结构化学讲义

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TODO.

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Gaussian 中提取分子积分的方法如下：

```
%chk=./h2.chk
#t rhf/gen scf=conventional symm=noint noraff ExtraLinks=L316 iop(3/33=3)

H2 minimal basis set

0 1
H 1. 0. 0.
H -1. 0. 0.
H 0. -1. 0.
H 0. 1. 0.

H 0
S 1 1.00
 0.480D+00 0.100D+01
****
```

```
 *** Overlap ***
                1             2             3             4
      1  0.100000D+01
      2  0.324446D-01  0.100000D+01
      3  0.180124D+00  0.180124D+00  0.100000D+01
      4  0.180124D+00  0.180124D+00  0.324446D-01  0.100000D+01
 *** Kinetic Energy ***
                1             2             3             4
      1  0.720000D+00
```

```
     2 -0.300290D-01  0.720000D+00
     3 -0.185119D-01 -0.185119D-01  0.720000D+00
     4 -0.185119D-01 -0.185119D-01 -0.300290D-01  0.720000D+00
```

...

```
 ***** Potential Energy *****
               1             2             3             4
     1  0.211838D+01
     2  0.680691D-01  0.211838D+01
     3  0.372883D+00  0.372883D+00  0.211838D+01
     4  0.372883D+00  0.372883D+00  0.680691D-01  0.211838D+01
 ****** Core Hamiltonian ******
               1             2             3             4
     1 -0.139838D+01
     2 -0.980981D-01 -0.139838D+01
     3 -0.391395D+00 -0.391395D+00 -0.139838D+01
     4 -0.391395D+00 -0.391395D+00 -0.980981D-01 -0.139838D+01
```

...

```
 *** Dumping Two-Electron integrals ***



 ISMode= 0 Mode= 1 IBase=        1 IBasD=        1    262145
 DBase=         0 DBasD=         0         0 IReset=        2    262139
 IntCnt=        0 ITotal=       55 NWIIB=    262144 ISym2E=0
 I=  4 J=  3 K=  2 L=  1 Int=  0.822923860669D-03
 I=  4 J=  1 K=  3 L=  2 Int=  0.120330383547D-01
 I=  4 J=  2 K=  3 L=  1 Int=  0.120330383547D-01
 I=  4 J=  4 K=  4 L=  4 Int=  0.781764019045D+00
 I=  4 J=  4 K=  4 L=  3 Int=  0.160685510571D-01
 I=  4 J=  4 K=  4 L=  2 Int=  0.109126261413D+00
```

```
I=  4 J=  4 K=  4 L=  1 Int=  0.109126261413D+00
I=  4 J=  3 K=  4 L=  3 Int=  0.822923860669D-03
I=  4 J=  4 K=  3 L=  3 Int=  0.264532250132D+00
I=  4 J=  3 K=  4 L=  2 Int=  0.354055434816D-02
I=  4 J=  4 K=  3 L=  2 Int=  0.600780522778D-01
I=  4 J=  3 K=  4 L=  1 Int=  0.354055434816D-02
I=  4 J=  4 K=  3 L=  1 Int=  0.600780522778D-01
I=  4 J=  2 K=  4 L=  2 Int=  0.253639954401D-01
I=  4 J=  4 K=  2 L=  2 Int=  0.370879913132D+00
I=  4 J=  2 K=  4 L=  1 Int=  0.160685510571D-01
I=  4 J=  4 K=  2 L=  1 Int=  0.160685510571D-01
I=  4 J=  1 K=  4 L=  1 Int=  0.253639954401D-01
I=  4 J=  4 K=  1 L=  1 Int=  0.370879913132D+00
I=  4 J=  3 K=  3 L=  3 Int=  0.160685510571D-01
I=  4 J=  2 K=  3 L=  3 Int=  0.600780522778D-01
I=  4 J=  3 K=  3 L=  2 Int=  0.354055434816D-02
I=  4 J=  1 K=  3 L=  3 Int=  0.600780522778D-01
I=  4 J=  3 K=  3 L=  1 Int=  0.354055434816D-02
I=  4 J=  2 K=  3 L=  2 Int=  0.160685510571D-01
I=  4 J=  3 K=  2 L=  2 Int=  0.160685510571D-01
I=  4 J=  1 K=  3 L=  1 Int=  0.160685510571D-01
I=  4 J=  3 K=  1 L=  1 Int=  0.160685510571D-01
I=  4 J=  2 K=  2 L=  2 Int=  0.109126261413D+00
I=  4 J=  1 K=  2 L=  2 Int=  0.600780522778D-01
I=  4 J=  2 K=  2 L=  1 Int=  0.354055434816D-02
I=  4 J=  1 K=  2 L=  1 Int=  0.354055434816D-02
I=  4 J=  2 K=  1 L=  1 Int=  0.600780522778D-01
I=  4 J=  1 K=  1 L=  1 Int=  0.109126261413D+00
I=  3 J=  3 K=  3 L=  3 Int=  0.781764019045D+00
I=  3 J=  3 K=  3 L=  2 Int=  0.109126261413D+00
I=  3 J=  3 K=  3 L=  1 Int=  0.109126261413D+00
I=  3 J=  2 K=  3 L=  2 Int=  0.253639954401D-01
I=  3 J=  3 K=  2 L=  2 Int=  0.370879913132D+00
I=  3 J=  2 K=  3 L=  1 Int=  0.160685510571D-01
I=  3 J=  3 K=  2 L=  1 Int=  0.160685510571D-01
I=  3 J=  1 K=  3 L=  1 Int=  0.253639954401D-01
I=  3 J=  3 K=  1 L=  1 Int=  0.370879913132D+00
I=  3 J=  2 K=  2 L=  2 Int=  0.109126261413D+00
I=  3 J=  1 K=  2 L=  2 Int=  0.600780522778D-01
I=  3 J=  2 K=  2 L=  1 Int=  0.354055434816D-02
I=  3 J=  1 K=  2 L=  1 Int=  0.354055434816D-02
```

```
I=  3 J=  2 K=  1 L=  1 Int=  0.600780522778D-01
I=  3 J=  1 K=  1 L=  1 Int=  0.109126261413D+00
I=  2 J=  2 K=  2 L=  2 Int=  0.781764019045D+00
I=  2 J=  2 K=  2 L=  1 Int=  0.160685510571D-01
I=  2 J=  1 K=  2 L=  1 Int=  0.822923860669D-03
I=  2 J=  2 K=  1 L=  1 Int=  0.264532250132D+00
I=  2 J=  1 K=  1 L=  1 Int=  0.160685510571D-01
I=  1 J=  1 K=  1 L=  1 Int=  0.781764019045D+00
```

