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APPENDIXES

Appendix I

Programme Generates Hondo Input/Output (Fortran)

```
************************************************************
*                    Programme proscf.f                    *
*                                                          *
************************************************************
*
* PLEASE READ THIS INSTRUCTION BEFORE MODIFYING.
*
*     Hondo programme provides ab intio SCF calculations. The programme
* needs the exact format of input file which can be served by 'proscf.f'.
*
*     The 'proscf.f' is suitable for using in the ion/molecule 2-body interaction.
* This process requires 5 important files
*
*   1. 'proscf.f' (this file): written as fortran language. Several places have to be
*      changed depended on what system are being studied. For example, Pls. go to
*      SUBROUTINE 'Geninput', and then XCl, YCl, & ZCl can be replaced by
*      XLi, YLi, & ZLi to evaluate Li coordinate.
*
*   2. 'part1' & 'part2': Two text files, some part of input, must be defined according
*      to type of calculation, basis set value etc.
*
*   3. '01, 02,...': The format inside these files are not difficult to define
*      if you understand this programme.
*    4. 'proscf.inp'  It is a batch file to assign which directions are run.
************************************************************************
*
      COMMON  R,Zeta,Phi
      CHARACTER  DN*2,Output*8,Text*5
*     DN = This is a file for indicated the Direction NO.of Ion.
      DATA  Pi/3.1415927/
      InpName = ' '
  1   FORMAT(A2)
      READ(*,1) DN
      DO WHILE (DN.NE.'99')
         OPEN(UNIT=7,FILE=DN)
         READ(7,*) Zeta,Phi
         READ(7,*) R
         DO WHILE (R.NE.-1.0)
            CALL  Geninput(R,Zeta,Phi)
            CALL  ToChar(R,Text)
            Output = Text//'-'//DN
            CALL  System('cp input '//Output//'.inp')
            CALL  System('hondo < input > '//Output//'.out')
            READ(7,*) R
```

```
            END DO
            CLOSE(7)
            READ(*,1) DN
          END DO
          STOP
          END
C-------------------------------------------------
          SUBROUTINE  Geninput(R,Zeta,Phi)
C         REAL  R,Zeta,Phi
          REAL  XCl,YCl,ZCl
          CHARACTER  S1*19
          DATA  Pi/3.1415927/
          XCl = R*sin(Zeta*Pi/180)*cos(Phi*Pi/180)
          YCl = R*sin(Zeta*Pi/180)*sin(Phi*Pi/180)
          ZCl = R*cos(Zeta*Pi/180)
          CALL  System('cp part1 input')
          S1 = 'Cl          0.    '
          OPEN(UNIT=8,FILE='input',ACCESS='APPEND')
  111     FORMAT((A),F12.6,8X,F12.6,8X,F12.6)
          WRITE(8,111) S1,XCl,YCl,ZCl
          CLOSE(8)
          Call System('cat part2 >> input')
          RETURN
          END
C-------------------------------------------------
          SUBROUTINE  ToChar(R,Text)
          REAL  R
          CHARACTER  Text*5
C
          OPEN(UNIT=8,FILE='temp',ACCESS='NEW')
  222     FORMAT(F5.2)
          WRITE(8,222) R
          CLOSE(8)
          OPEN(UNIT=8,FILE='temp')
  333     FORMAT(A5)
          READ(8,333) Text
          CLOSE(8)
          RETURN
          END
```

Appendix II

Hondo Input File

```
 $CNTRL runflg= 0, iprint=0, $end
 $GUESS       nguess  norb uhfflg
      2      11    0
 $INTGRL      nkfil
      0
 $WFN    wfnflg
      0
 $SCF    nco  nseto  no  maxit  uhfflg  acurcy
      11    0     10*0   99       0    0.0001
 $BASIS
 *** NH2OH Only INTERACTION ***
   0   0  12   1  ...  ECP
 Cl
 Cl         17.       0.000000          -0.559902          -5.659210
   1   S   2
   1      2.225          -0.33098
   2      1.173           0.11528
   2   S   2
   1      0.3851          0.84717
   2      0.1301          0.26534
   3   P   2
   1      2.225          -0.12604
   2      1.173           0.29952
   4   P   2
   1      0.3851          0.58357
   2      0.1301          0.34097

 N          7.       0.000000          0.000000          0.000000
   1   SP   3
   1      6.403        -0.13955          0.10336
   2      1.580         0.05492          0.33205
   3      0.5094        0.71678          0.48708
   2   SP   1
   1      0.1623        0.33210          0.31312
   3   D   1
   1      0.8640        1.00000

 O          8.       0.000000          -0.559902          1.340790
   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         1.00000

H         1.      -0.818050        0.604221        0.000000
  1   S   1  DZV

H         1.       0.818050        0.604221        0.000000
  1   S   1  DZV

H         1.       0.000000       -1.503310        1.152904
  1   S   1  DZV

 $END
 $ECP
CL-ECP    10   2  Stevens-Basch-Kraus Core
   1 -- CL -- D  POTENTIAL
-3.40738    1  4.87483
   2 -- CL -- S-D POTENTIAL
 6.50966    0 17.00367
42.27785    2  4.10380
   2 -- CL -- P-D POTENTIAL
 3.42860    0  8.90029
22.15256    2  3.52648
N - ECP   02   1
   1 -- N -- L=1 POTENTIAL
 -0.91212   1  11.99686
   2 -- N -- SP POTENTIAL
  1.93565   0   3.83895
 21.73355   2  11.73247
O - ECP    2   1
   1 --  O -- P -POTENTIAL
 -0.92550   1 16.11718
   2 --  O -- SP-POTENTIAL
  1.96069   0  5.05348
 29.13442   2 15.95333
                NO-POTENTIAL
                NO-POTENTIAL
                NO-POTENTIAL
 $END
```

Appendix III

Programme Calculates Stabilization Energy and Coordinate from Hondo Output

```
                    UNIX Programme
**************************************************************
*                                                            *
*                  Programme GenFitInp                       *
*                                                            *
**************************************************************


for i {
echo $i>>info
awk '
 /COORDINATES/&&!/INPUT/ {cco=NR}
 /FINAL/  {eco=$10;  ecal=($10+27.049494211)*627.5}
 /INTERNUCLEAR/ {ecnl=NR}
 {line[NR]=$0}
END {
 printf        "%f",ecal        ;        printf        substr(line[cco+5],46,45);printf
"%s",substr(line[ecnl+8],17,10); printf "%15.9f\n",eco
  }' $i >> data
cp data data1
awk '{
 printf      "%10.2f      %10.5f      %10.5f      %10.5f      %15.9f      %5.2f\n"
,$1,$2*0.529167,$3*0.529167,$4*0.529167,$6,$5

} ' data
rm data
}
```

