Gaussianの使い方

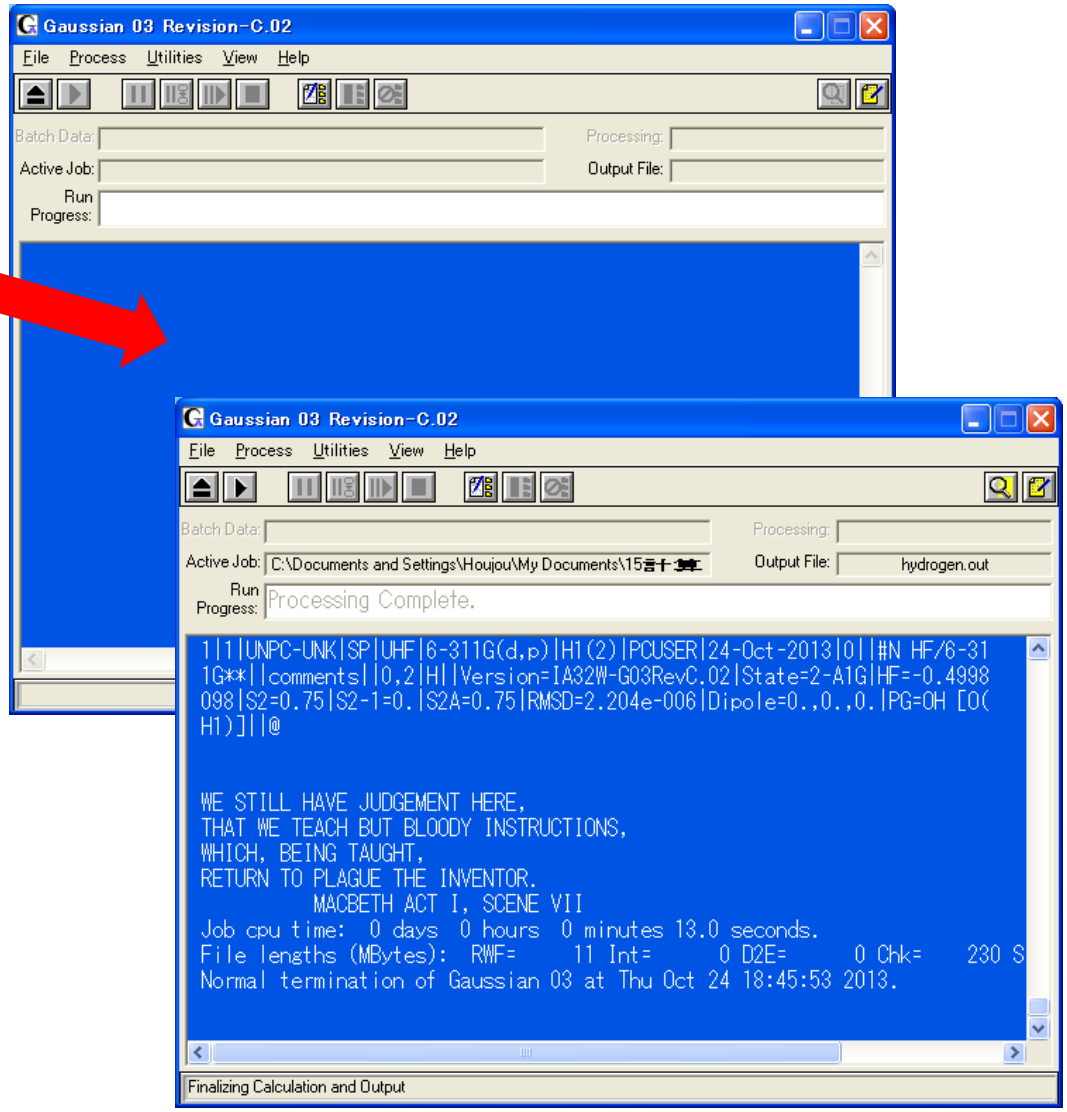
Hydrogen.gjf

```
%chk=default

#N HF/6-311G**

comments

0 2
H
```



入力ファイル

%chk=default	チェックポイントファイルの指定
#N HF/6-311G**	出力フォーマット(Normal, Print, Terse) Hartree-Fock法,6-311G**基底関数
comments	コメント
0 2	電荷、スピン多重度
H	元素記号

分子構造の情報

XYZ座標で指定

```
water molecule

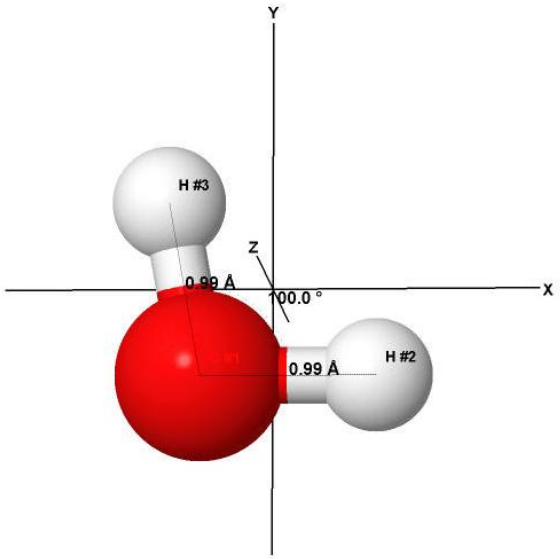
0 1
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
```

