東京大学　生産技術研究所
北條　博彦

化学生命工学専攻

有機機能材料学特論II

Gaussianの使い方

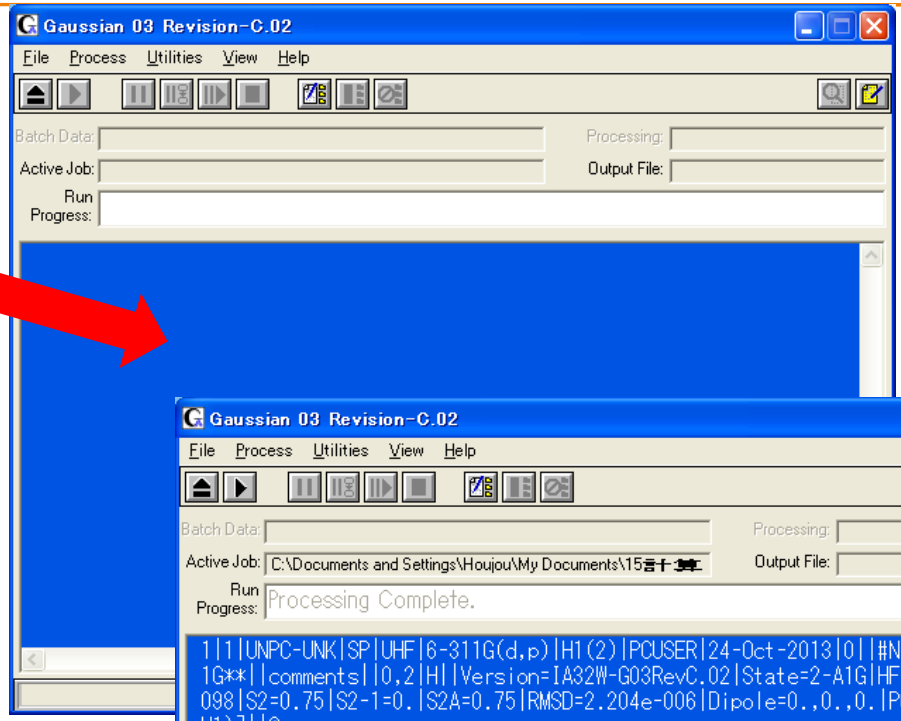
Hydrogen.gjf

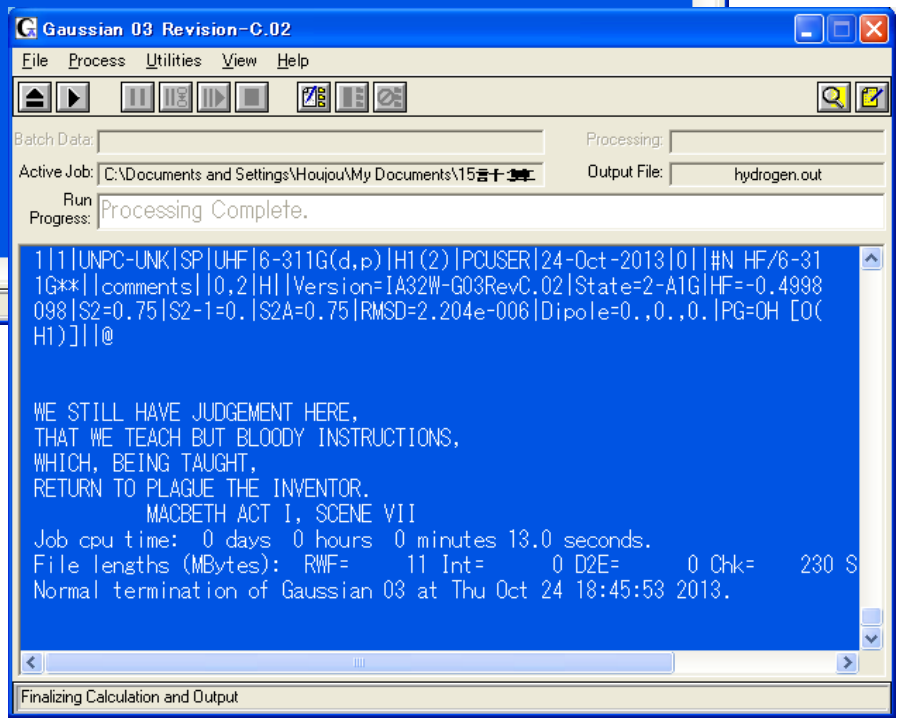
```
%chk=default

#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** Terse)	**出力フォーマット（**Normal, Print,
	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

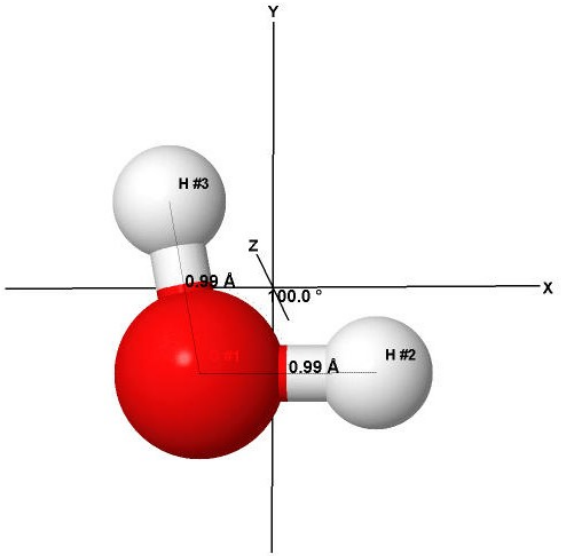
0 1
O -0.464 0.177 0.0
H -0.464 1.137 0.0
H 0.441 -0.143 0.0
```