Appendix IV

Fitting Input File

```
        -792.0
        103.1
        1.01
        1164.48
        -1975.81
        133.5
        0.4
        5116.66
        -3293.02
        240.181
        0.594765
        6564.23
        -516.759
        5.96242
        0.06
        853.493
   -0.81805,  0.60422,  0.00000,
    0.81805,  0.60422,  0.00000,
    0.00000,  0.00000,  0.00000,
    0.00000, -0.55990,  1.34079,
    0.00000, -1.50331,  1.15290
END
        1,1,      1,2,3,4
        2,1,      1,2,3,4
        3,1,      5,6,7,8
        4,1,      9,10,11,12
        5,1,      13,14,15,16
    28.22 ,    1.48527,  2.01090,  0.00000,  2.50
     7.02 ,    1.60410,  2.17177,  0.00000,  2.70
    -3.18 ,    1.72292,  2.33264,  0.00000,  2.90
    -5.92 ,    1.78233,  2.41308,  0.00000,  3.00
    -8.66 ,    1.90115,  2.57395,  0.00000,  3.20
    -9.30 ,    2.01997,  2.73482,  0.00000,  3.40
    -8.94 ,    2.13879,  2.89570,  0.00000,  3.60
    -7.20 ,    2.37644,  3.21744,  0.00000,  4.00
    -3.70 ,    2.97055,  4.02180,  0.00000,  5.00
    -2.18 ,    3.56466,  4.82616,  0.00000,  6.00
     2.98 ,    1.99996,  1.99996,  2.82837,  4.00
     1.63 ,    2.49995,  2.49995,  3.53547,  5.00
     0.85 ,    3.49993,  3.49993,  4.94965,  7.00
```

Appendix V

Explanations to input-variables for MC91 Programme

USED MC91-PARAMETER SETTING (DEFINES SIZE OF ARRAYS) : MNS = 5
MNSS = 5
MNPB = 1414

PART 1 : SYS

TITLE ... NAME OF MC-SIMULATION => FOR DOCUMENTATION ONLY
MAX.: 70 CHARACTERS

TK ... TEMPERATURE OF SYSTEM IN KELVIN.
DEFAULT = 298.15

DEN ... DENSITY OF YOUR SYSTEM IN G/CM**3 (ACC. TO TK).

ELB ... ELEMENTARY LENGTH OF THE EDGE OF THE BOX IN ANGSTROEM
(ACC. TO DEN).

YOU HAVE TO SPECIFY EITHER DEN OR ELB .GT. 0.0 !!!

RCS ... CUTOFF-RADIUS FOR SHORT-RANGE POTENTIAL-TERMS IN ANGSTROEM.
SHOULD NOT BE SET LOWER THAN 7.0 ANGSTROEM !
DEFAULT = ELB/2.0

DMC ... MINIMAL DISTANCE OF 2 MOLECULAR CENTERS IN ANGSTROEM.
3-TIMES MINIMAL DISTANCE OF 2 MOLECULAR SITES.
IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
DEFAULT = ELB/((NPSX(NPT)**(1/3))*SQRT(3))
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)
(SQRT(3) = ARBITRARY FACTOR > 1.0 !)

EWALD ... 0 : CALCULATION OF ALL 1/R INTERACTIONS WITHOUT EWALD-SUM
BUT INCLUDING SUMMATION OVER IMAGINARY-BOXES.
1 : CALCULATION OF 1/R INTERACTIONS WITH
EWALD-SUMMATION FOR ION-ION ENERGIES.
2 : CALCULATION OF 1/R INTERACTIONS WITH
EWALD-SUMMATION FOR ION-ION AND ION-DIPOLE ENERGIES.
3 : CALCULATION OF ALL 1/R INTERACTIONS WITH EWALD-SUM.
!!! EWALD > 0 ONLY FOR ELECTRICALLY NEUTRAL SYSTEMS !!!
DEFAULT = 3

NIBD ... MAXIMUM NUMBER OF IMAGINARY-BOXES IN ONE AXIS DIRECTION(+/-)
FOR SUMMATION OF 1/R ION-ION INTERACTIONS AND EWALD=0.
SUMMATION FROM OUTSIDE TO INSIDE (SMALLER TERMS FIRST !).
NIBD=0 CORRESPONDS TO A TOTAL OF 1 BOX (NO IMAGINARY-BOXES)
NIBD=1 CORRESPONDS TO A TOTAL OF 7 BOXES (6 IMAGINARY-BOXES)
NIBD=2 CORRESPONDS TO A TOTAL OF 33 BOXES
(32 IMAGINARY-BOXES).
NIBD=10 CORRESPONDS TO A TOTAL OF 4168 BOXES

```
        MAX. VALUE : 10 !!!
 DEFAULT = 2

EPSC ... DIELECTRIC-CONSTANT ( EPSILON ) OUTSIDE YOUR BOX(ES)
        FOR ENERGY-CORRECTION ACCORDING TO SURFACE-TERM.
        EPSC < 0.0 : NO CORRECTION WILL BE CALCULATED.
        0.0 <= EPSC < 1.0 : EPSILON = INFINITE : METALLIC SURROUNDING.
        1.0 <= EPSC : EPSILON = EPSC ( EPSILON = 1.0 : VACUUM SURROUNDING ).
 DEFAULT = 0.0

MCY ... USE OF CF2-POTENTIAL ( MCY=0 ) OR MCY-POTENTIAL ( MCY=1 )
        FOR WATER-WATER-INTERACTIONS.
 DEFAULT = 0

RDVRES ... RESOLUTION OF RADIAL-DENSITY-VECTORS IN ANGSTROEM.
 DEFAULT = 0.05

NRDVS ... NUMBER OF STEPS FOR COLLECTION OF RDV'S
          AND CALCULATION OF RDF'S.
  NRDVS = 0 : CALCULATED BY RDVRES -> ALL DISTANCES INCLUDED !
  NRDVS = 1 : CALCULATED BY RDVRES -> DISTANCES UP TO ELB/2 INCLUDED !
  NRDVS = 2 - 499 : THIS VALUE WILL BE USED !
 DEFAULT = 0

TSF ... MAXIMUM TRANSLATIONAL SHIFT FOR A PARTICLE-MOVE IN ANGSTROEM.
      IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
 DEFAULT = DMC/12

ASF ... MAXIMUM ANGULAR SHIFT FOR A PARTICLE-MOVE IN RAD.
      IF YOU SPECIFY 0.0, THE DEFAULT-VALUE IS USED !
 DEFAULT = 2*PI/SQRT(3)/12

TSF AND ASF INFLUENCE THE RATIO OF ACCEPTED TO REJECTED CONFIGURATIONS
( METROPOLIS-METHOD ). FOR AUTOMATIC ADAPTION BY VARIABLE RRARC
THEY ARE JUST START-VALUES.

RRARC ... REQUESTED RATIO OF ACCEPTED TO REJECTED CONFIGURATIONS.
       USED FOR AUTOMATIC ADAPTION OF TSF AND ASF.
  RRARC <= 0.0 : NO AUTOMATIC ADAPTION OF TSF AND ASF.
  RRARC = 3.0 : 75% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.
  RRARC = 1.0 : 50% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.
  RRARC = 0.5 : 33% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.
  RRARC = 0.3 : 23% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.
  RRARC = 0.1 : 9% OF ALL CONFIGURATIONS SHOULD BE ACCEPTED.
  %(ACCEPTED CONFIGURATIONS) = 100*RRARC/(1+RRARC) !
 DEFAULT = 0.5

$SYS
TITLE=' CHLORIDE ION & HYDROXYLAMINE  32.00 deg C 1 / 216   PARTICLES  ',
TK=305.15,DEN=1.204,ELB=0.0,RCS=0.0,DMC=1.5,EWALD=0,NIBD=2,EPSC=-1.0,MCY=0,
RDVRES=0.025,NRDVS=1,TSF=0.0,ASF=0.0,RRARC=0.5,
$END
```