内部参照座標（Zマトリクス）で指定

```
water molecule

0 1
O
H 1 r2
H 1 r3   2 a3

r2 1.0
r3 1.0
a3 104.5
```



出力ファイル

注意書き

```
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開発者

```
Cite this work as:
Gaussian 03, Revision C.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Wallingford CT, 2004.
```

入力された情報にもとづく内容

```
*****************************************
Gaussian 03:  IA32W-G03RevC.02 12-Jun-2004
              26-Apr-2011
*****************************************
%chk=default
--------------
#N HF/6-311G**
--------------
1/38=1/1;
2/17=6,18=5,40=1/2;
3/5=4,6=6,7=101,11=9,16=1,25=1,30=1/1,2,3;
4//1;
5/5=2,32=1,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
99/5=1,9=1/99;
--------
comments
--------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 2
H

                         Input orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1             0        0.000000    0.000000    0.000000
---------------------------------------------------------------------
Stoichiometry    H(2)
Framework group  OH[O(H)]
Deg. of freedom     0
Full point group                 OH      NOp  48
Largest Abelian subgroup         D2H     NOp   8
Largest concise Abelian subgroup C1      NOp   1
                        Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic              Coordinates (Angstroms)
Number     Number      Type              X           Y           Z
---------------------------------------------------------------------
   1          1             0        0.000000    0.000000    0.000000
---------------------------------------------------------------------
```

基底関数について

```
Standard basis: 6-311G(d,p) (5D, 7F)
There are     3 symmetry adapted basis functions of AG  symmetry.
There are     0 symmetry adapted basis functions of B1G symmetry.
There are     0 symmetry adapted basis functions of B2G symmetry.
There are     0 symmetry adapted basis functions of B3G symmetry.
There are     0 symmetry adapted basis functions of AU  symmetry.
There are     1 symmetry adapted basis functions of B1U symmetry.
There are     1 symmetry adapted basis functions of B2U symmetry.
There are     1 symmetry adapted basis functions of B3U symmetry.
Integral buffers will be    262144 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
    6 basis functions,     8 primitive gaussians,     6 cartesian basis functions
    1 alpha electrons        0 beta electrons
      nuclear repulsion energy         0.0000000000 Hartrees.
```

6-311G**基底関数

・内殻電子軌道は6個のガウス関数の線形和

・価電子軌道は3個+1個+1個のガウス関数の線形和

・＊印はp軌道に対してd型の分極関数を加える（H以外）

・＊＊印はさらにHのs軌道にもp型の分極関数を加える

・Hの場合：1s, 2s, 3s軌道として3+1+1で3個の基底関数、5個の原始ガウス関数

4px, 4py, 4pz軌道として3個の基底関数、3個の原始ガウス関数

合計6個の基底関数、8個の原始ガウス関数

SCF計算について

```
 NAtoms=     1 NActive=     1 NUniq=     1 SFac= 1.00D+00 NAtFMM=    60 Big=F
 One-electron integrals computed using PRISM.
 NBasis=      6 RedAO= T  NBF=      3      0      0      0      0      1      1      1
 NBsUse=      6 1.00D-06 NBFU=      3      0      0      0      0      1      1      1
 Harris functional with IExCor=  205 diagonalized for initial guess.
 ExpMin= 1.03D-01 ExpMax= 3.39D+01 ExpMxC= 3.39D+01 IAcc=1 IRadAn=          1
AccDes= 1.00D-06
 HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=          1 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Initial guess orbital symmetries:
 Alpha Orbitals:
       Occupied  (A1G)
       Virtual   (A1G) (T1U) (T1U) (T1U) (A1G)
 Beta  Orbitals:
       Virtual   (A1G) (A1G) (T1U) (T1U) (T1U) (A1G)
 The electronic state of the initial guess is 2-A1G.
 <S**2> of initial guess= 0.7500
 Warning!  Cutoffs for single-point calculations used.
 Requested convergence on RMS density matrix=1.00D-04 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-02.
 Requested convergence on                 energy=5.00D-05.
 No special actions if energy rises.
 Keep R1 and R2 integrals in memory in canonical form, NReq=      419469.
 SCF Done:  E(UHF) = -0.499809815090     A.U. after    4 cycles
             Convg  =    0.2204D-05             -V/T =  2.0000
             S**2   =   0.7500
 Annihilation of the first spin contaminant:
 S**2 before annihilation     0.7500,   after     0.7500
```

スピンの計算値

$$\langle S^2 \rangle = s(s+1) = \frac{1}{2}\left(\frac{1}{2}+1\right)$$

$$= 0.75$$

SCFで収束したエネルギー
（解析解は－0.5 A.U.）

```
 ********************************************************************

           Population analysis using the SCF density.

