

第一章 量子化学

1.1 量化理论

TODO.

1.2 量化软件实现

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

O 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

1.3 量化软件使用心得：Gaussian

1.3.1 Gaussian 中优化不收敛的解决办法

1.4 量化软件使用心得：Material Studio

1.4.1 MS xxx