PART 2 : PAR - NO DEFAULT VALUES !

NPS(X) (X=1,5) ... NUMBER OF PARTICLES OF TYPE X.
X=1 : WATER
X=2 : COPPER OR ZINC (2 PROGRAM-VERSIONS !)
X=3 : LITHIUM
X=4 : HYDROXYLAMINE
X=5 : CHLORIDE

```
$PAR
NPS(1)=0,
NPS(2)=0,
NPS(3)=0,
NPS(4)=216,
NPS(5)=1,
$END
```

PART 3 : RUN

RSC ... DETERMINES, HOW STARTING CONFIGURATION IS OBTAINED.
1 : READ START-CONFIGURATION FROM FILE MC91SC.
0 : START-CONFIGURATION GENERATED RANDOMLY.
DEFAULT = 0

USC ... DETERMINES CONTENTS OF FILE MC91SC.
1 : MC91SC WILL BE PERIODICALLY UPDATED. THIS NEW COORDINATES CAN BE USED LATER ON AS IMPROOVED START-COORDINATES.
0 : MC91SC RETAINS ORIGINAL FORM.
DEFAULT = 1

WCON ... DETERMINES WHETHER FILE MCCON WILL BE WRITTEN OR NOT.
BESTIMMT, OB DER FILE MCCON BESCHRIEBEN WIRD ODER NICHT.
1 : MCCON WILL BE EXPANDED EVERY MACRO-STEP.
0 : MCCON WILL NOT BE WRITTEN.
DEFAULT = 1

RNGO ... RANDOM-NUMBER-GENERATOR OPTION (CHOICE OF TYPE OF RNG).
1 : INTERNAL RNG OF THIS PROGRAM (NORMAL CASE).
2 : CYBER 840 (NOS/VE) RNG.
CYBER 840 (NOS/VE) RNG.
DEFAULT = 1

IJC, KLC ... THIS ARE THE SEED-VALUES FOR THE RANDOM-NUMBER-GENERATOR :
0 <= IJC <= 31328 , 0 <= KLC <= 30081
DEFAULT = 10443, 20054

EXPM ... LARGEST X FOR EXP(X) AND
SMALLEST -X FOR EXP(-X) FOR YOUR COMPUTER.
CHECK THIS VARIABLE-SETTING ON YOUR MACHINE (TEST PROGRAM)
FOR CYBER 840 : 2839.823
FOR 32-BIT MACHINES NORMALLY 88. IS O.K.
DEFAULT = 88.

MAXCON ... TOTAL NUMBER OF CONFIGURATIONS FOR THIS SIMULATION.
DEFAULT = 1000*NPSX(NPT)
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)

NUPDAT ... NUMBER OF STEPS (CONFIGURATIONS / MACRO-STEP) FOR UPDATING
OF STATISTICAL DATA.
(NPSX(NPT) = TOTAL NUMBER OF PARTICLES IN THE BOX)

NCONB ... NUMBER OF STEPS (CONFIGURATIONS) UNTIL THE SIMULATION BREAKS.
USE THIS FEATURE FOR SUBMITTING NUMEROUS SHORT JOBS RATHER
THAN ONE LONG JOB. NORMALLY, SET NCONB=+INTEGER*NUPDAT
(ACCORDING TO THE RESOURCES ON YOUR MACHINE) - TEST !
THE SUBMISSION OF SHORT JOBS IN A CHAIN CAN BE MANAGED
AUTOMATICALLY VIA A SHELL-SCRIPT OR PROCEDURE ETC..
DEFAULT = 0 (ONLY ONE BREAK AFTER INITIALIZING (STEP 0 : START-RUN))

UCV ... DETERMINES WHETHER RADIAL-DENSITY-VECTORS AND
RADIAL-DENSITY-FUNCTIONS (INCLUDING INTEGRATIONS
-> COORDINATION-NUMBERS) ARE EVALUATED OR NOT.
1 : CONTINUOUS EVALUATION AND SUMMATION OF RDV'S.
RDV'S STORED IN FILE MC91CV.
0 : NO RDV-EVALUATION.
DEFAULT = 1

NCF ... SPEFIFIES HOW OFTEN RADIAL-DENSITY-FUNCTIONS ARE EVALUATED
AND UPDATED ON FILES MC91CFxxxx (ONLY ACTIVE FOR UCV=1).
NCF = 1 : EVERY MACRO-STEP
NCF = 10 : EVERY 10th MACRO-STEP
NCF = 100 : EVERY 100th MACRO-STEP
DEFAULT = MAXCON/NUPDAT

MWCF ... MODE (FORMAT) FOR WRITING TO FILES MC91CFxxxx.
0 : PARALLEL (4 COLUMNS)
1 : SERIAL (3-TIMES 2 COLUMNS)
DEFAULT = 0