 ********************************************************************

 Orbital symmetries:
 Alpha Orbitals:
       Occupied  (A1G)
       Virtual   (A1G) (T1U) (T1U) (T1U) (A1G)
 Beta  Orbitals:
       Virtual   (A1G) (A1G) (T1U) (T1U) (T1U) (A1G)
 The electronic state is 2-A1G.
 Alpha  occ. eigenvalues --   -0.49981
 Alpha virt. eigenvalues --    0.34890   1.49076   1.49076   1.49076   2.46995
  Beta virt. eigenvalues --    0.05625   0.49238   1.62201   1.62201   1.62201
  Beta virt. eigenvalues --    2.60147
          Condensed to atoms (all electrons):
                1
     1  H    1.000000
 Mulliken atomic charges:
                1
     1  H    0.000000
 Sum of Mulliken charges=   0.00000
 Atomic charges with hydrogens summed into heavy atoms:
                1
     1  H    0.000000
 Sum of Mulliken charges=   0.00000
          Atomic-Atomic Spin Densities.
                1
     1  H    1.000000
 Mulliken atomic spin densities:
                1
     1  H    1.000000
 Sum of Mulliken spin densities=   1.00000
 Electronic spatial extent (au):  <R**2>=     2.9910
 Charge=     0.0000 electrons
```

分子軌道係数をつかった解析

軌道エネルギー

ポピュレーション解析

分子軌道係数をつかった解析

多極子モーメント

```
Dipole moment (field-independent basis, Debye):
    X=      0.0000    Y=      0.0000    Z=      0.0000  Tot=      0.0000
Quadrupole moment (field-independent basis, Debye-Ang):
   XX=     -1.3410   YY=     -1.3410   ZZ=     -1.3410
   XY=      0.0000   XZ=      0.0000   YZ=      0.0000
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=      0.0000   YY=      0.0000   ZZ=      0.0000
   XY=      0.0000   XZ=      0.0000   YZ=      0.0000
Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=      0.0000  YYY=      0.0000  ZZZ=      0.0000  XYY=      0.0000
  XXY=      0.0000  XXZ=      0.0000  XZZ=      0.0000  YZZ=      0.0000
  YYZ=      0.0000  XYZ=      0.0000
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX=     -1.6553 YYYY=     -1.6553 ZZZZ=     -1.6553 XXXY=      0.0000
XXXZ=      0.0000 YYYX=      0.0000 YYYZ=      0.0000 ZZZX=      0.0000
ZZZY=      0.0000 XXYY=     -0.5518 XXZZ=     -0.5518 YYZZ=     -0.5518
XXYZ=      0.0000 YYXZ=      0.0000 ZZXY=      0.0000
```

```
N-N= 0.000000000000D+00 E-N=-9.996005737518D-01  KE= 4.997907584786D-01
Symmetry AG   KE= 4.997907584786D-01
Symmetry B1G  KE= 0.000000000000D+00
Symmetry B2G  KE= 0.000000000000D+00
Symmetry B3G  KE= 0.000000000000D+00
Symmetry AU   KE= 0.000000000000D+00
Symmetry B1U  KE= 0.000000000000D+00
Symmetry B2U  KE= 0.000000000000D+00
Symmetry B3U  KE= 0.000000000000D+00
```

エネルギーの内訳

分子軌道係数をつかった解析

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 H(1)	0.28744	1284.83861	458.46234	428.57603

Center	Spin Dipole Couplings 3XX-RR	3YY-RR	3ZZ-RR
1 Atom	0.000000	0.000000	0.000000

	XY	XZ	YZ
1 Atom	0.000000	0.000000	0.000000

Anisotropic Spin Dipole Couplings in Principal Axis System

Atom		a.u.	MegaHertz	Gauss	10(-4) cm-1	Axes		
1 H(1)	Baa	0.0000	0.000	0.000	0.000	1.0000	0.0000	0.0000
	Bbb	0.0000	0.000	0.000	0.000	0.0000	1.0000	0.0000
	Bcc	0.0000	0.000	0.000	0.000	0.0000	0.0000	1.0000

計算結果のまとめ

```
1|1|UNPC-UNK|SP|UHF|6-311G(d,p)|H1(2)|PCUSER|26-Apr-2011|0||#N HF/6-31
1G**||comments||0,2|H||Version=IA32W-G03RevC.02|State=2-A1G|HF=-0.4998
098|S2=0.75|S2-1=0.|S2A=0.75|RMSD=2.204e-006|Dipole=0.,0.,0.|PG=OH [O(
H1)]||@
```

今日の格言

