
80      continue
        stop
        end
```

2.) Fortran program to calculate stabilization energy (kcal/mol) from the total energy (hartree).

```
C   This program is written by Yongyos Yongyai
C   ********************************************
      real dis(30),et(30),ee(30),st(30)
      integer i,n
      ref=-79.509
      print*, 'Pls enter the number of data : '
      read*, n
      open(5,file='znwa.dat')
      open(6,file='znwa.pt')
      write(6,1)
1     format(/'O-H Distance',5x,'Total Energy',6x,'  Escf')
      write(6,4)
4     format(3x,'<Ang.>',6x,' <Hatree>',4x,'  <Kcal/mol>'/)
      do 2 i=1,n
      read(5,3) dis(i),et(i)
3     format(60x,f8.3/65x,f15.5)
2     continue
      do 5 i=1,n
      st(i)=(et(i)-ref)*627.5
      write(6,10) dis(i),et(i),st(i)
10    format(2x,f5.3,5x,f15.5,3x,f15.5)
5     continue
      stop
      end
C   ****************************************
```

3.) Awk program to collect important information from Hondo Output file.

```
rm info
echo""
echo Concentrated Hondo Output Information collected
in file info
echo""
for i {
echo $i
echo $i>>info
awk '
/COORDINATES/&&!/INPUT/ {cco=NR}
/CONTRACTED/ {ccoe=NR}
/COORDINATES/&&!/INPUT/ {ccoo=NR}
/INTERNUCLEAR/ {ccooe=NR}
/FINAL/  {eco=$10;  ecal=($10+96.46142)*627.5}
```

```
/CONDENSED/ {pco=NR}
/--- BOND INDICES/ {pcoe=NR}
{line[NR]=$0}
END {
printf"\n E tot = %f", eco
printf"              E stab = %f\n", ecal
for (i=cco+4;i<ccoe-2 ;i++) print substr(line[i],17,70)
for (i=pco+1 ;i<pcoe-1;i++) print substr(line[i],17,60)
printf"*****************************************\n"
} ' $i  >>info
}
echo""
echo Mission completed !
exit
```

4.) **Awk program to transform data from Hondo Output file to fiting input file.**

```
date
echo""
echo  Hondo Output Data transformed for Rodfit
Input to file  fit.inp
echo""
for i {
echo $i
echo $i>>info
awk '
/COORDINATES/&&!/INPUT/ {cco=NR}
/CONTRACTED/ {ccoe=NR}
/FINAL/  {eco=$10;  ecal=($10+96.46142)*627.5}
{line[NR]=$0}
END {
printf"%f,%f", ecal,angle(j)
for (i=cco+7;i<ccoe-11 ;i++)
if (substr(line[i],1,42)!=" ")
print substr(line[i],47,40)} ' $i >> data
}
awk '{if ($3!="") {print
$1*0.52914,$2*0.52914,$3*0.52914}
else if ($1!="") {print $1} } ' data >fit.inp
rm data
date
echo""
echo Mission completed !
exit
```

5.) Input file for HONDO program

```
$CNTRL  runflg=0 , iprint=0 , $END
$MASS                 amass*50  50*0.0
$GUESS                nguess  norb uhfflg
          2       13   0
$INTGRL               nkfil
          0
$WFN    wfnflg
          0
$SCF    nco  nseto  no     maxit  uhfflg accurcy
          13   0      10*0  90      0      0.001
$BASIS
Zn (II) + 2 H2O
0   0   12    1  ...  ECP
C1
ZN  1      30.        0.            0.          0.
1   D   5
1     68.850000        .0214335
2     18.320000        .1368916
3      5.922000        .3704352
4      1.927000        .4834232
5      0.552800       0.3315150
2   S   1
1       .799700       -.2517637

O          8.       0.00000     0.00000     -1000.00000
1   SP   3
1      8.519          -0.1455          0.11007
2      2.073          0.08286          0.34969
3      0.6471          0.74325          0.48093
2   SP   1
4      0.2000          0.28472          0.30727
3   D   1
1      1.154           1.0

H          1.       0.00000     0.75670     -1000.58580
1   DZ   3  DZV
H          1.       0.00000    -0.75670     -1000.58580
1   DZ   3  DZV

O          8.       0.0         0.0           2.0
1   SP   3
1      8.519          -0.1455          0.11007
2      2.073          0.08286          0.34969
3      0.6471          0.74325          0.48093
2   SP   1
```

