付録Ⅰ　出力ファイルの見方－過酸化水素の場合

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 ** [MOPAC] Ver.6 ;                    by Dr. James J.P. Stewart,      **
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 ** MOPAC6.03 ON Windows95,NT,XP ;          by N.Senda(Tencube)  2008.04.26 **
 *******************************************************************************

                          PM3 CALCULATION RESULTS
  Winmostar

 *******************************************************************************
 *         MOPAC:  VERSION  6.03              CALC'D. 09-Jun-09
 *  VECTORS  - FINAL EIGENVECTORS TO BE PRINTED
 *  BONDS    - FINAL BOND-ORDER MATRIX TO BE PRINTED
 *  GEO-OK   - OVERRIDE INTERATOMIC DISTANCE CHECK
 *  GRAPH    - GENERATE FILE FOR GRAPHICS
 *   T=      - A TIME OF  3600.0 SECONDS REQUESTED
 *  DUMP=N   - RESTART FILE WRITTEN EVERY  3600.0 SECONDS
 *  EF       - USE EF ROUTINE FOR MINIMUM SEARCH
 *  PM3      - THE PM3 HAMILTONIAN TO BE USED
 *  PRECISE  - CRITERIA TO BE INCREASED BY 100 TIMES
 *  NOINTER  - INTERATOMIC DISTANCES NOT TO BE PRINTED
 *  GNORM=   - EXIT WHEN GRADIENT NORM DROPS BELOW .500E-01
 *******************************************************************************070BY090
 0
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 PM3 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS BONDS GEO-OK  ←指定したキーワード

 Winmostar

   ATOM   CHEMICAL  BOND LENGTH    BOND ANGLE     TWIST ANGLE
   NUMBER  SYMBOL    (ANGSTROMS)     (DEGREES)      (DEGREES)
   (I)               NA:I         NB:NA:I      NC:NB:NA:I     NA   NB   NC

     1     O
     2     O        1.41620  *                                  1
     3     H         .96000  *    101.70310  *                  1    2          ←入力データ
     4     H         .96000  *    101.70310  *  150.00000  *    2    1    3

        CARTESIAN COORDINATES

    NO.       ATOM        X         Y         Z

     1         O        .0000     .0000     .0000
     2         O       1.4162     .0000     .0000                                ←XYZ 座標値
     3         H       -.1947     .9400     .0000
     4         H       1.6109    -.8141     .4700
 H: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).          ←使用パラメータの出典
 O: (PM3): J. J. P. STEWART, J. COMP. CHEM.     10, 209 (1989).

        RHF CALCULATION, NO. OF DOUBLY OCCUPIED LEVELS =  7
 CYCLE:   1 TIME:    .00 TIME LEFT:   3600.0 GRAD.:    34.495 HEAT:-38.79316
 CYCLE:   2 TIME:    .00 TIME LEFT:   3600.0 GRAD.:    24.431 HEAT:-39.31034
 CYCLE:   3 TIME:    .02 TIME LEFT:   3600.0 GRAD.:    19.178 HEAT:-40.06055
 CYCLE:   4 TIME:    .00 TIME LEFT:   3600.0 GRAD.:    16.372 HEAT:-40.23603
 CYCLE:   5 TIME:    .00 TIME LEFT:   3600.0 GRAD.:     3.843 HEAT:-40.44753
 CYCLE:   6 TIME:    .00 TIME LEFT:   3600.0 GRAD.:     1.972 HEAT:-40.45535
 CYCLE:   7 TIME:    .02 TIME LEFT:   3600.0 GRAD.:     1.806 HEAT:-40.45936
 CYCLE:   8 TIME:    .00 TIME LEFT:   3600.0 GRAD.:     2.314 HEAT:-40.46496     ←計算の収束過程
 CYCLE:   9 TIME:    .00 TIME LEFT:   3600.0 GRAD.:     2.972 HEAT:-40.47186
 CYCLE:  10 TIME:    .02 TIME LEFT:   3600.0 GRAD.:     4.039 HEAT:-40.48376
 CYCLE:  11 TIME:    .00 TIME LEFT:   3600.0 GRAD.:     5.952 HEAT:-40.50786
 CYCLE:  12 TIME:    .02 TIME LEFT:   3599.9 GRAD.:     8.715 HEAT:-40.55837
 CYCLE:  13 TIME:    .00 TIME LEFT:   3599.9 GRAD.:    10.631 HEAT:-40.64389
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CYCLE:  14 TIME:    .02 TIME LEFT:   3599.9 GRAD.:    8.372 HEAT:-40.73147
CYCLE:  15 TIME:    .00 TIME LEFT:   3599.9 GRAD.:    3.207 HEAT:-40.77332
CYCLE:  16 TIME:    .00 TIME LEFT:   3599.9 GRAD.:     .539 HEAT:-40.77835
CYCLE:  17 TIME:    .02 TIME LEFT:   3599.9 GRAD.:     .073 HEAT:-40.77849
CYCLE:  18 TIME:    .00 TIME LEFT:   3599.9 GRAD.:     .010 HEAT:-40.77849
```

←計算が収束した！

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PM3 EF PRECISE GNORM=0.05 NOINTER GRAPHF VECTORS BONDS GEO-OK

Winmostar

   GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
   SCF FIELD WAS ACHIEVED

                    PM3    CALCULATION
                                VERSION  6.03
                                09-Jun-09

      FINAL HEAT OF FORMATION =       -40.77849 KCAL
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←標準生成エンタルピーの計算値