2.3 ¶ÔPyQuanteÖÐ¹ØÓÚ»ù×é»ý · Ö´úÂëµÄ×¢ÊÍ

2.3.1 ¸ÅÊö

ÒÔÏÂ×¢½â»ùÓÚPyQuante-1.6.5°æ±¾£¬Ô´ÎÄ¼þÎ»ÓÚÄ¿Â¼£º~`\PyQuante\`¡£Ò»ÏÂ¶ÔÃ¿¸öÎÄ¼þÒÔÒÔÒ

2.3.2 PGBF.py

°üº¬¹ØÓÚÔÊ¼¸ßË¹»ùº¯ÊýµÄ»ù±¾²Ù×÷

²Î¿¼ÎÄÏ×£º

’Gaussian Expansion Methods for Molecular Orbitals.’ H. Taketa, S. Huzinaga, and K. O-ohata. H. Phys. Soc. Japan, 21, 2313, 1966.[THO paper]

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$$g(x,y,z) = Ax^i y^j z^k \exp\left[-a(r-r_0)^2\right] \tag{2.1}$$

±¾Ä£¿é°üº¬Ò»ÏÂ · ½ · ¨£º

overlap(g’): ¼ÆËãgÓëg’µÄÖØµþ¾ØÕó: Int(g*g’)

kinetic(g’): ¼ÆËãgÓëg’µÄ¶¯ÄÜ»ý · Ö£ºInt(G*lapl(G’)), ÆäÖÐlapl±íÊ¾ÀÆÕÀË¹Ëã · û.

nuclear(g’,r): ¼ÆËãºËÎüÒýÄÜ»ý · Ö

Int(g*(1/r)*g’). Only programmed for 1s gaussians.

coulomb(g,g’,g”,g”’): Compute the two-electron colombic repulsion

integral Int(g(1)g’(1)(1/r12)g”(2)g”’(2)).

2.4 量化软件实现

2.4.1 CGBF.py

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2.4.2 Ints.py

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2.4.3 pyints.py

Python implementations of work functions for Gaussian integrals in the PyQuante package.
The equations herein are based upon
'Gaussian Expansion Methods for Molecular Orbitals.' H. Taketa, S. Huzinaga, and K. O-ohata. H. Phys. Soc. Japan, 21, 2313, 1966.[THO paper]

2.5 量化软件使用心得:Gaussian

2.5.1 Gaussian 中优化不收敛的解决办法

2.6 量化软件使用心得:Material Studio

2.6.1 MS1