```
Distributed Data Interface kickoff program.
Initiating 2 compute processes on 2 nodes to run the following command:
C:\WinGAMESS/gamess.10.exe water_sym

         ***************************************************
         *         GAMESS VERSION =  1 OCT 2010 (R1)       *
         *             FROM IOWA STATE UNIVERSITY          *
         * M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT, *
         *   M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,   *
         *          K.A.NGUYEN, S.J.SU, T.L.WINDUS,          *
         *       TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY      *
         *         J.COMPUT.CHEM.  14, 1347-1363(1993)       *
         *************** 32 BIT LINUX VERSION ***************

 SINCE 1993, STUDENTS AND POSTDOCS WORKING AT IOWA STATE UNIVERSITY
 AND ALSO IN THEIR VARIOUS JOBS AFTER LEAVING ISU HAVE MADE IMPORTANT
 CONTRIBUTIONS TO THE CODE:
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 ADDITIONAL CODE HAS BEEN PROVIDED BY COLLABORATORS IN OTHER GROUPS:
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    MIE UNIVERSITY: HIROAKI UMEDA
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         OLIVIER QUINET, BENOIT CHAMPAGNE
    UNIVERSITY OF CALIFORNIA - SANTA BARBARA: BERNARD KIRTMAN
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         SHARON HAMMES-SCHIFFER
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    UNIVERSITY OF NEBRASKA:
         PEIFENG SU, DEJUN SI, YALI WANG, HUI LI
    UNIVERSITY OF ZURICH:
         ROBERTO PEVERATI, KIM BALDRIDGE
    N. COPERNICUS UNIVERSITY AND JACKSON STATE UNIVERSITY:
         MARIA BARYSZ


PARALLEL VERSION RUNNING ON     2 PROCESSORS IN     2 NODES.

EXECUTION OF GAMESS BEGUN Mon Apr 11 13:58:57 2011

           ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD>!   File created by MacMolPlt 7.4
INPUT CARD> $CONTRL SCFTYP=RHF RUNTYP=ENERGY MAXIT=30 MULT=1 $END
INPUT CARD> $SYSTEM TIMLIM=525600 MEMORY=1000000 $END
INPUT CARD> $BASIS GBASIS=STO NGAUSS=3 $END
INPUT CARD> $SCF DIRSCF=.TRUE. $END
INPUT CARD> $DATA
INPUT CARD>Title
INPUT CARD>CNV 2
INPUT CARD>
INPUT CARD>O     8.0     0.00000     0.00000    -0.06673
INPUT CARD>H     1.0     0.76334     0.00000     0.52965
INPUT CARD> $END
   1000000 WORDS OF MEMORY AVAILABLE
```

```
    BASIS OPTIONS
    -------------
    GBASIS=STO          IGAUSS=       3      POLAR=NONE
    NDFUNC=       0     NFFUNC=       0     DIFFSP=       F
    NPFUNC=       0      DIFFS=       F     BASNAM=


    RUN TITLE
    ---------
Title

THE POINT GROUP OF THE MOLECULE IS CNV
THE ORDER OF THE PRINCIPAL AXIS IS     2

ATOM      ATOMIC                      COORDINATES (BOHR)
          CHARGE         X                Y                Z
O           8.0     0.0000000000        0.0000000000       -0.1261014152
H           1.0    -1.4425034355        0.0000000000        1.0008933694
H           1.0     1.4425034355        0.0000000000        1.0008933694

         INTERNUCLEAR DISTANCES (ANGS.)