```
Age does not diminish the extreme disappointment of
having a scoop of ice cream fall from the cone.
-- Jim Fiebig
Job cpu time:  0 days  0 hours  0 minutes 13.0 seconds.
File lengths (MBytes):  RWF=     11 Int=      0 D2E=      0 Chk=    230 Scr=      1
Normal termination of Gaussian 03 at Thu Oct 24 19:29:45 2013.
```

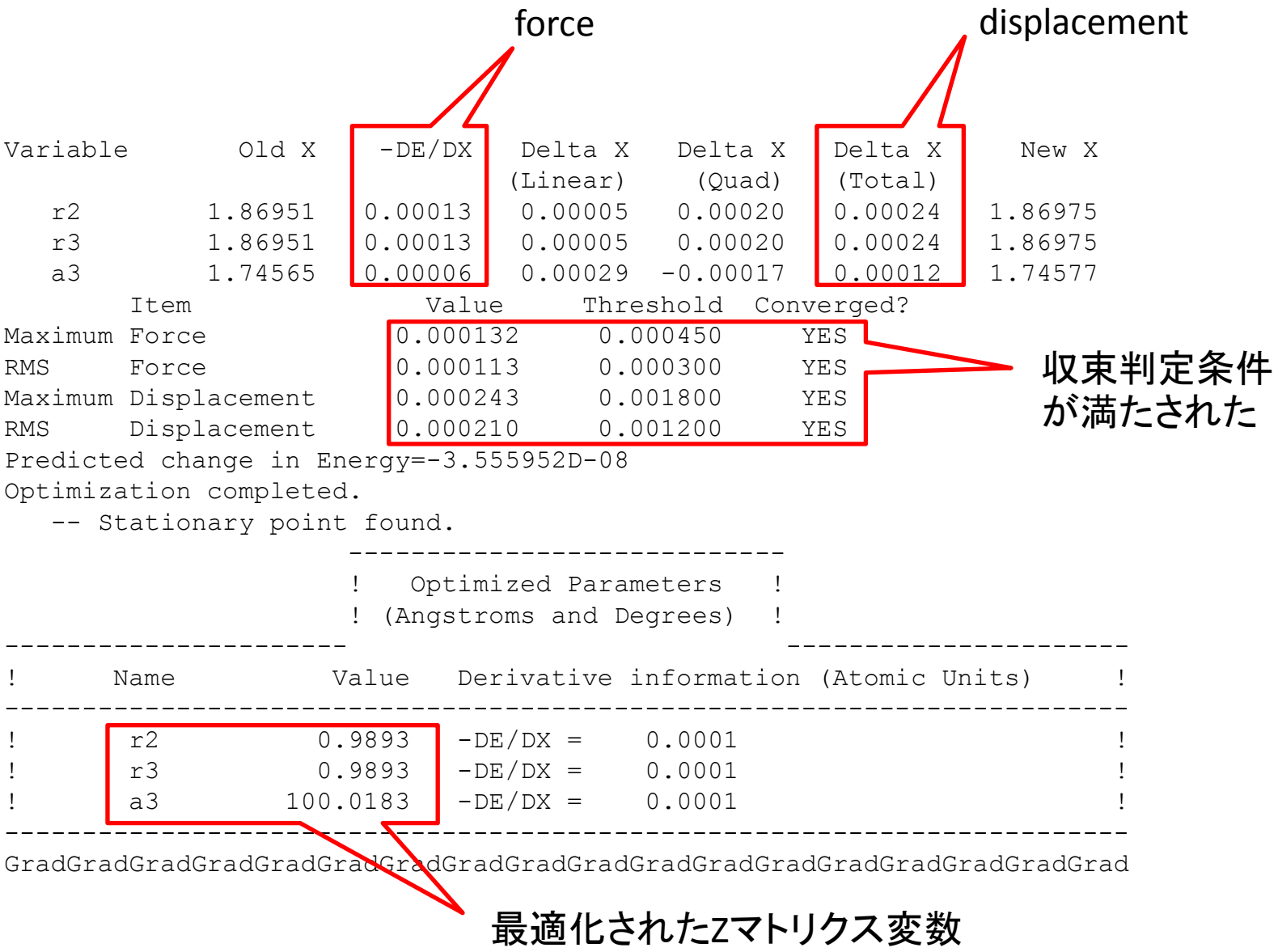
いろいろなキーワード

#N HF/STO-3G opt=z-matrix gfprint pop=full

分子軌道の係数を書き出す

構造を最適化する（Zマトリクスの変数を使う）