UNIT21: STES: TABLE FOR EWALD-SUM VALUES (UNFORMATTED).
DEFAULT = 'STES'
UNIT22: SRNG: RESTART-INFORMATION FOR INTERNAL RNG (UNFORMATTED).
DEFAULT = 'SRNG'
MACNNL: Maximum Number of Nearest Neighbour Ligands considered
Default = 20

```
$RUN
RSC=1,USC=1,WCON=1,RNGO=1,IJC=10443,KLC=20054,EXPM=88.,
MAXCON=1000000,NUPDAT=1000,NCONB=0,UCV=1,NCF=10,MWCF=0,
MC91SC='MC91SC     ',MC91CV='MC91CV     ',
MCOUT='MCOUT      ',MCENE='MCENE      ',MCCON='MCCON      ',
STES='STES       ',SRNG='SRNG       ',MACNNL=0,
$END
```

Appendix VI

MC91 Output File

```
**************************************************************************
* CHLORIDE ION & HYDROXYLAMINE 32.00 deg C 1 / 216   PARTICLES     *
**************************************************************************

 SOLVENT-SPECIES FOR CALCULATION OF MOLALITIES          HYDROXYLAMI

 NUMBER OF  HYDROXYLAMI PARTICLES                       216
 NUMBER OF SITES IN  HYDROXYLAMINE                      5
 TOTAL CHARGE ON  HYDROXYLAMI IN A.U                    .0000000
 CALCULATED MOLALITY FOR  HYDROXYLAMI                   30.2756904
 CALCULATED MOLARITY FOR  HYDROXYLAMI                   36.2716872
   COORDINATES ( X / Y / Z ) AND CHARGE FOR CENTER
      .0000000      .0000000      .0000000     -.4820000
   COORDINATES ( X / Y / Z ) AND CHARGE FOR SITE  2
     -.8180500      .6042200      .0000000      .3010000
   COORDINATES ( X / Y / Z ) AND CHARGE FOR SITE  3
      .8180500      .6042200      .0000000      .3010000
   COORDINATES ( X / Y / Z ) AND CHARGE FOR SITE  4
      .0000000     -.5599000     1.3407900     -.5250000
   COORDINATES ( X / Y / Z ) AND CHARGE FOR SITE  5
      .0000000    -1.5033100     1.1529000      .4050000

 NUMBER OF    CL (-)   PARTICLES                        1
 NUMBER OF SITES IN    CL (-)                          1
 TOTAL CHARGE ON    CL (-)   IN A.U.                   -1.0000000
 CALCULATED MOLALITY FOR    CL (-)                     .1401652
 CALCULATED MOLARITY FOR    CL (-)                     .1679245

 TOTAL NUMBER OF PARTICLES IN THE BOX                  217
 TOTAL NUMBER OF DIFFERENT SITES                       6
 TOTAL NUMBER OF COORDINATES IN THE BOX                3243;  3894
 TOTAL CHARGE FOR THE SYSTEM IN A.U                    -1.0000000
 ACTIVE CHARGE-FACTORS ( DEFAULT FOR ALL )             1.0000000

 DENSITY IN THE SIMULATION-BOX IN G/CM**3              1.2040000
 EDGE-LENGTH OF THE SIMULATION-BOX IN ANG.             21.4641650

 TEMPERATURE IN KELVIN                                 305.1500000
 KT ( BOLTZMANN-FACTOR ) IN KCAL/MOL                   .6063941

 CUTOFF RADIUS FOR SHORT-RANGE TERMS IN ANG.           10.7320825
 MINIMAL DISTANCE OF MOLECULAR CENTERS (ANG.)          1.5000000
 MINIMAL DISTANCE OF MOLECULAR SITES (ANG.)            .5000000

 REQUESTED ACCEPTANCE RATIO (+CONF.)/(-CONF.)          .5000000
 START VALUE MAX. TRANSLATIONAL SHIFT ( ANG. )         ±.1250000
 START VALUE MAX. ANGULAR SHIFT ( RAD )                ±.3022999
```

(DEGREES) ±17.3205081

USE OF EWALD-SUMMATION FOR 1/R INTERACTIONS ALL OFF
NUMBER OF IMAGINARY-BOXES/AXIS-DIRECTION(+/-) 2
EPSILON FOR ENERGY-CORRECTION (SURFACE-TERM) NO CORR.

CALCULATION OF RADIAL-DENSITY-VECTORS ON
RESOLUTION OF THE RDV'S IN ANG. (RDVRES) .0250000
NUMBER OF RDV- AND RDF-POINTS PER SITE-SITE 428
MAXIMUM DISTANCE FOR RDV'S AND RDF'S IN ANG 10.7125000
FREQUENCY OF CALC. OF RDF'S IN MACRO-STEPS 10
FORMAT-MODE FOR WRITING TO MC91CF.xxx PARALLEL

MAX. NUMBER OF ITERATION-STEPS (CONFIG.) 1000000
NUMBER OF ITERATION-STEPS PER MACRO-STEP 1000
ONLY ONE BREAK AFTER INITIALIZING (STEP 0)

MAX. NUMBER OF NNL CONSIDERED FOR CORRECTION 0

USED RANDOM-NUMBER-GENERATOR INTERNAL

LARGEST USED X FOR CALCULATION OF EXP(X) AND
SMALLEST USED -X FOR CALCULATION OF EXP(-X) : X = 88.0000000

FILE-NAME UNIT 9 (FORMATTED) MC91I
FILE-NAME UNIT 10 (UNFORMATTED) MC91IS
FILE-NAME UNIT 22 (UNFORMATTED) SRNG
FILE-NAME UNIT 11 (FORMATTED) MC91SC
UNIT 11 : READ STARTCONFIGURATION AS INPUT ON
UNIT 11 : UPDATE STARTCONFIGURATION ON
FILE-NAME UNIT 12 (FORMATTED) MC91CV
UNIT 12 : UPDATE RADIAL-DENSITY-VECTORS ON
FILE-NAME UNIT 15 (FORMATTED + APPEND) MCCON
UNIT 15 : EXPAND HISTORY EVERY MACRO-STEP ON
FILE-NAME UNIT 14 (FORMATTED + APPEND) MCENE
FILE-NAME UNIT 13 (FORMATTED + APPEND) MCOUT

TOTAL NUMBER OF INDEPENDENT TWO-PARTICLE INTERACTIONS 23436
TOTAL NUMBER OF INDEPENDENT SITE-SITE DISTANCES IN BOX 581580

EVALUATING DISTANCES AND ENERGIES :
START-ENERGY OF THE SYSTEM = -5411.2747028 KCAL/MOL

STATISTICS NR. 0 :
TOTAL NUMBER OF CONFIGURATIONS (LOOPS) : 0
ACCEPTED CONFIGURATIONS (+ CONFIG.) : 0
REJECTED CONFIGURATIONS (- CONFIG.) : 0