         ------------------------------

               1 O          2 H          3 H

  1 O       0.0000000    0.9686883 *  0.9686883 *
  2 H       0.9686883 *  0.0000000    1.5266800 *
  3 H       0.9686883 *  1.5266800 *  0.0000000

 * ... LESS THAN  3.000


    ATOMIC BASIS SET
    ----------------
THE CONTRACTED PRIMITIVE FUNCTIONS HAVE BEEN UNNORMALIZED
THE CONTRACTED BASIS FUNCTIONS ARE NOW NORMALIZED TO UNITY

 SHELL TYPE  PRIMITIVE        EXPONENT          CONTRACTION COEFFICIENT(S)

O

     1   S       1           130.7093214    0.154328967295
     1   S       2            23.8088661    0.535328142282
     1   S       3             6.4436083    0.444634542185

     2   L       4             5.0331513   -0.099967229187    0.155916274999
     2   L       5             1.1695961    0.399512826089    0.607683718598
     2   L       6             0.3803890    0.700115468880    0.391957393099

H

     4   S       7             3.4252509    0.154328967295
     4   S       8             0.6239137    0.535328142282
     4   S       9             0.1688554    0.444634542185

TOTAL NUMBER OF BASIS SET SHELLS             =    4
NUMBER OF CARTESIAN GAUSSIAN BASIS FUNCTIONS =    7
NUMBER OF ELECTRONS                          =   10
CHARGE OF MOLECULE                           =    0
SPIN MULTIPLICITY                            =    1
NUMBER OF OCCUPIED ORBITALS (ALPHA)          =    5
NUMBER OF OCCUPIED ORBITALS (BETA )          =    5
TOTAL NUMBER OF ATOMS                        =    3
THE NUCLEAR REPULSION ENERGY IS       9.0871358664

    $CONTRL OPTIONS
    ---------------
SCFTYP=RHF          RUNTYP=ENERGY       EXETYP=RUN
MPLEVL=       0     CITYP =NONE         CCTYP =NONE         VBTYP =NONE
DFTTYP=NONE         TDDFT =NONE
MULT  =       1     ICHARG=       0     NZVAR =       0     COORD =UNIQUE
PP    =NONE         RELWFN=NONE         LOCAL =NONE         NUMGRD=       F
ISPHER=      -1     NOSYM =       0     MAXIT =      30     UNITS =ANGS
PLTORB=       F     MOLPLT=       F     AIMPAC=       F     FRIEND=
NPRINT=       7     IREST =       0     GEOM  =INPUT
NORMF =       0     NORMP =       0     ITOL  =      20     ICUT  =       9
INTTYP=BEST         GRDTYP=BEST         QMTTOL= 1.0E-06

    $SYSTEM OPTIONS
    ---------------
 REPLICATED MEMORY=     1000000 WORDS (ON EVERY NODE).
DISTRIBUTED MEMDDI=           0 MILLION WORDS IN AGGREGATE,
MEMDDI DISTRIBUTED OVER   2 PROCESSORS IS           0 WORDS/PROCESSOR.
TOTAL MEMORY REQUESTED ON EACH PROCESSOR=     1000000 WORDS.
```

```
TIMLIM=      525600.00 MINUTES, OR     365.0 DAYS.
PARALL= T  BALTYP=  DLB     KDIAG=    0  COREFL= F
MXSEQ2=     300 MXSEQ3=     150

         ----------------
         PROPERTIES INPUT
         ----------------

    MOMENTS            FIELD           POTENTIAL          DENSITY
IEMOM =       1   IEFLD =       0   IEPOT =       0   IEDEN =       0
WHERE =COMASS     WHERE =NUCLEI     WHERE =NUCLEI     WHERE =NUCLEI
OUTPUT=BOTH       OUTPUT=BOTH       OUTPUT=BOTH       OUTPUT=BOTH
IEMINT=       0   IEFINT=       0                     IEDINT=       0
                                                      MORB  =       0
         EXTRAPOLATION IN EFFECT
ORBITAL PRINTING OPTION: NPREO=     1     7     2     1

    ------------------------------
    INTEGRAL TRANSFORMATION OPTIONS
    ------------------------------
    NWORD  =            0
    CUTOFF = 1.0E-09     MPTRAN =       0
    DIRTRF =       T     AOINTS =DUP

         ----------------------
         INTEGRAL INPUT OPTIONS
         ----------------------
NOPK  =       1 NORDER=       0 SCHWRZ=       T

    ----------------------------------------
    THE POINT GROUP IS CNV, NAXIS= 2, ORDER= 4
    ----------------------------------------

    DIMENSIONS OF THE SYMMETRY SUBSPACES ARE
A1  =    4     A2  =    0     B1  =    2     B2  =    1

..... DONE SETTING UP THE RUN .....
