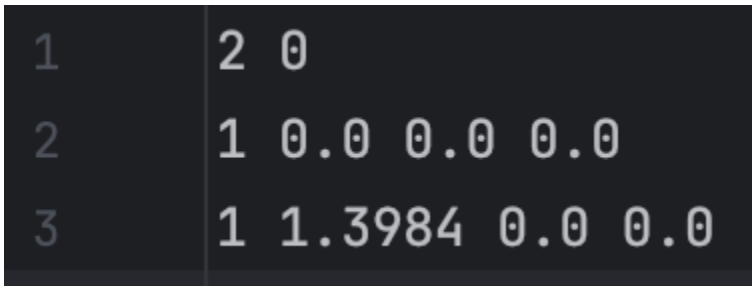
Vitto Resnick | CHEM 179 | HW3 | 3035806760
Link: https://github.com/chemclown21/CHEM_179_HW3

<table>
<tr><td>Input</td><td>

```
(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % g++ -std=c++11 -o main main.cpp -larmadillo
-I/usr/local/opt/armadillo/include -L/usr/local/opt/armadillo/lib

(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % ./main /Users/vittor/Documents/CLASSES/SPRING\
2024/CHEM_179_HW3/sample_input/H2.txt
```



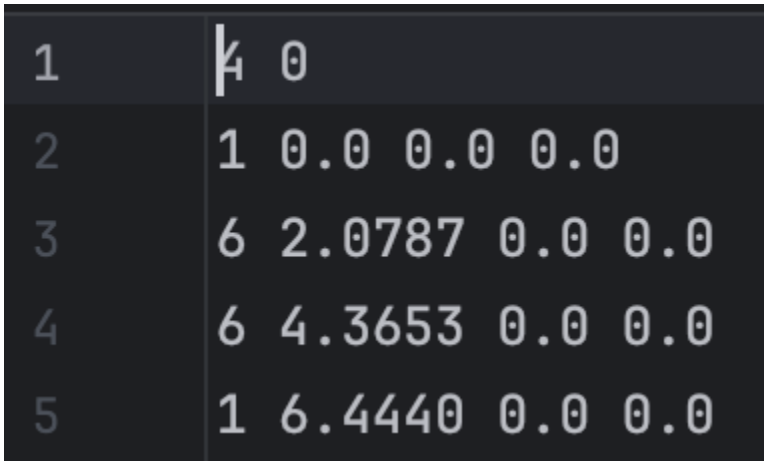

</td></tr>
<tr><td>My Ans</td><td>

```
S: Contracted overlap integral, overlap matrix:
   1.0000   0.6599
   0.6599   1.0000
H: Hamiltonian matrix
  -13.6000  -15.7050
  -15.7050  -13.6000
X_mat: Inverse square root of S:
   1.2454  -0.4692
  -0.4692   1.2454
C: MO coefficients (C matrix)
   0.5488  -1.2125
   0.5488   1.2125
The molecule in file /Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW3/sample_input/H2.txt has energy -35.3099 eV%
```

</td></tr>
<tr><td>Input</td><td>

```
(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % g++ -std=c++11 -o main main.cpp -larmadillo
-I/usr/local/opt/armadillo/include -L/usr/local/opt/armadillo/lib

(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % ./main /Users/vittor/Documents/CLASSES/SPRING\
2024/CHEM_179_HW3/sample_input/C2H2.txt
```