ALL ENERGIES IN KCAL / MOL :

```
 TOTAL SYSTEM-ENERGY :   -5411.2747045  (  /  217 =   -24.936750  ) .
   TOTAL SYSTEM-ENERGY-ALTERATION      :     -5411.27470445526615

---------------------- INTERACTION - ENERGIES ----------------------
| HYDROXYLAMI <-> HYDROXYLAMI : -5250.55814  ( NEW - OLD :  -5250.55814 ) |
| HYDROXYLAMI <-> HYDROXYLAMI / HYDROXYLAMI:        -24.3081395        |
| HYDROXYLAMI <-> HYDROXYLAMI /   PAIR   :          -.0565306        |
---------------------- INTERACTION - ENERGIES ----------------------
| HYDROXYLAMI <->   CL (-)   :  -160.71656  ( NEW - OLD :  -160.71656 ) |
| HYDROXYLAMI <->   CL (-)   / HYDROXYLAMI:          -.7440582        |
| HYDROXYLAMI <->   CL (-)   /   PAIR   :          -.7440582        |
---------------------- INTERACTION - ENERGIES ----------------------
|   CL (-)   <-> HYDROXYLAMI :  -160.71656  ( NEW - OLD :  -160.71656 ) |
|   CL (-)   <-> HYDROXYLAMI /  CL (-)  :        -160.7165630        |
|   CL (-)   <-> HYDROXYLAMI /   PAIR   :          -.7440582        |
---------------------- INTERACTION - ENERGIES ----------------------
|   CL (-)   <->   CL (-)   :     .00000  ( NEW - OLD :      .00000 ) |
|   CL (-)   <->   CL (-)   /  CL (-)  :           .0000000        |
|   CL (-)   <->   CL (-)   /   PAIR   :           .0000000        |
---------------------- INTERACTION - ENERGIES ----------------------
|   SUM OF INTERACTION-ENERGIES  -  SYSTEM-ENERGY  =     .00000000000    |
---------------------- INTERACTION - ENERGIES ----------------------

 RADIAL-DENSITY-VECTORS WRITTEN TO FILE MC91CV.

 SEED-VALUES ( STATUS ) OF RANDOM-NUMBER-GENERATOR STORED.

 RESTART-INFORMATIONS-FILE MC91IS UPDATED.


*** START-RUN FINISHED ! ***
```