CPU     0: STEP CPU TIME=     0.02 TOTAL CPU TIME=        0.0 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.0 SECONDS, CPU UTILIZATION IS  93.75%

         ********************
         1 ELECTRON INTEGRALS
         ********************
...... END OF ONE-ELECTRON INTEGRALS ......
CPU     0: STEP CPU TIME=     0.00 TOTAL CPU TIME=        0.0 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.0 SECONDS, CPU UTILIZATION IS  93.75%

         -------------
         GUESS OPTIONS
         -------------
         GUESS =HUCKEL            NORB  =       0          NORDER=       0
         MIX   =       F          PRTMO =       F          PUNMO =       F
         TOLZ  = 1.0E-08          TOLE  = 1.0E-05
         SYMDEN=       F          PURIFY=       F

INITIAL GUESS ORBITALS GENERATED BY HUCKEL   ROUTINE.
HUCKEL GUESS REQUIRES      2569 WORDS.

SYMMETRIES FOR INITIAL GUESS ORBITALS FOLLOW.   BOTH SET(S).
    5 ORBITALS ARE OCCUPIED (    1 CORE ORBITALS).
    2=A1       3=B1       4=A1       5=B2       6=B1       7=A1
...... END OF INITIAL ORBITAL SELECTION ......
CPU     0: STEP CPU TIME=     0.00 TOTAL CPU TIME=        0.0 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.0 SECONDS, CPU UTILIZATION IS  93.75%

                  ----------------------
                  AO INTEGRAL TECHNOLOGY
                  ----------------------
    S,P,L SHELL ROTATED AXIS INTEGRALS, REPROGRAMMED BY
       KAZUYA ISHIMURA (IMS) AND JOSE SIERRA (SYNSTAR).
    S,P,D,L SHELL ROTATED AXIS INTEGRALS PROGRAMMED BY
       KAZUYA ISHIMURA (INSTITUTE FOR MOLECULAR SCIENCE).
    S,P,D,F,G SHELL TO TOTAL QUARTET ANGULAR MOMENTUM SUM 5,
       ERIC PROGRAM BY GRAHAM FLETCHER (ELORET AND NASA ADVANCED
       SUPERCOMPUTING DIVISION, AMES RESEARCH CENTER).
    S,P,D,F,G,L SHELL GENERAL RYS QUADRATURE PROGRAMMED BY
       MICHEL DUPUIS (PACIFIC NORTHWEST NATIONAL LABORATORY).

         --------------------
         2 ELECTRON INTEGRALS
         --------------------

DIRECT SCF METHOD SKIPS INTEGRAL STORAGE ON DISK.
DIRECT TRANSFORMATION SKIPS AO INTEGRAL STORAGE ON DISK.
 ...... END OF TWO-ELECTRON INTEGRALS .....
```

```
CPU     0: STEP CPU TIME=     0.05 TOTAL CPU TIME=        0.1 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.1 SECONDS, CPU UTILIZATION IS  79.49%

         -------------------------
                RHF SCF CALCULATION
         -------------------------

    NUCLEAR ENERGY =         9.0871358664
    MAXIT =   30     NPUNCH=    2
    EXTRAP=T  DAMP=F  SHIFT=F  RSTRCT=F  DIIS=F  DEM=F  SOSCF=F
    DENSITY MATRIX CONV=  2.00E-05
    MEMORY REQUIRED FOR RHF ITERS=     44817 WORDS.

