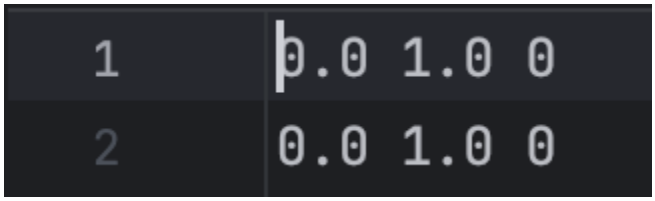
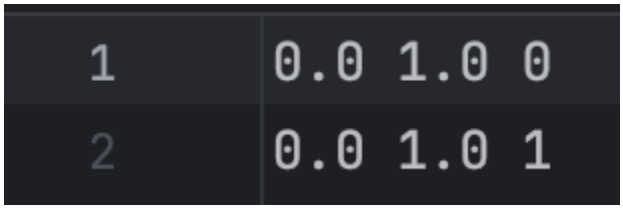
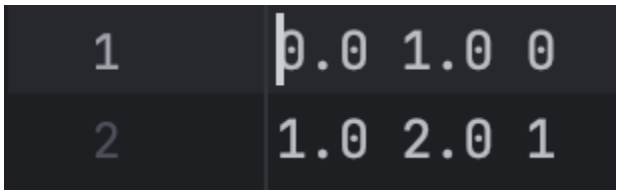
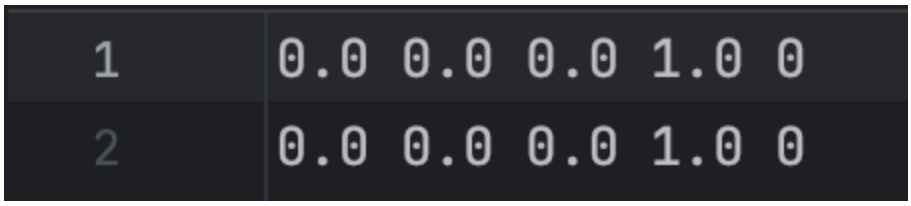
Vitto Resnick | CHEM 179 | HW2 | 3035806760
Link: https://github.com/chemclown21/CHEM_179_HW2

1.1 Input	
1.1 My Ans	"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2" 1d numerical overlap integral between Gaussian functions is 1.25331 Process finished with exit code 0
1.1 Xiao	1 1d numerical overlap integral between Gaussian functions is 1.25331413731550456e+00
1.2 Input	
1.2 My Ans	"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2" 1d numerical overlap integral between Gaussian functions is 2.21768e-17 Process finished with exit code 0
1.2 Xiao	1 1d numerical overlap integral between Gaussian functions is 0.00000000000000000e+00
1.3 Input	
1.3 My Ans	"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2" 1d numerical overlap integral between Gaussian functions is -0.175131 Process finished with exit code 0
1.3 Xiao	1 1d numerical overlap integral between Gaussian functions is -1.75131150074330832e-01

2.1 Input



2.1 My Ans

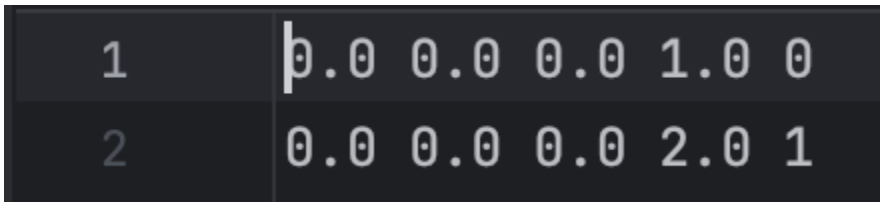
```
"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2"
Shell 1 has 1 functions.
This shell info: R(0, 0, 0), with angular momentum: 0, coefficient: 1
Shell 2 has 1 functions.
This shell info: R(0, 0, 0), with angular momentum: 0, coefficient: 1
Overlap integral between Shell 1 and Shell 2
   1.9687
The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (0, 0, 0).
The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (0, 0, 0).

Process finished with exit code 0
```