```
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
                          ----------------------------
                          !    Initial Parameters    !
                          ! (Angstroms and Degrees)  !
----------------------                                ----------------------
!      Name           Value   Derivative information (Atomic Units)     !
-------------------------------------------------------------------------
!       r2           1.0      estimate D2E/DX2                           !
!       r3           1.0      estimate D2E/DX2                           !
!       a3         104.5      estimate D2E/DX2                           !
-------------------------------------------------------------------------
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run=  20 maximum allowed number of steps= 100.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
```


force
displacement
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
r2 1.86951 0.00013 0.00005 0.00020 0.00024 1.86975
r3 1.86951 0.00013 0.00005 0.00020 0.00024 1.86975
a3 1.74565 0.00006 0.00029 -0.00017 0.00012 1.74577
Item Value Threshold Converged?
Maximum Force 0.000132 0.000450 YES
RMS Force 0.000113 0.000300 YES
Maximum Displacement 0.000243 0.001800 YES
RMS Displacement 0.000210 0.001200 YES
収束判定条件
が満たされた
Predicted change in Energy=-3.555952D-08
Optimization completed.
-- Stationary point found.
! Optimized Parameters !
! (Angstroms and Degrees) !
! Name Value Derivative information (Atomic Units) !
! r2 0.9893 -DE/DX = 0.0001 !
! r3 0.9893 -DE/DX = 0.0001 !
! a3 100.0183 -DE/DX = 0.0001 !
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
最適化されたZマトリクス変数

分子軌道係数

Molecular Orbital Coefficients

				1	2	3	4	5
				(A1)--O	(A1)--O	(B2)--O	(A1)--O	(B1)--O
	EIGENVALUES --			-20.25157	-1.25761	-0.59389	-0.45976	-0.39263
1	1	O	1S	0.99422	-0.23376	0.00000	-0.10405	0.00000
2			2S	0.02585	0.84441	0.00000	0.53823	0.00000
3			2PX	0.00000	0.00000	0.00000	0.00000	1.00000
4			2PY	0.00000	0.00000	0.61271	0.00000	0.00000
5			2PZ	-0.00417	-0.12288	0.00000	0.75587	0.00000
6	2	H	1S	-0.00558	0.15560	0.44922	-0.29507	0.00000
7	3	H	1S	-0.00558	0.15560	-0.44922	-0.29507	0.00000

				6	7
				(A1)--V	(B2)--V
	EIGENVALUES --			0.58191	0.69277
1	1	O	1S	-0.12583	0.00000
2			2S	0.82030	0.00000
3			2PX	0.00000	0.00000
4			2PY	0.00000	0.95983
5			2PZ	-0.76360	0.00000
6	2	H	1S	-0.76922	-0.81475
7	3	H	1S	-0.76922	0.81475

密度行列

DENSITY MATRIX.

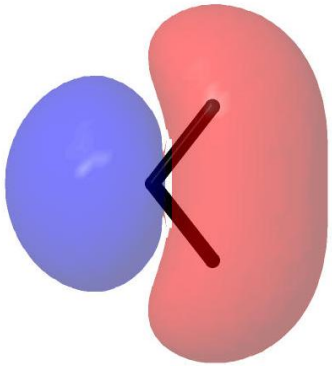
				1	2	3	4	5
1	1	O	1S	2.10787				
2			2S	-0.45538	2.00677			
3			2PX	0.00000	0.00000	2.00000		
4			2PY	0.00000	0.00000	0.00000	0.75083	
5			2PZ	-0.10813	0.60593	0.00000	0.00000	1.17292
6	2	H	1S	-0.02245	-0.05514	0.00000	0.55049	-0.48427
7	3	H	1S	-0.02245	-0.05514	0.00000	-0.55049	-0.48427

				6	7
6	2	H	1S	0.62622	
7	3	H	1S	-0.18098	0.62622

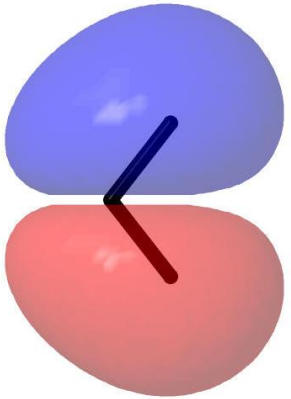
分子軌道の可視化

-20.25

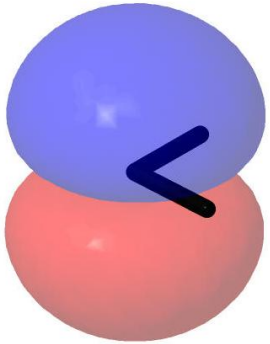
-1.26



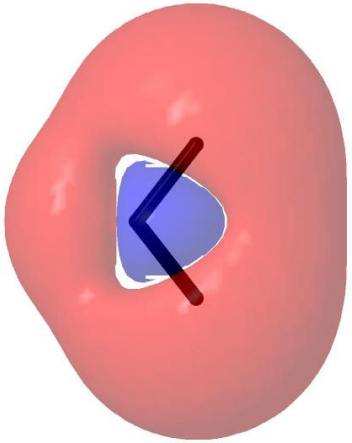
-0.59



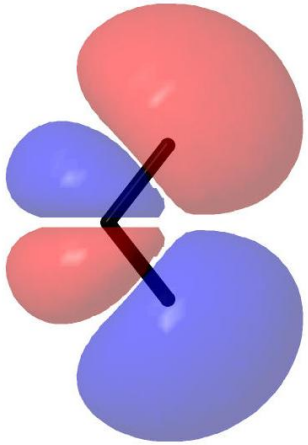
-0.46



-0.39



0.58



0.69

基準振動解析