DIRECT SCF CALCULATION, SCHWRZ=T   FDIFF=T,  DIRTHR=  0.00E+00 NITDIR=10
SCHWARZ INEQUALITY OVERHEAD:        28 INTEGRALS, T=        0.00

                                                                                NONZERO     BLOCKS
ITER EX DEM     TOTAL ENERGY        E CHANGE  DENSITY CHANGE    DIIS ERROR    INTEGRALS    SKIPPED
  1  0  0      -74.7974092796   -74.7974092796   0.596869468   0.000000000          141          0
  2  1  0      -74.9507257506    -0.1533164709   0.181657794   0.000000000          141          0
  3  2  0      -74.9629281338    -0.0122023833   0.059598419   0.000000000          141          0
  4  3  0      -74.9642035242    -0.0012753904   0.020216252   0.000000000          141          0
  5  4  0      -74.9643795359    -0.0001760117   0.007366384   0.000000000          141          0
  6  0  0      -74.9644088533    -0.0000293174   0.004742101   0.000000000          141          0
  7  1  0      -74.9644154231    -0.0000065699   0.000070104   0.000000000          141          0
  8  2  0      -74.9644154252    -0.0000000021   0.000025327   0.000000000          141          0
  9  3  0      -74.9644154256    -0.0000000003   0.000009752   0.000000000          141          0

         -----------------
         DENSITY CONVERGED
         -----------------
    TIME TO FORM FOCK OPERATORS=       0.0 SECONDS (       0.0 SEC/ITER)
    FOCK TIME ON FIRST ITERATION=       0.0, LAST ITERATION=       0.0
    TIME TO SOLVE SCF EQUATIONS=       0.0 SECONDS (       0.0 SEC/ITER)

FINAL RHF ENERGY IS      -74.9644154256 AFTER   9 ITERATIONS

         ------------
         EIGENVECTORS
         ------------

                    1          2          3          4          5
                -20.2438    -1.2632    -0.6111    -0.4529    -0.3909
                   A1         A1         B1         A1         B2
   1  O  1  S    0.994158  -0.233200  -0.000000   0.102889   0.000000
   2  O  1  S    0.026315   0.837618  -0.000000  -0.534598   0.000000
   3  O  1  X   -0.000000   0.000000   0.606792  -0.000000   0.000000
   4  O  1  Y   -0.000000   0.000000  -0.000000  -0.000000   1.000000
   5  O  1  Z    0.004251   0.126155  -0.000000   0.772609   0.000000
   6  H  2  S   -0.005841   0.157816  -0.446042   0.282964   0.000000
   7  H  3  S   -0.005841   0.157816   0.446042   0.282964   0.000000

                    6          7
                 0.5952     0.7274
                   A1         B1
   1  O  1  S   -0.130529   0.000000
   2  O  1  S    0.863693   0.000000
   3  O  1  X    0.000000   0.982566
   4  O  1  Y    0.000000   0.000000
   5  O  1  Z    0.744429   0.000000
   6  H  2  S   -0.788315   0.828700
   7  H  3  S   -0.788315  -0.828700
...... END OF RHF CALCULATION ......
CPU     0: STEP CPU TIME=     0.00 TOTAL CPU TIME=        0.1 (    0.0 MIN)
TOTAL WALL CLOCK TIME=        0.1 SECONDS, CPU UTILIZATION IS  79.49%

    ---------------------------------------------------------------
    PROPERTY VALUES FOR THE RHF   SELF-CONSISTENT FIELD WAVEFUNCTION
    ---------------------------------------------------------------

         -----------------
         ENERGY COMPONENTS
         -----------------

        WAVEFUNCTION NORMALIZATION =       1.0000000000

              ONE ELECTRON ENERGY =    -122.1793235802
              TWO ELECTRON ENERGY =      38.1277722882
         NUCLEAR REPULSION ENERGY =       9.0871358664
                                    ------------------
                     TOTAL ENERGY =     -74.9644154256

ELECTRON-ELECTRON POTENTIAL ENERGY =      38.1277722882
 NUCLEUS-ELECTRON POTENTIAL ENERGY =    -196.7417484352
  NUCLEUS-NUCLEUS POTENTIAL ENERGY =       9.0871358664
```

```
                                    ------------------
           TOTAL POTENTIAL ENERGY =    -149.5268402806
             TOTAL KINETIC ENERGY =      74.5624248550
               VIRIAL RATIO (V/T) =       2.0053913291

 ...... PI ENERGY ANALYSIS ......