```
4      0.2000          0.28472         0.30727
3   D   1
1      1.154           1.0

H          1.      0.75695     0.          2.58588
1   DZ    3  DZV

H          1.     -0.75695     0.          2.58588
1   DZ    3  DZV

$END
$ECP
ZN-ECP     18   3
5 -- Z -- L=F POTENTIAL
-18.00000    1 386.73797
-124.35274    2  72.85874
-30.66018    2  15.90662
-10.63590    2   4.35023
-.76836    2   1.28422
5
3.00000    0  19.08679
22.52342    1   5.02311
48.44659    2   1.27017
-44.55601    2   1.06713
12.99840    2    .92642
5
5.00000    0  43.49277
20.74356    1  20.86927
90.30272    2  21.71184
74.66103    2   6.36169
9.88944    2   1.22912
3
-4.84904    2  13.58518
3.69134    2   9.83730
-.50373    2    .83731
O-ECP     02    1
1 -- O -- L=1 POTENTIAL
-0.92550    1  16.11718
2 -- O -- S-P POTENTIAL
1.96069    0   5.05348
29.13442    2  15.95333

O-ECP     02    1

$END
```

6.) Fortran program to produce probability data for water ligands probability plot.

```
*************************************************************
        Program MC_grid : written by YongYos Yongyai
          Austrian-Thai Computation Chemistry Center
*************************************************************
        PROGRAM GRID
        IMPLICIT INTEGER (I-N),REAL (A-H,O-Z)
        PARAMETER (MOLALL = 282)
        PARAMETER (BOXLH = 19.62260)
        PARAMETER (NUM_HISTO = 1000)
        REAL XKOORD (MOLALL),
+       YKOORD (MOLALL),
+       ZKOORD (MOLALL),
+       ALPHA (MOLALL),
+       BETA (MOLALL),
+       GAMA (MOLALL)
        INTEGER SPEC(MOLALL),STEPO
        B2 = BOXLH/2.
        OPEN(10,FILE = 'HISTORY' ,STATUS = 'OLD')
        OPEN(11,FILE = 'DAT' ,STATUS = 'UNKNOWN')
        OPEN(12,FILE = 'BASKET1' ,STATUS = 'UNKNOWN')
        DO 100 K=1,NUM_HISTO
        READ (10,'(///)')
        READ (10,'(4X,I2,6F10.5)')
+       (SPEC(I),XKOORD(I),YKOORD(I),ZKOORD(I),ALPHA(I),
+       BETA(I),GAMA(I), I=1,MOLALL)
        DO 10 I=1,20
        X1 = XKOORD(I)
        Y1 = YKOORD(I)
        Z1 = ZKOORD(I)
        XZN = X1 - XKOORD(I)
        YZN = Y1 - YKOORD(I)
        ZZN = Z1 - ZKOORD(I)
        DO 20 J=61,282
        X2  = XKOORD(J)
        Y2  = YKOORD(J)
        Z2  = ZKOORD(J)
        XO  = X2 - X1
        YO  = Y2 - Y1
        ZO  = Z2 - Z1
********** MINIMAL IMAGE **********
        IF (XO.GE.(XZN+B2)) THEN
        XO = XO - BOXLH
        ELSEIF (XO.LE.(XZN-B2)) THEN
        XO = XO + BOXLH
        ENDIF
```

```
      IF (YO.GE.(YZN+B2)) THEN
      YO = YO - BOXLH
      ELSEIF (YO.LE.(YZN-B2)) THEN
      YO = YO + BOXLH
      ENDIF
      IF (ZO.GE.(ZZN+B2)) THEN
      ZO = ZO - BOXLH
      ELSEIF (ZO.LE.(ZZN-B2)) THEN
      ZO = ZO + BOXLH
      ENDIF
*     RZNO = distance ZN-O ,[RRZNO = distance ZN-O for the
*     first          water]
      RZNO = SQRT((XO-XZN)**2+(YO-YZN)**2+(ZO-ZZN)**2)
      IF (RZNO .LE. 3.5) THEN
      STEPO = STEPO + 1
      IF (STEPO.EQ.1) THEN
      WRITE(12,'("  ")')
      CALL PAR1(XO,YO,ZO,RZNO,ZETA,ZFIX)
      CALL TransXY(XO,YO,ZO,RZNO,ZFIX,TX,TY,TZ)
      RRZNO = RZNO
      CALL PAR2(TX,TY,TZ,RXY,PHI,ZZ)
      CALL TurnToX(TX,TY,TZ,RXY,PHI,ZZ,XF,YF,ZF)
      WRITE(12,'(5x,4f10.5)') XF,YF,ZF
      ELSE
      CALL TransXY(XO,YO,ZO,RRZNO,ZFIX,TX,TY,TZ)
      CALL TurnToX(TX,TY,TZ,RXY,PHI,ZZ,XF,YF,ZF)
      WRITE(12,'(5x,3f10.5)') XF,YF,ZF
      ENDIF
      ENDIF
20    CONTINUE
      STEPO=0
10    CONTINUE
100   CONTINUE
      END