```
%chk=default
```
チェックポイントファイルの指定

```
#N HF/6-311G** Opt Freq
```
最適化の後、基準振動解析を行う

```
water molecule
```
コメント

```
0 1
O
H 1 r2
H 1 r3   2 a3

r2 1.0
r3 1.0
a3 104.5
```
電荷、スピン多重度
構造情報

【重要】基準振動解析は最適化された座標で行わないと意味がない

Inside Gaussian (1)

- Freqルーチンでは何を計算しているか

$$\left.\begin{aligned} D &= M^{-1/2} K M^{-1/2} \\ W &= M^{1/2} X \end{aligned}\right\}$$

$$\Rightarrow DW = W\Omega^2$$

D: 入力座標系での動力学行列
W: 質量荷重座標
→Wは直交しているが，縮退した6個の固有ベクトルとの関係は分からない

T: 分子の自由並進ベクトルの組（x, y, z）
R: 分子の自由回転ベクトルの組（x, y, z）

$$C \equiv (T \mid R) \qquad [3N \times 6]$$

$$T = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ & \vdots & \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad R = \begin{pmatrix} 0 & z_1 \sin\theta_y + x_1(\cos\theta_y - 1) & x_1(\cos\theta_z - 1) - y_1 \sin\theta_z \\ y_1(\cos\theta_x - 1) - z_1 \sin\theta_x & 0 & x_1 \sin\theta_z + y_1(\cos\theta_z - 1) \\ y_1 \sin\theta_x + z_1(\cos\theta_x - 1) & z_1(\cos\theta_y - 1) - x_1 \sin\theta_y & 0 \\ & \vdots & \\ 0 & z_N \sin\theta_y + x_N(\cos\theta_y - 1) & x_N(\cos\theta_z - 1) - y_N \sin\theta_z \\ y_N(\cos\theta_x - 1) - z_N \sin\theta_x & 0 & x_N \sin\theta_z + y_N(\cos\theta_z - 1) \\ y_N \sin\theta_x + z_N(\cos\theta_x - 1) & z_N(\cos\theta_y - 1) - x_N \sin\theta_y & 0 \end{pmatrix}$$

$$\theta_a = 2\sin^{-1}\left(2\sqrt{\sum_i (r_i^2 - a_i^2)} \right)^{-1}$$

Inside Gaussian (2)

- 慣性主軸系での動力学行列を解く

$$P \equiv M^{1/2} C \qquad [3N \times 6]$$

$$P^t P = C^t M C \equiv \Gamma^{-1} \qquad [6 \times 6]$$

$$U^t \Gamma^{-1} U = \gamma^{-1}$$

$$Q \equiv \left(PU\gamma^{1/2} \,|\, Q' \right),\ Q^t Q = 1 \qquad [3N \times 3N]$$

$$\begin{cases} DW = W\Omega^2 \\ Q^t D Q = D^\circ & [(3N-6)\times(3N-6)] \\ Q^t W = L & [(3N-6)\times(3N-6)] \end{cases}$$

$$\Rightarrow D^\circ L = L\Omega^2,\ L^t L = 1$$

$$X \equiv M^{-1/2} W = M^{-1/2} Q L$$

$$\tilde{M}^{-1} \equiv X^t X = L^t Q^t M^{-1} Q L$$

$$\Rightarrow X = \tilde{X}\tilde{M}^{-1/2},\ \tilde{X}^t \tilde{X} = 1$$

P:荷重変位行列
Γ^{-1}:慣性負荷行列(対称)
U:Γ^{-1}を対角化するユニタリ行列
γ:慣性負荷の主値(対角)
Q:規格直交化された荷重変位行列
Q':PUγ$^{1/2}$に直交するように(Schmidt直交化によって)つくった行列

D°:慣性主軸系での動力学行列

L:D°を対角化するユニタリ行列

X:座標変位ベクトル
M~$^{-1}$:換算質量行列
X~:規格化された座標変位ベクトル

Inside Gaussian (3)

- 二原子分子の場合

$$Dw = \begin{pmatrix} \mu_1 K & -\sqrt{\mu_1\mu_2}K \\ -\sqrt{\mu_1\mu_2}K & \mu_2 K \end{pmatrix}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}\omega^2$$

D: 動力学行列（任意座標系）

$$R = \sqrt{\frac{1}{\mu_1+\mu_2}}\begin{pmatrix} \sqrt{\mu_1} & \sqrt{\mu_1} \\ \sqrt{\mu_2} & -\sqrt{\mu_2} \end{pmatrix}$$

R: 慣性主軸系での固有ベクトル
（純並進をx軸に一致させた）

$$D^\circ = \begin{pmatrix} 0 & 0 \\ 0 & (\mu_1+\mu_2)K \end{pmatrix}$$

$$L = 1$$

L: D° の部分行列[1×1]の固有ベクトル

$$X = \sqrt{\frac{1}{\mu_1+\mu_2}}\begin{pmatrix} \sqrt{\mu_1} & 0 \\ 0 & \sqrt{\mu_2} \end{pmatrix}\begin{pmatrix} \sqrt{\mu_2} & \sqrt{\mu_1} \\ \sqrt{\mu_1} & -\sqrt{\mu_2} \end{pmatrix}$$

$$= \sqrt{\frac{1}{\mu_1+\mu_2}}\begin{pmatrix} \sqrt{\mu_1\mu_2} & \mu_1 \\ \sqrt{\mu_1\mu_2} & -\mu_2 \end{pmatrix}$$

X: 質量荷重の逆変換

$$m^* = \frac{\mu_1+\mu_2}{\mu_1^2+\mu_2^2}$$

Xの規格化定数の二乗を換算質量m*と定義

基準振動ベクトル