ENERGY ANALYSIS:
          FOCK ENERGY=    -45.9237766278
         BARE H ENERGY=   -122.1793235802
    ELECTRONIC ENERGY =    -84.0515501040
        KINETIC ENERGY=     74.5624248550
         N-N REPULSION=      9.0871358664
          TOTAL ENERGY=    -74.9644142376
       SIGMA PART(1+2)=    -76.2127294486
             (K,V1,2)=     69.5049624030   -176.7884643168     31.0707724652
          PI PART(1+2)=     -7.8388206554
             (K,V1,2)=      5.0574624520    -19.9532841185      7.0570010110
 SIGMA SKELETON, ERROR=    -67.1255935822      0.0000000000
           MIXED PART= 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
...... END OF PI ENERGY ANALYSIS ......

         ---------------------------------------
         MULLIKEN AND LOWDIN POPULATION ANALYSES
         ---------------------------------------

    ATOMIC MULLIKEN POPULATION IN EACH MOLECULAR ORBITAL

                      1          2          3          4          5

                  2.000000   2.000000   2.000000   2.000000   2.000000

   1              2.001361   1.617307   1.068623   1.667555   2.000000
   2             -0.000680   0.191347   0.465688   0.166222   0.000000
   3             -0.000680   0.191347   0.465688   0.166222   0.000000

              ----- POPULATIONS IN EACH AO -----
                            MULLIKEN      LOWDIN
              1  O  1  S      1.99768     1.99607
              2  O  1  S      1.83410     1.68593
              3  O  1  X      1.06862     1.09728
              4  O  1  Y      2.00000     2.00000
              5  O  1  Z      1.45445     1.46728
              6  H  2  S      0.82258     0.87672
              7  H  3  S      0.82258     0.87672

         ----- MULLIKEN ATOMIC OVERLAP POPULATIONS -----
         (OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

            1          2          3

   1    7.8326767
   2    0.2610849   0.6079246
   3    0.2610849  -0.0464327   0.6079246

         TOTAL MULLIKEN AND LOWDIN ATOMIC POPULATIONS
      ATOM         MULL.POP.    CHARGE          LOW.POP.     CHARGE
   1 O             8.354846   -0.354846         8.246557   -0.246557
   2 H             0.822577    0.177423         0.876722    0.123278
   3 H             0.822577    0.177423         0.876722    0.123278

         -------------------------------
         BOND ORDER AND VALENCE ANALYSIS     BOND ORDER THRESHOLD=0.050
         -------------------------------

                  BOND                        BOND                        BOND
 ATOM PAIR DIST  ORDER      ATOM PAIR DIST  ORDER      ATOM PAIR DIST  ORDER
   1   2  0.969  0.957        1   3  0.969  0.957

                     TOTAL       BONDED        FREE
      ATOM           VALENCE     VALENCE     VALENCE
   1 O                 1.913       1.913       0.000
   2 H                 0.969       0.969       0.000
   3 H                 0.969       0.969       0.000

         ---------------------
         ELECTROSTATIC MOMENTS
         ---------------------

POINT   1           X           Y           Z (BOHR)    CHARGE
              0.000000    0.000000    0.000026        0.00 (A.U.)
         DX          DY          DZ          /D/  (DEBYE)
    0.000000    0.000000    1.713972    1.713972
...... END OF PROPERTY EVALUATION ......
CPU     0: STEP CPU TIME=     0.02 TOTAL CPU TIME=        0.1 (    0.0 MIN)
```

```
 TOTAL WALL CLOCK TIME=        0.1 SECONDS, CPU UTILIZATION IS  81.91%
      580000  WORDS OF DYNAMIC MEMORY USED
 EXECUTION OF GAMESS TERMINATED NORMALLY Mon Apr 11 13:58:57 2011
 DDI: 263224 bytes (0.3 MB / 0 MWords) used by master data server.

 ----------------------------------------
 CPU timing information for all processes
 ========================================
 0: 0.171 + 0.62 = 0.233
 1: 0.140 + 0.00 = 0.140
 2: 0.00 + 0.15 = 0.15
 3: 0.00 + 0.31 = 0.31
 ----------------------------------------
 ddikick.x: exited gracefully.
----- accounting info -----
```