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,
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K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
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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
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
```

収束判定条件が満たされた

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

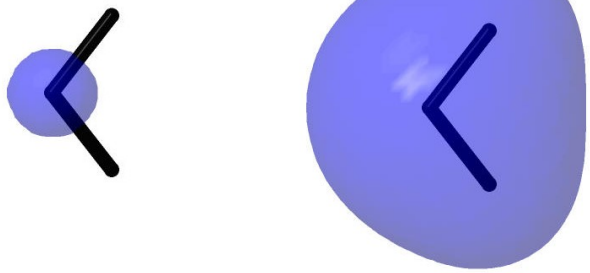
密度行列

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

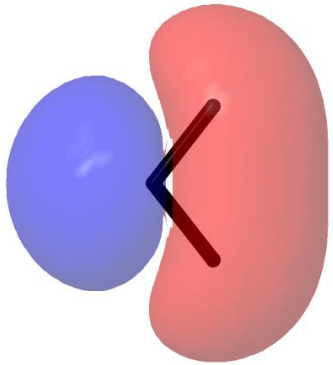
				6	7
6	2	H	1S	0.62622	
7	3	H	1S	-0.18098	0.62622

分子軌道の可視化

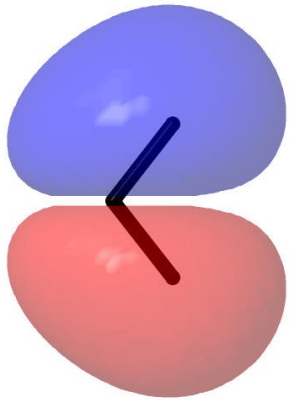


-20.25

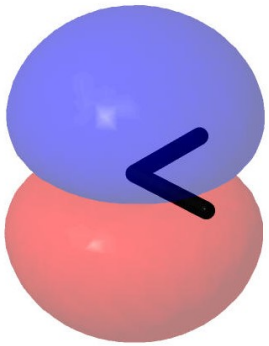
-1.26



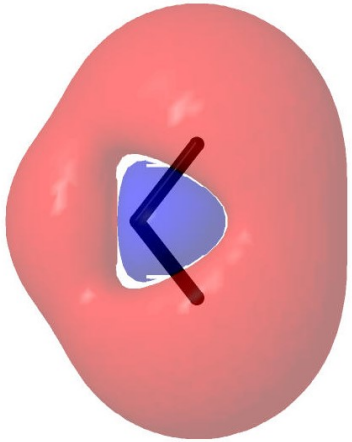
-0.59



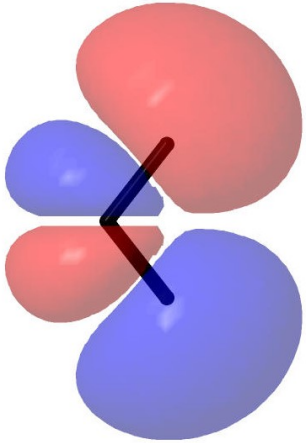
-0.46



-0.39



0.58



0.69