```
Full mass-weighted force constant matrix:
Low frequencies ---   -49.1758   -48.7150   -47.8111     0.0009     0.0013     0.0013
Low frequencies ---  1750.6155  4143.9531  4239.2189
Diagonal vibrational polarizability:
       0.0000000       0.0857239       0.7214610
Diagonal vibrational hyperpolarizability:
       0.0000000       0.0000000      -6.7501010
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:
                      1          2          3
                     A1         A1         B2
      Frequencies ---  1750.6155  4143.9531  4239.2189
   Reduced masses ---     1.0822     1.0456     1.0828
  Force constants ---     1.9541    10.5791    11.4650
   IR Intensities ---    78.9900    17.7638    57.2454
 Raman Activities ---     6.3854    65.3982    32.4046
   Depol. (Plane) ---     0.5156     0.1838     0.7500
   Depol. (Unpol) ---     0.6804     0.3105     0.8571
Coord Atom Element:
  1     1     8          0.00000    0.00000    0.00000
  2     1     8          0.00000    0.00000    0.07073
  3     1     8          0.07045    0.05021    0.00000
  1     2     1          0.00000    0.00000    0.00000
  2     2     1         -0.43012    0.58309   -0.56129
  3     2     1         -0.55903   -0.39843    0.42714
  1     3     1          0.00000    0.00000    0.00000
  2     3     1          0.43012   -0.58309   -0.56129
  3     3     1         -0.55903   -0.39843   -0.42714
```

低振動数の解（負値か0に近ければよい）

振動数（大きめにでる→非調和項を入れると改善される）

モード質量とモード剛性

IRとラマンの強度

原子の座標変位

熱力学諸量(1)

```
-------------------
- Thermochemistry -
-------------------
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Atom  1 has atomic number  8 and mass  15.99491
Atom  2 has atomic number  1 and mass   1.00783
Atom  3 has atomic number  1 and mass   1.00783
Molecular mass:    18.01056 amu.
Principal axes and moments of inertia in atomic units:
                          1         2         3
    EIGENVALUES --     2.07515   4.03496   6.11011
          X            0.00000   0.00000   1.00000
          Y            1.00000   0.00000   0.00000
          Z            0.00000   1.00000   0.00000
This molecule is an asymmetric top.
Rotational symmetry number  2.
Rotational temperatures (Kelvin)      41.73861    21.46583    14.17549
Rotational constants (GHZ):          869.69251   447.27574   295.36958
Zero-point vibrational energy       60613.5 (Joules/Mol)
                                    14.48698 (Kcal/Mol)
Vibrational temperatures:   2518.74  5962.22  6099.28
          (Kelvin)
```

温度、圧力、同位体は指定可能

慣性モーメントの主値と慣性主軸

回転温度、回転定数、零点エネルギー、振動温度

熱力学諸量(2)

```
Zero-point correction=                           0.023086 (Hartree/Particle)
 Thermal correction to Energy=                    0.025921
 Thermal correction to Enthalpy=                  0.026865
 Thermal correction to Gibbs Free Energy=         0.005509
 Sum of electronic and zero-point Energies=           -76.023926
 Sum of electronic and thermal Energies=              -76.021091
 Sum of electronic and thermal Enthalpies=            -76.020147
 Sum of electronic and thermal Free Energies=         -76.041503

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  16.266             5.992            44.948
 Electronic              0.000             0.000             0.000
 Translational           0.889             2.981            34.608
 Rotational              0.889             2.981            10.335
 Vibrational            14.488             0.030             0.004
                           Q            Log10(Q)             Ln(Q)
 Total Bot        0.292489D-02          -2.533891         -5.834499
 Total V=0        0.121654D+09           8.085125         18.616687
 Vib (Bot)        0.240479D-10         -10.618922        -24.450972
 Vib (V=0)        0.100021D+01           0.000093          0.000214
 Electronic       0.100000D+01           0.000000          0.000000
 Translational    0.300432D+07           6.477746         14.915562
 Rotational       0.404842D+02           1.607285          3.700911
```

= 25.0 J K^{-1} mol^{-1}
(実験値（水蒸気）
28.8 J K^{-1} mol^{-1})

= 12.47 J K^{-1} mol^{-1}
= $3R/2$

励起状態の計算