</td></tr>
</table>

My Ans

```
S: Contracted overlap integral, overlap matrix:
   1.0000e+00   4.8501e-01  -4.6382e-01           0           0   7.2952e-02  -9.7547e-02           0           0   7.3985e-03
   4.8501e-01   1.0000e+00           0           0           0   4.6629e-01  -4.5219e-01           0           0   7.2952e-02
  -4.6382e-01           0   1.0000e+00           0           0   4.5219e-01  -3.1207e-01           0           0   9.7547e-02
           0           0           0   1.0000e+00           0           0           0   2.9737e-01           0           0
           0           0           0           0   1.0000e+00           0           0           0   2.9737e-01           0
   7.2952e-02   4.6629e-01   4.5219e-01           0           0   1.0000e+00  -6.7317e-16           0           0   4.8501e-01
  -9.7547e-02  -4.5219e-01  -3.1207e-01           0           0  -6.7317e-16   1.0000e+00           0           0   4.6382e-01
           0           0           0   2.9737e-01           0           0           0   1.0000e+00           0           0
           0           0           0           0   2.9737e-01           0           0           0   1.0000e+00           0
   7.3985e-03   7.2952e-02   9.7547e-02           0           0   4.8501e-01   4.6382e-01           0           0   1.0000e+00
H: Hamiltonian matrix
  -1.3600e+01  -1.4854e+01   1.0146e+01           0           0  -2.2342e+00   2.1338e+00           0           0  -1.7609e-01
  -1.4854e+01  -2.1400e+01           0           0           0  -1.7462e+01   1.2978e+01           0           0  -2.2342e+00
   1.0146e+01           0  -1.1400e+01           0           0  -1.2978e+01   6.2258e+00           0           0  -2.1338e+00
           0           0           0  -1.1400e+01           0           0           0  -5.9325e+00           0           0
           0           0           0           0  -1.1400e+01           0           0           0  -5.9325e+00           0
  -2.2342e+00  -1.7462e+01  -1.2978e+01           0           0  -2.1400e+01   1.9320e-14           0           0  -1.4854e+01
   2.1338e+00   1.2978e+01   6.2258e+00           0           0   1.9320e-14  -1.1400e+01           0           0  -1.0146e+01
           0           0           0  -5.9325e+00           0           0           0  -1.1400e+01           0           0
           0           0           0           0  -5.9325e+00           0           0           0  -1.1400e+01           0
  -1.7609e-01  -2.2342e+00  -2.1338e+00           0           0  -1.4854e+01  -1.0146e+01           0           0  -1.3600e+01
X_mat: Inverse square root of S:
   1.2686e+00  -2.9295e-01   3.9220e-01   4.4535e-17   6.6318e-17  -8.6119e-02   7.2306e-02   2.1271e-17  -4.8305e-17  -1.2048e-02