Appendix VII

Radial Distribution Functions for the solvent

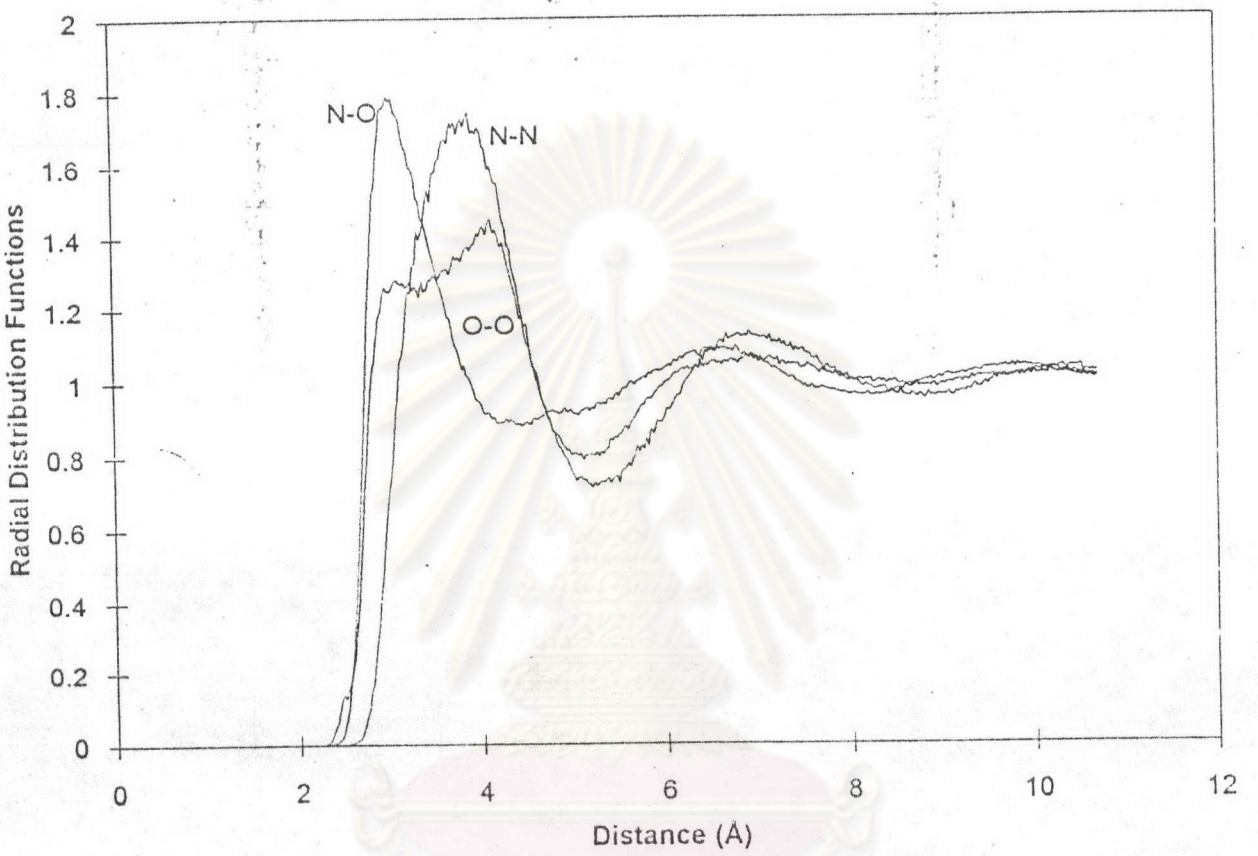

Figure (a) N-O, N-N, O-O

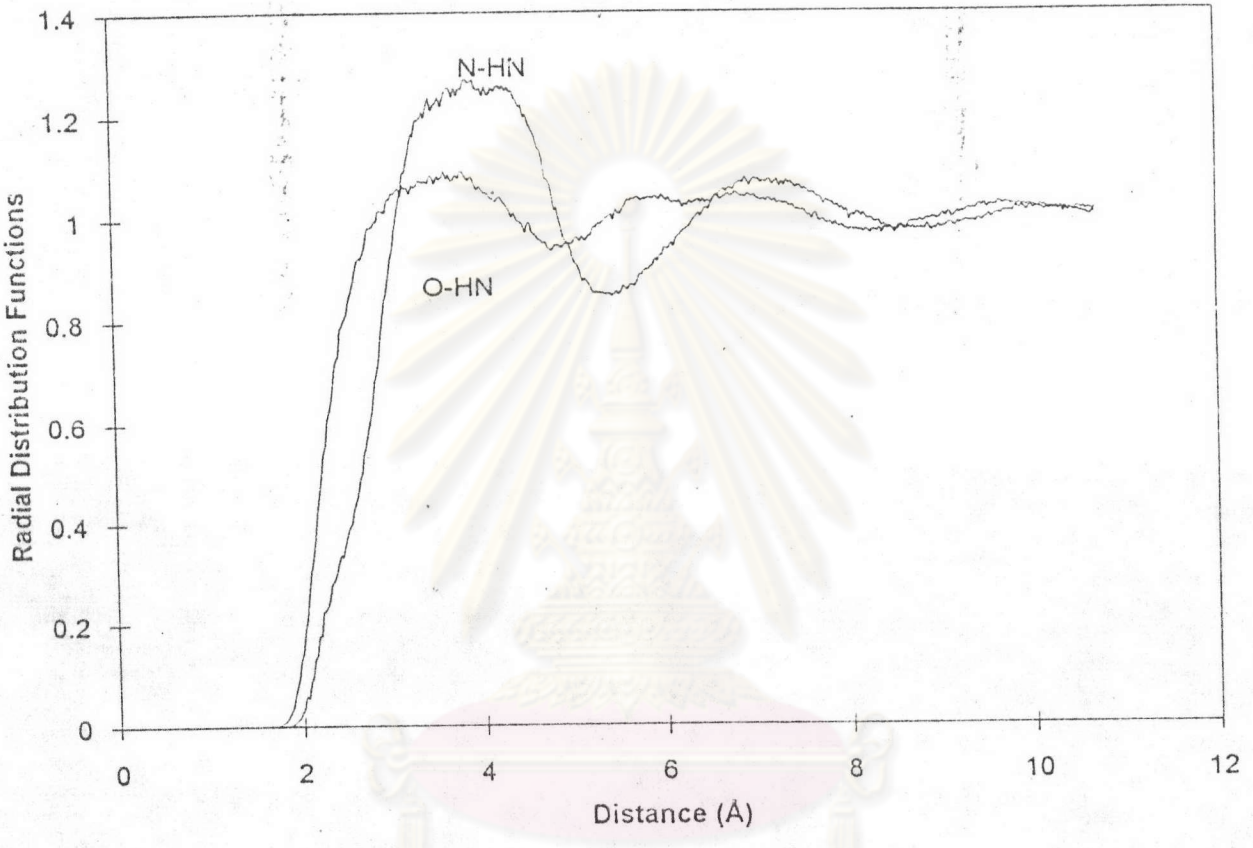

Figure (b) $N\text{-}H_N$, $O\text{-}H_N$

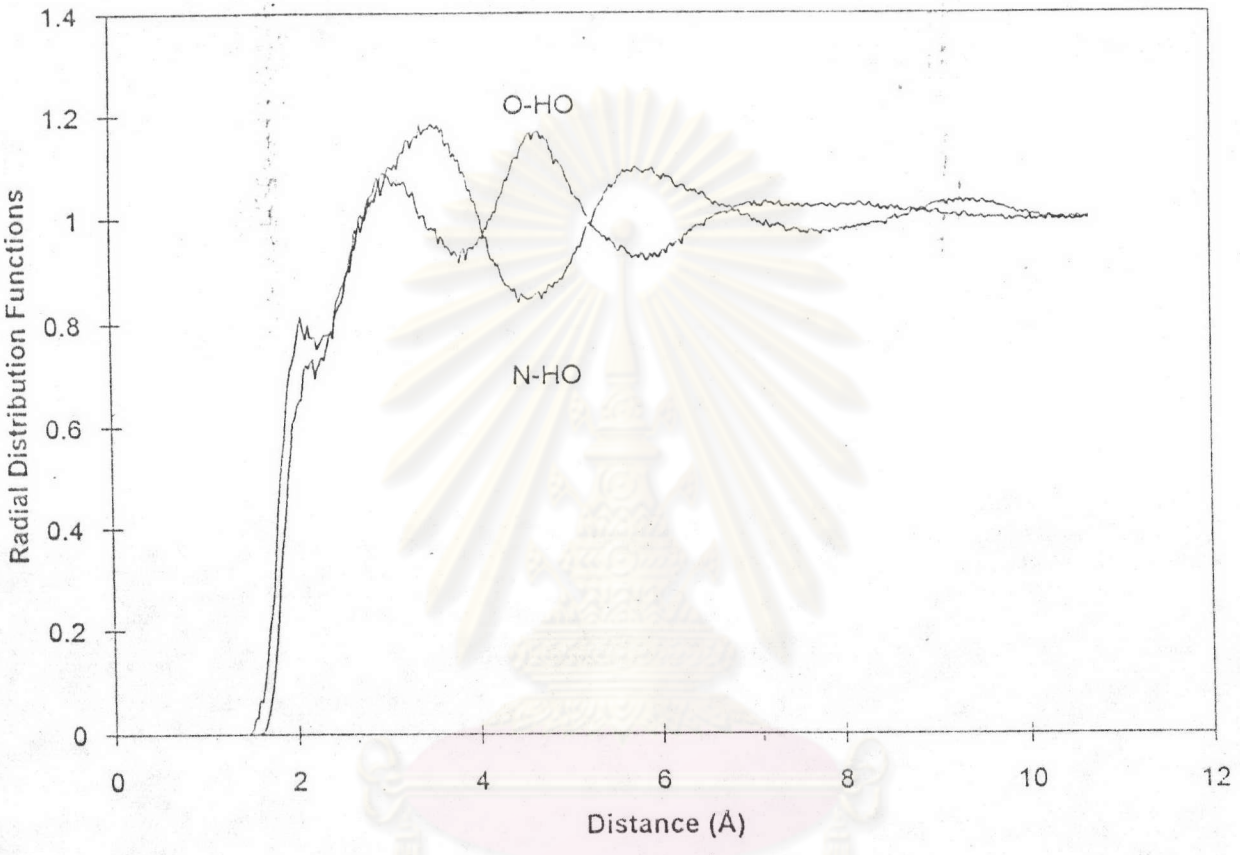

Figure (c) N-H_o, O-H_o

Appendix VIII

Coordination Number and Energy Distribution Programme for MC91 (C Programme)

```
#include <stdio.h>
#include <float.h>
#include <math.h>
#define eldim 21.4357     /* elementary box length       */
#define spec1 1      /* particles of species 1      */
#define az1 1
#define spec2 216       /* particles of species 2      */
#define az2 1
#define spec3 0       /* particles of species 3      */
#define az3 1
#define spec4 0       /* particles of species 4      */
#define az4 1
#define spec5 0       /* particles of species 5      */
#define az5 1
#define rm12 10.0       /* radius for 1st shell 2-1     */
#define erm12 5.0       /* radius for energy distribution 2-1     */
#define rm13 3.5       /* radius for 1st shell 3-1     */
#define rm25 3.4       /* radius for 1st shell 2-5     */
#define rm15 4.0      /* radius for 1st shell 1-5   */
#define rm35 3.5       /* radius for 1st shell 3-5     */
#define iupfak 1000      /* no. of history files to read */
#define mb 20          /* maximal coord. no. expected  */
#define elow12 -50.   /*lowest value for 2-1 interaction */
#define elow25 -300.  /*lowest value for 2-5 interaction */
#define mz  (spec1+spec2+spec3+spec4+spec5)

main(void)
{
float x[mz], y[mz],z[mz],alf[mz],bet[mz],gam[mz],rr,xx,yy,zz,r;
float xx1,xx2,yy1,yy2,zz1,zz2,rh1,rh2,xxs,yys,zzs,ewt;
float xx3,xx4,xx5,yy3,yy4,yy5,zz3,zz4,zz5,rh3,rh4;
float b12p[mb],b13p[mb],b25p[mb],b15p[mb],b35p[mb],e12p[mb];
float aco12,aco13,aco25,aco15,aco35,eco12,dum4[mz],dum6,dum7,dum8;
float h1x[spec2],h1y[spec2],h1z[spec2],o1x[spec2],o1y[spec2],o1z[spec2];
float h3x[spec2],h3y[spec2],h3z[spec2];
float h2x[spec2],h2y[spec2],h2z[spec2],estep12,estep25,kfloat,uli,oli;
int b12[mb],b13[mb],b25[mb],b15[mb],b35[mb],ctot,m1,m23,m1234,m12,m123;
int bct, i12,i15,i13,i25,i35,i,k,l,m,n,dum1[mz],dum2[mz],dum3[mz],dum5[mz];
int e12[mb],e25[mb],ect;
float nul, inc,nn;
```

```
char textline[132];
FILE *fn;
FILE *pf1;
FILE *pf2;
FILE *pf3;
FILE *pf4;
FILE *pf5;
FILE *pf6;
FILE *pf7;

float fuckmin (float cord);
float ene (float rr,float rh1, float rh2,float rh3,float rh4);
float fuck1 (float cord);

estep12 = elow12/20;
estep25 = elow25/20;
fn=fopen("MCCON","r");
for (n=0;n<mb;n++)
 {b12[n]=0;
 b13[n]=0;
 b25[n]=0;
 b15[n]=0;
 b35[n]=0;
 e12[n]=0;
 e25[n]=0;
 }

 m1=spec1;
 m12=spec1+spec2;
 m123=spec1+spec2+spec3;
 m1234=spec1+spec2+spec3+spec4;
 /* printf("mz,m1,m12,m123,m1234= %d %d %d %d %d\n",mz,m1,m12,m123,m1234); */
 for (i=1;i<iupfak+1;++i)     /* loop over history file(s) */
  {
   fgets(textline,132,fn); /* headlines to skip */
   fgets(textline,132,fn); /* headlines to skip */
   fgets(textline,132,fn); /* headlines to skip */
   for(k=0;k<mz;++k)
   {
    fscanf(fn,"%d %d %f %f %f %f %f %f %d %f
 %d",&dum1[k],&dum2[k],&alf[k],&bet[k],&gam[k],&x[k],&y[k],&z[k],&dum3[k],&du