```
%chk=default
```
チェックポイントファイルの指定

```
#N B3LYP/6-311G** TD=(Nstates=5)
```
時間依存DFT

```
water molecule
```
コメント

```
0 1
```
電荷、スピン多重度

```
O
H 1 r2
H 1 r3   2 a3
```
構造情報

```
r2 1.0
r3 1.0
a3 104.5
```

通常のDFT計算の結果

```
Initial guess orbital symmetries:
       Occupied  (A1) (A1) (B2) (A1) (B1)
       Virtual   (A1) (B2) (B2) (A1) (B1) (A1) (B2) (A1) (A1) (A2)
                 (B1) (B2) (B2) (A1) (A1) (B2) (B1) (A2) (A1) (A1)
                 (B2) (B1) (A1) (B2) (A1)
 The electronic state of the initial guess is 1-A1.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 Keep R1 integrals in memory in canonical form, NReq=      614236.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved.  Increase integral accuracy.
 SCF Done:  E(RB+HF-LYP) =  -76.4459738120     A.U. after    9 cycles
             Convg  =    0.9400D-08             -V/T =  2.0028
             S**2   =   0.0000
ExpMin= 1.03D-01 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=1 IRadAn=         1 AccDes=
1.00D-06
 HarFok:  IExCor= 205 AccDes= 1.00D-06 IRadAn=         1 IDoV=1
 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 Range of M.O.s used for correlation:     2    30
 NBasis=    30 NAE=     5 NBE=     5 NFC=     1 NFV=     0
 NROrb=     29 NOA=     4 NOB=     4 NVA=    25 NVB=    25
 R1, R2, and R3 integrals will be kept in memory, NReq=      799768.
 Orbital symmetries:
       Occupied  (A1) (A1) (B2) (A1) (B1)
       Virtual   (A1) (B2) (B2) (A1) (A1) (B1) (B2) (A1) (A1) (A2)
                 (B1) (B2) (B2) (A1) (A1) (B2) (B1) (A2) (A1) (A1)
                 (B2) (B1) (A1) (B2) (A1)
```

励起状態の計算結果

```
20 initial guesses have been made.
Convergence on wavefunction:    0.001000000000000
Iteration     1 Dimension    20 NMult    20
CISAX will form  20 AO SS matrices at one time.
Iteration     2 Dimension    30 NMult    30
Iteration     3 Dimension    40 NMult    40
Iteration     4 Dimension    44 NMult    44
**********************************************************************
Excited states from <AA,BB:AA,BB> singles matrix:
**********************************************************************

Ground to excited state Transition electric dipole moments (Au):
      state          X           Y           Z          Osc.
        1         0.3692      0.0000      0.0000      0.0238
        2         0.0000      0.0000      0.0000      0.0000
        3         0.0000      0.0000      0.6169      0.0904
        4         0.0000      0.4270      0.0000      0.0519
        5         0.0000      0.8867      0.0000      0.2501
Ground to excited state transition velocity dipole Moments (Au):
      state          X           Y           Z          Osc.
        1        -0.2005      0.0000      0.0000      0.1022
        2         0.0000      0.0000      0.0000      0.0000
        3         0.0000      0.0000     -0.2903      0.1576
        4         0.0000     -0.1762      0.0000      0.0485
        5         0.0000     -0.4169      0.0000      0.2428
```

Ground to excited state transition magnetic dipole Moments (Au):

state	X	Y	Z
1	0.0000	0.1874	0.0000
2	0.0000	0.0000	-0.2790
3	0.0000	0.0000	0.0000
4	0.2776	0.0000	0.0000
5	-0.0895	0.0000	0.0000

<0|del|b> * <b|rxdel|0> (Au), Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	X	Y	Z	R(velocity)
1	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000

<0|r|b> * <b|rxdel|0> (Au), Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	X	Y	Z	R(length)
1	0.0000	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	0.0000	0.0000
4	0.0000	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	0.0000

<0|del|b> * <b|r|0> (Au)

state	X	Y	Z	Osc.(frdel)
1	-0.0740	0.0000	0.0000	0.0494
2	0.0000	0.0000	0.0000	0.0000
3	0.0000	0.0000	-0.1791	0.1194
4	0.0000	-0.0752	0.0000	0.0501
5	0.0000	-0.3697	0.0000	0.2464

Ground to excited state transition densities written to RWF 633

励起配置・吸収波長・振動子強度など

```
Excitation energies and oscillator strengths:

Excited State   1:   Singlet-B1     7.1349 eV  173.77 nm  f=0.0238
      5 ->  6         0.69252
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:   Singlet-A2     9.0146 eV  137.54 nm  f=0.0000
      5 ->  7         0.70011

Excited State   3:   Singlet-A1     9.7004 eV  127.81 nm  f=0.0904
      4 ->  6         0.68703

Excited State   4:   Singlet-B2    11.6169 eV  106.73 nm  f=0.0519
      4 ->  7         0.68969

Excited State   5:   Singlet-B2    12.9866 eV   95.47 nm  f=0.2501
      3 ->  6         0.68673
```