  -2.9295e-01   1.4802e+00   2.0371e-01  -2.3977e-17  -6.0025e-17  -4.6197e-01   4.8690e-01   1.6824e-16   1.2823e-16  -8.6119e-02
   3.9220e-01   2.0371e-01   1.4501e+00  -4.0930e-18   3.3422e-17  -4.8690e-01   4.2301e-01   1.1902e-16  -9.6934e-17  -7.2306e-02
   4.4535e-17  -2.3977e-17  -4.0930e-18   1.0355e+00  -2.9678e-17  -1.7063e-17  -6.0156e-17  -1.5752e-01  -3.6256e-16   1.5606e-18
   6.6318e-17  -6.0025e-17   3.3422e-17  -5.1489e-17   1.0355e+00  -3.0651e-17  -1.5112e-17   1.0926e-16  -1.5752e-01   5.4850e-17
  -8.6119e-02  -4.6197e-01  -4.8690e-01  -1.7063e-17  -3.0651e-17   1.4802e+00  -2.0371e-01  -5.6511e-17   2.3884e-18  -2.9295e-01
   7.2306e-02   4.8690e-01   4.2301e-01  -6.0156e-17  -1.5112e-17  -2.0371e-01   1.4501e+00   9.1220e-17  -7.3526e-17  -3.9220e-01
   2.1271e-17   1.6824e-16   1.1902e-16  -1.5752e-01   1.3658e-16  -5.6511e-17   9.1220e-17   1.0355e+00   3.4276e-16  -4.1398e-17
  -4.8305e-17   1.2823e-16  -9.6934e-17  -3.3733e-16  -1.5752e-01   2.3884e-18  -7.3526e-17   3.3929e-16   1.0355e+00  -4.5307e-17
  -1.2048e-02  -8.6119e-02  -7.2306e-02   1.5606e-18   5.4850e-17  -2.9295e-01  -3.9220e-01  -4.1398e-17  -4.5307e-17   1.2686e+00
C: MO coefficients (C matrix)
  -9.1509e-02   3.3303e-01  -3.7688e-01  -3.8473e-16  -4.5763e-16   1.1591e-16   1.3644e-16  -9.0554e-01  -8.7300e-01  -1.3580e-01
  -5.3539e-01   3.7953e-01   3.9308e-02  -3.9703e-16   1.0070e-17   6.4914e-18   3.0409e-16   5.2740e-01   5.8491e-01  -1.3129e+00
  -3.5750e-02  -2.3725e-01   4.2622e-01   1.1681e-16   5.3657e-16   3.0050e-16  -1.2724e-16  -6.2436e-01  -6.6014e-01  -1.2863e+00
   1.6188e-17   2.3403e-16   5.6659e-16  -1.6018e-02  -6.2060e-01   6.3285e-01  -5.5778e-01   2.1440e-17  -3.7594e-17   8.8199e-17
   5.0978e-17   1.1522e-16  -2.6875e-16   6.2060e-01  -1.6018e-02   5.5778e-01   6.3285e-01   1.8102e-17  -9.3009e-17   9.3209e-18
  -5.3539e-01  -3.7953e-01   3.9308e-02   1.5331e-16   2.7454e-16   1.9279e-16  -1.2698e-16  -5.2740e-01   5.8491e-01   1.3129e+00
   3.5750e-02  -2.3725e-01  -4.2622e-01  -1.7659e-16  -7.2259e-16  -9.3599e-17   2.6625e-16  -6.2436e-01   6.6014e-01  -1.2863e+00
  -2.9072e-16  -6.6101e-17   1.1292e-15  -1.6018e-02  -6.2060e-01  -6.3285e-01   5.5778e-01  -7.9920e-17  -3.9904e-17  -3.9384e-16
  -2.8873e-16   1.1025e-15   2.3674e-16   6.2060e-01  -1.6018e-02  -5.5778e-01  -6.3285e-01   2.0394e-16   2.0293e-16   8.1989e-17
  -9.1509e-02  -3.3303e-01  -3.7688e-01   4.2514e-16  -5.1056e-16  -2.3476e-16  -1.8145e-16   9.0554e-01  -8.7300e-01   1.3580e-01
The molecule in file /Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW3/sample_input/C2H2.txt has energy -177.17 eV%
```