 m4[k],&dum5[k]);
     if(k>=m1&&k<m12){
      fscanf(fn,"%f %f %f",&h1x[k],&h1y[k],&h1z[k]);
```

```
fscanf(fn,"%f %f %f",&h2x[k],&h2y[k],&h2z[k]);
fscanf(fn,"%f %f %f",&o1x[k],&o1y[k],&o1z[k]);
fscanf(fn,"%f %f %f",&h3x[k],&h3y[k],&h3z[k]);

/* this part has to be modified or extended if spec1#cf-water*/
/* or if other species are not 1-atomic (use at1..at5) */
}

}
/* The following two lines let you check the progress of long jobs */
/* you may erase them, if you are not interested in it */
/* printf("History file number %d read in\n",i); */
/* printf("Position: %ld\n",ftell(fn)); */
bct=0;
ect=0;
for(l=0;l<m1;++l)   /* evaluate species 2 with 1 */
{
 for(m=m1;m<m12;++m)
 {  xxs = fuck1(x[l]-x[m]);
    yys = fuck1(y[l]-y[m]);
    zzs = fuck1(z[l]-z[m]);
  xx = (x[l]+xxs)-x[m];
  yy = (y[l]+yys)-y[m];
  zz = (z[l]+zzs)-z[m];
  rr = xx*xx + yy*yy + zz*zz;

  xx1 = (h1x[l]+xxs)-x[m];
  yy1 = (h1y[l]+yys)-y[m];
  zz1 = (h1z[l]+zzs)-z[m];
  rh1 = xx1*xx1 + yy1*yy1 + zz1*zz1;
  xx2 = (h2x[l]+xxs)-x[m];
  yy2 = (h2y[l]+yys)-y[m];
  zz2 = (h2z[l]+zzs)-z[m];
  rh2 = xx2*xx2 + yy2*yy2 + zz2*zz2;
  xx4 = (h3x[l]+xxs)-x[m];
  yy4 = (h3y[l]+yys)-y[m];
  zz4 = (h3z[l]+zzs)-z[m];
  rh4 = xx3*xx3 + yy3*yy3 + zz3*zz3;
  xx3 = (o1x[l]+xxs)-x[m];
  yy3 = (o1y[l]+yys)-y[m];
  zz3 = (o1z[l]+zzs)-z[m];
  rh3 = xx4*xx4 + yy4*yy4 + zz4*zz4;
  if(rr<rm12*rm12)bct=bct+1;
  if(rr<erm12*erm12)
```

```
    {
    ewt=  ene(rr,rh1,rh2,rh3,rh4)/estep12;
    ect= floor(ewt);
    e12[ect]=e12[ect]+1;
    }
   }
  b12[bct]+=1;
  bct=0;
 }
}

fclose(fn);

/* normalize the baskets */

ctot=0;
for (i12=0;i12<mb;++i12) { ctot+=b12[i12];}
for (i12=0;i12<mb;++i12) { b12p[i12]=(float) b12[i12]*100./(float)ctot;}

ctot=0;
for (i12=0;i12<mb;++i12) { ctot+=e12[i12];}
for (i12=0;i12<mb;++i12) { e12p[i12]=(float) e12[i12]*100./(float)ctot;}

aco12=aco13=aco35=aco15=aco25=0.;
eco12=0.;
for (n=0;n<mb;++n)
 {aco12+=b12p[n]*n/100.;
  eco12+=e12p[n]*n*estep12/100.;
 }
/* print results */

 printf("\n\n PERCENTUAL OCCURRENCE OF COORDINATION
NUMBERS\n\n\n");
 printf("\n   Species 2  by  Species 1  :\n\n");
 for (k=0;k<mb;++k) {printf("Coord.No. %2d    %.2f  percent\n",k,b12p[k]);}
 printf("  ");
 printf("Limit = %.2f A     Av.Coord.No. = %.2f  \n\n",rm12,aco12);


 printf("\n\n PERCENTUAL DISTRIBUTION OF INTERACTION ENERGIES\n\n\n");
 printf("\n   Species 2  by  Species 1  :\n\n");
 for (k=0;k<mb;++k)
  {kfloat=(float)k;
```

```
uli= kfloat * estep12;
oli= uli + estep12;
/*  printf("kfloat,uli,oli = %f %f %f\n",kfloat,uli,oli); */
printf("E-Band No. %2d    %.2f  percent ",k+1,e12p[k]);
printf("  ( %.1f to %.1f kcal/mole )\n",uli,oli);
}
printf("  ");
printf("Limit = %.2f A     Av.Energy = %.2f  \n\n",erm12,eco12);


/* Prepare data files for Histogram */


inc=0.5;
nul=0.;
pf1 =fopen("higra12.dat","w+");

for (n=0;n<mb;++n)
  {nn=(float)n;
  fprintf(pf1,"%f %f\n",nn-inc,nul);
  fprintf(pf1,"%f %f\n",nn-inc,b12p[n]);
  fprintf(pf1,"%f %f\n",nn+inc,b12p[n]);
  fprintf(pf1,"%f %f\n",nn+inc,nul);
  }
 close(pf1);

pf6 =fopen("egra12.dat","w+");

for (n=0;n<mb;++n)
  {nn=(float)n;
  fprintf(pf6,"%f %f\n",(nn-inc)*estep12,nul);