      SUBROUTINE PAR1(X,Y,Z,R,ZET,ZZ)
      ZZ = Z
      RETURN
      END

      SUBROUTINE TransXY(X,Y,Z,R,ZF,TTX,TTY,TTZ)
      TTZ = Z-ZF
      TTY = Y*R/(SQRT(X**2+Y**2))
      TTX = X*R/(SQRT(X**2+Y**2))
      RETURN
      END

      SUBROUTINE PAR2(X,Y,Z,R,PI,ZZZ)
```

```
R = SQRT(X**2+Y**2)
IF(X.EQ.0) THEN
PI = 3.14159/2.
ELSE
PI = ATAN(Y/X)
ENDIF
ZZZ=Z
RETURN
END

SUBROUTINE TurnToX (X,Y,Z,RR,PP,ZZZ,XX,YY,ZZ)
IF(X.GT.0 .AND. Y.GT.0) THEN
XX = X+(RR-RR*COS(PP))
YY = Y-RR*SIN(PP)
ENDIF
IF(X.LE.0 .AND. Y.LE.0) THEN
XX = X-(RR-RR*COS(PP))
YY = Y+RR*SIN(PP)
ENDIF
IF(X.GT.0.AND. Y.LT.0) THEN
XX = X+(RR-RR*COS(PP))
YY = Y-RR*SIN(PP)
ENDIF
IF(X.LT.0.AND. Y.GT.0) THEN
XX = X-(RR-RR*COS(PP))
YY = Y+RR*SIN(PP)
ENDIF
ZZ = Z
RETURN
END
```

7.) **PV-WAVE program to plot the probabity plot of water ligands around Zn^{2+} ion.**

```
; WAVE Version 3.02 (ultrix mipsel)
; Journal File for yod@ATC
; Working directory: /work2/yod2/mc5m
; Date: Mon Sep  9 20:04:38 1991
a=fltarr(3,4900)
openr,1,'xyclw3M'
readf,1,a
a=transpose(a)
x=a(*,0)
y=a(*,1)
p=a(*,2)
x=rebin(x,700)
y=rebin(y,700)
```

```
p=rebin(p,700)
window,1,xsize=600,ysize=500,color=7
xyp=grid(x,y,p,nx=50,nghbr=20)
surface,xyp
b=fltarr(3,4900)
openr,2,'xzclw3M'
readf,2,b
b=transpose(b)
x1=b(*,0)
y1=b(*,1)
p1=b(*,2)
x1=rebin(x1,700)
y1=rebin(y1,700)
p1=rebin(p1,700)
xzp=grid(x1,y1,p1,nx=50,nghbr=20)
com=xyp+xzp
surface,com,zrange=[0,500],az=40
surface,com,zrange=[0,500],az=45
surface,smooth(com,6),az=45
END;
```

CURRICULUM VITAE

Yongyos Yongyai

1968	Born August, 31st in Songkla, Thailand Father : Mr. Puchong Yongyai Mother : Mrs. Wanlee Yongyai
1974-1980	Elementary School
1980-1986	High school (Triam Udom Seuksa,Bangkok)
1986-1990	Bachelor of Science(Chemistry),Chulalongkorn University, Bangkok
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Chem. Phys, 156, 403 (1991).

2. "Computational methods in solution chemistry",
Pure & Appl. Chem., 63(12), 1725 (1991).

3. "Microstructure and species distribution of aqueous zinc chloride solutions: results from Monte Carlo simulations",
J.Chem.Soc. Faraday II, in press