2.1 Xiao

```
1    Shell 1 has 1 functions.
2    This shell info: R( 0.00, 0.00, 0.00), with angular momentum: 0, coefficient: 1.00
3    Shell 2 has 1 functions.
4    This shell info: R( 0.00, 0.00, 0.00), with angular momentum: 0, coefficient: 1.00
5    Overlap integral between Shell 1 and Shell 2
6       1.9687
7    The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (0, 0, 0).
8    The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (0, 0, 0).
```

2.2 Input



2.2 My Ans

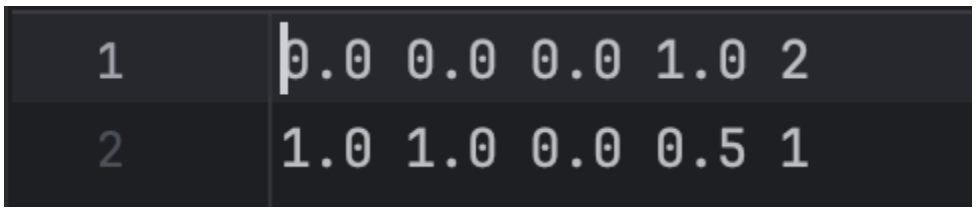
```
"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2"
Shell 1 has 1 functions.
This shell info: R(0, 0, 0), with angular momentum: 0, coefficient: 1
Shell 2 has 3 functions.
This shell info: R(0, 0, 0), with angular momentum: 1, coefficient: 2
Overlap integral between Shell 1 and Shell 2
       0       0       0
The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (0, 0, 0).
The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (1, 0, 0), (0, 1, 0), (0, 0, 1).

Process finished with exit code 0
```

2.2 Xiao

```
1    Shell 1 has 1 functions.
2    This shell info: R( 0.00, 0.00, 0.00), with angular momentum: 0, coefficient: 1.00
3    Shell 2 has 3 functions.
4    This shell info: R( 0.00, 0.00, 0.00), with angular momentum: 1, coefficient: 2.00
5    Overlap integral between Shell 1 and Shell 2
6            0       0       0
7    The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (0, 0, 0).
8    The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (1, 0, 0), (0, 1, 0), (0, 0,
```

2.3 Input



2.3 My Ans	"/Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW2/cmake-build-debug/CHEM_179_HW2" Shell 1 has 6 functions. This shell info: R(0, 0, 0), with angular momentum: 2, coefficient: 1 Shell 2 has 3 functions. This shell info: R(1, 1, 0), with angular momentum: 1, coefficient: 0.5 Overlap integral between Shell 1 and Shell 2 -0.1153 -0.4611 0 0.0576 0.0576 0 0 0 0.1729 -0.4611 -0.1153 0 0 0 0.1729 -0.3458 -0.3458 0 The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (2, 0, 0), (1, 1, 0), (1, 0, 1), (0, 2, 0), (0, 1, The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (1, 0, 0), (0, 1, 0), (0, 0, 1). Process finished with exit code 0
2.3 Xiao	Shell 1 has 6 functions. This shell info: R(0.00, 0.00, 0.00), with angular momentum: 2, coefficient: 1.00 Shell 2 has 3 functions. This shell info: R(1.00, 1.00, 0.00), with angular momentum: 1, coefficient: 0.50 Overlap integral between Shell 1 and Shell 2 −0.1153 −0.4611 0 0.0576 0.0576 0 0 0 0.1729 −0.4611 −0.1153 0 0 0 0.1729 −0.3458 −0.3458 0 The components of angular momentum (l, m, n) for the matrix column, from top to bottom, are listed sequentially as: (2, 0, 0), (1, 1, 0), (1, 0, 1), The components of angular momentum (l, m, n) for the matrix row, from left to right, are listed sequentially as: (1, 0, 0), (0, 1, 0), (0, 0, 1).