  fprintf(pf6,"%f %f\n",(nn-inc)*estep12,e12p[n]);
  fprintf(pf6,"%f %f\n",(nn+inc)*estep12,e12p[n]);
  fprintf(pf6,"%f %f\n",(nn+inc)*estep12,nul);
  }
 close(pf6);
}
float fuckmin (float cord)
{
float fuck,dcord;
dcord=(float) floor ((cord/eldim) + 0.5);
fuck= fabs(cord - dcord*eldim);
 /* printf("cord= %f,dcord= %f,fuck= %f\n",cord,dcord,fuck); */
return(fuck);
```

```
}

float fuck1 (float cord)
{
 float fucku,dcord;
 dcord=(float) floor ((cord/eldim)+0.5) ;
 fucku= -dcord*eldim;
  /* printf("cord= %f,dcord= %f,fucku= %f\n",cord,dcord,fucku); */
 return(fucku);
}


float ene (float rr,float rh1, float rh2,float rh3,float rh4)
{
 float energy,charn,charnh,charo,charoh;
 double rro,rrh1,rrh2,rrh3,rrh4;
 float A1N,A2N,A3N,A4N,A1H,A2H,A3H,A4H,A1O,A2O,A3O,A4O;
 float A1HO,A2HO,A3HO,A4HO,RSQ,CUTLIM;

          A1N = -2490.941;
          A2N = 6580.365;
          A3N = 2.145;
          A4N = 4743.527;
          A1H = -294.882;
          A2H = 377.458;
          A3H = 1.266;
          A4H = 499.368;
          A1O = 438.151;
          A2O = 553645.735;
          A3O = 4.829;
          A4O = -7202.369;
          A1HO = -659.565;
          A2HO = 690.983;
          A3HO = 1.472;
          A4HO = 1160.711;
      RSQ = rr;
      rro=sqrt((double)rr);
      rrh1=sqrt((double)rh1);
      rrh2=sqrt((double)rh2);
      rrh3=sqrt((double)rh3);
      rrh4=sqrt((double)rh4);
      CUTLIM = eldim/2.;

      if(rro==0.||rrh1==0.||rrh2==0.||rrh3==0.||rrh4==0.) return(0);
```

```
charn=332.15*-0.482 ;
charnh=332.15*0.301 ;
charo=332.15*-0.525 ;
charoh=332.15*0.405 ;
energy = charn/rro + charnh/rrh1 + charnh/rrh2
  + charo/rrh3 + charoh/rrh4;


      energy = energy + A1N*pow(rro,-4.)
        + A4N*pow(rro,-7.)
        + A1H*pow(rrh1,-4.)
        + A4H*pow(rrh1,-7.)
        + A1H*pow(rrh2,-4.)
        + A4H*pow(rrh2,-7.)
        + A1O*pow(rrh3,-4.)
        + A4O*pow(rrh3,-7.)
        + A1HO*pow(rrh4,-4.)
        + A4HO*pow(rrh4,-7.);
      if ( rro <= CUTLIM ) {
        energy = energy+A2N*exp(-A3N*rro)
            +A2H*exp(-A3H*rrh1)
            +A2H*exp(-A3H*rrh2)
            +A2O*exp(-A3O*rrh3)
            +A2HO*exp(-A3HO*rrh4);
            }

   if(energy >= 0.) energy=0.;
   if(energy < elow12)
    {
     /* printf("Low energy encountered: %f\n",energy); */
     /* printf("rro,rrh1,rrh2 = %f %f %f\n",rro,rrh1,rrh2);*/
     return(0);
    }
  /*   printf("Energy = %f\n",energy);  */
return(energy);
}
```

CURRICULUM VITAE

Pornthep Sompornpisut

1969	Born March, 31st in Bangkok, Thailand Father : Mr. Pornprasert Sompornpisut Mother : Mrs. Pornwipa Sompornpisut
1975-1981	Elementary School
1981-1987	Highschool (Chinoroswittayalai, Bangkok)
1987-1991	Bachelor of Science (Chemistry), Chulalongkorn University, Bangkok
1992-	Master degree study at Department of Chemistry, Chulalongkorn University, Bangkok

The paper which has been published in international journal out of this Master thesis is:

- "Li^+ in Liquid Hydroxylamine: Intermolecular Potential Function and Monte Carlo Simulation" ,

Sompornpisut P. , Kokpol S. U., and Rode B.M. Chem Phys. 7, 1993.