```
      TOTAL ENERGY            =      -616.28331 EV
      ELECTRONIC ENERGY       =     -1151.31038 EV
      CORE-CORE REPULSION     =       535.02707 EV

      IONIZATION POTENTIAL    =        11.60220
      NO. OF FILLED LEVELS    =        7
      MOLECULAR WEIGHT        =     34.015

      SCF CALCULATIONS  =             19
      COMPUTATION TIME =    .094 SECONDS
```

←全エネルギー
←電子エネルギー
←核反発エネルギー
←イオン化ポテンシャル
←分子量

```
  ATOM   CHEMICAL  BOND LENGTH    BOND ANGLE     TWIST ANGLE
 NUMBER  SYMBOL    (ANGSTROMS)    (DEGREES)      (DEGREES)
 (I)               NA:I        NB:NA:I     NC:NB:NA:I     NA   NB   NC

   1     O
   2     O       1.48195  *                                  1
   3     H        .94450  *     96.48942  *                  1    2
   4     H        .94450  *     96.49018  * -179.97740  *    2    1    3
```

←最適構造の核間距離および結合角，二面角

```
          EIGENVECTORS

  ROOT NO.    1         2         3         4         5         6
       -36.42348  -32.90999  -18.40264  -17.01393  -14.48160  -14.27379

 S  O   1   .63424    -.65078    -.21400    -.04405    -.00067     .23595
PX  O   1   .12347     .10086    -.01201     .66841     .00059    -.19432
PY  O   1   .06069    -.09184     .57259    -.16055     .00152    -.54582
PZ  O   1  -.00001    -.00001     .00007     .00005    -.70710    -.00198

 S  O   2   .63424     .65078     .21399    -.04405    -.00067     .23595
PX  O   2  -.12347     .10086    -.01203    -.66841    -.00059     .19432
PY  O   2  -.06069    -.09184     .57259     .16053    -.00124     .54582
PZ  O   2  -.00003    -.00003     .00016     .00012    -.70711    -.00176

 S  H   3   .28073    -.24057     .35525    -.15975     .00090    -.32961

 S  H   4   .28074     .24057    -.35525    -.15974     .00090    -.32961
```

←分子軌道の番号
←分子軌道のエネルギー
←分子軌道における各原子軌道につく係数（重み）

```
 ROOT NO.   7         8         9        10

      -11.60220    1.57742    4.23870    4.78625

 S  O   1  -.00002    .13426   -.20031   -.11252
PX  O   1   .00000    .66135    .01504    .22868
PY  O   1   .00005    .15382   -.41548   -.37422
PZ  O   1  -.70711    .00000    .00000    .00000

 S  O   2   .00002   -.13427   -.20031    .11252
PX  O   2   .00000    .66135   -.01505    .22869
PY  O   2  -.00022    .15382    .41547   -.37423
PZ  O   2   .70711    .00006    .00016   -.00015

 S  H   3   .00004   -.14466    .53576    .54313

 S  H   4  -.00004    .14466    .53574   -.54314

        NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

     ATOM NO.   TYPE         CHARGE       ATOM  ELECTRON DENSITY
       1         O          -.2059         6.2059
       2         O          -.2059         6.2059          ←O 原子の部分電荷と電子数
       3         H           .2059          .7941
       4         H           .2059          .7941

DIPOLE          X        Y        Z      TOTAL
POINT-CHG.     .000     .000     .000     .000
HYBRID         .000     .000     .000     .000
SUM            .000     .000    -.001     .001          ←双極子モーメント

     CARTESIAN COORDINATES

  NO.       ATOM            X        Y        Z

   1         O             .0000    .0000    .0000
   2         O            1.4819    .0000    .0000      ←各原子の XYZ 座標値
   3         H            -.1067    .9384    .0000
   4         H            1.5887   -.9384   -.0004

     ATOMIC ORBITAL ELECTRON POPULATIONS    ←電子密度

 1.85837   1.02018   1.32735   2.00000   1.85837   1.02018   1.32735   2.00000
  .79410    .79410

     BONDING CONTRIBUTION OF EACH M.O.      ←各 MO の結合への寄与

 .8440   .6567  1.2326  1.9158   .0000  1.1771   .0000 -1.9613 -1.9369 -1.9280

          BOND ORDERS AND VALENCIES          ←下表に結合次数と原子価
            O 1          O 2          H 3          H 4
------------------------------------------------------------------------

   O   1  1.955504                                    ←O(1)の原子価は 1.955504
   O   2  1.001240   1.955504                         ←O(1)とO(2)の結合次数は 1.00124 次
   H   3   .949685   .004580   .957604                ←O(1)とH(3)の結合次数は 0.949685 次
   H   4   .004580   .949685   .003339   .957604      ←O(1)とH(4)との結合次数は 0.00458 次

     DATA FOR GRAPH WRITTEN TO DISK←図を書くためのデータはディスクに書き込んだ

TOTAL CPU TIME:          .09 SECONDS                  ←計算に 0.09 秒かかった
== MOPAC DONE ==                                      ←MOPAC 計算はできた！
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