Input

```
(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % g++ -std=c++11 -o main main.cpp -larmadillo
-I/usr/local/opt/armadillo/include -L/usr/local/opt/armadillo/lib

(base) vittor@wifi-10-43-187-53 CHEM_179_HW3 % ./main /Users/vittor/Documents/CLASSES/SPRING\
2024/CHEM_179_HW3/sample_input/C2H4.txt
```

```
1  6 0
2  6       1.266     0.000       0.0
3  6      -1.266    -0.000       0.0
4  1       2.305     1.800       0.0
5  1       2.305    -1.800       0.0
6  1      -2.305     1.800       0.0
7  1      -2.305    -1.800       0.0
```

My Ans

```
S: Contracted overlap integral, overlap matrix:
   1.0000        0        0        0   0.3954   0.4094        0        0   0.4851   0.4851   0.1045   0.1045
        0   1.0000        0        0  -0.4094  -0.3281        0        0   0.2319   0.2319  -0.1193  -0.1193
        0        0   1.0000        0        0        0   0.2373        0   0.4018  -0.4018   0.0601  -0.0601
        0        0        0   1.0000        0        0        0   0.2373        0        0        0        0
   0.3954  -0.4094        0        0   1.0000        0        0        0   0.1045   0.1045   0.4851   0.4851
   0.4094  -0.3281        0        0        0   1.0000        0        0   0.1193   0.1193  -0.2319  -0.2319
        0        0   0.2373        0        0        0   1.0000        0   0.0601  -0.0601   0.4018  -0.4018
        0        0        0   0.2373        0        0        0   1.0000        0        0        0        0
   0.4851   0.2319   0.4018        0   0.1045   0.1193   0.0601        0   1.0000   0.1390   0.0554   0.0149
   0.4851   0.2319  -0.4018        0   0.1045   0.1193  -0.0601        0   0.1390   1.0000   0.0149   0.0554
   0.1045  -0.1193   0.0601        0   0.4851  -0.2319   0.4018        0   0.0554   0.0149   1.0000   0.1390
   0.1045  -0.1193  -0.0601        0   0.4851  -0.2319  -0.4018        0   0.0149   0.0554   0.1390   1.0000
H: Hamiltonian matrix
  -21.4000         0         0         0  -14.8089  -11.7485         0         0  -14.8569  -14.8569   -3.2014   -3.2014
         0  -11.4000         0         0   11.7485    6.5465         0         0   -5.0729   -5.0729    2.6097    2.6097
         0         0  -11.4000         0         0         0   -4.7345         0   -8.7885    8.7885   -1.3154    1.3154
         0         0         0  -11.4000         0         0         0   -4.7345         0         0         0         0
  -14.8089   11.7485         0         0  -21.4000         0         0         0   -3.2014   -3.2014  -14.8569  -14.8569
  -11.7485    6.5465         0         0         0  -11.4000         0         0   -2.6097   -2.6097    5.0729    5.0729
         0         0   -4.7345         0         0         0  -11.4000         0   -1.3154    1.3154   -8.7885    8.7885
         0         0         0   -4.7345         0         0         0  -11.4000         0         0         0         0
  -14.8569   -5.0729   -8.7885         0   -3.2014   -2.6097   -1.3154         0  -13.6000   -3.3093   -1.3190   -0.3547
  -14.8569   -5.0729    8.7885         0   -3.2014   -2.6097    1.3154         0   -3.3093  -13.6000   -0.3547   -1.3190
   -3.2014    2.6097   -1.3154         0  -14.8569    5.0729   -8.7885         0   -1.3190   -0.3547  -13.6000   -3.3093
   -3.2014    2.6097    1.3154         0  -14.8569    5.0729    8.7885         0   -0.3547   -1.3190   -3.3093  -13.6000
X_mat: Inverse square root of S:
   1.4763e+00  -8.2761e-02  -3.2306e-16  -1.4025e-16  -3.2686e-01  -3.4116e-01  -8.4944e-16   4.0155e-17  -3.2802e-01  -3.2802e-01  -1.8394e-02  -1.8394e-02
  -8.2761e-02   1.2645e+00   3.4272e-16  -1.1290e-16   3.4116e-01   3.1015e-01   1.7077e-16  -6.9972e-17  -1.7446e-01  -1.7446e-01   2.5852e-02   2.5852e-02
  -3.2306e-16   3.4272e-16   1.2210e+00  -5.7111e-17   3.3472e-17   6.5372e-16  -1.5062e-01  -9.2650e-17  -3.0473e-01   3.0473e-01   1.9158e-02  -1.9158e-02
  -1.4025e-16  -1.1290e-16  -5.7111e-17   1.0220e+00   6.5694e-17  -9.4342e-17   7.8829e-17  -1.2303e-01   2.0612e-16  -1.7813e-18  -3.4745e-17  -3.6949e-17
  -3.2686e-01   3.4116e-01   3.3472e-17   6.5694e-17   1.4763e+00   8.2761e-02   1.1198e-15   1.5899e-17  -1.8394e-02  -1.8394e-02  -3.2802e-01  -3.2802e-01
  -3.4116e-01   3.1015e-01   6.5372e-16  -9.4342e-17   8.2761e-02   1.2645e+00   4.6630e-17   1.3656e-17  -2.5852e-02  -2.5852e-02   1.7446e-01   1.7446e-01
  -8.4944e-16   1.7077e-16  -1.5062e-01   7.8829e-17   1.1198e-15   4.6630e-17   1.2210e+00   1.1286e-16   1.9158e-02  -1.9158e-02  -3.0473e-01   3.0473e-01
   4.0155e-17  -6.9972e-17  -9.2650e-17  -1.2303e-01   1.5899e-17   1.3656e-17   1.1286e-16   1.0220e+00  -1.4088e-17   6.4352e-17  -3.1987e-16   9.3497e-17
  -3.2802e-01  -1.7446e-01  -3.0473e-01   2.0612e-16  -1.8394e-02  -2.5852e-02   1.9158e-02  -1.4088e-17   1.2624e+00  -3.5047e-02  -2.0930e-02  -1.5135e-03
  -3.2802e-01  -1.7446e-01   3.0473e-01  -1.7813e-18  -1.8394e-02  -2.5852e-02  -1.9158e-02   6.4352e-17  -3.5047e-02   1.2624e+00  -1.5135e-03  -2.0930e-02
  -1.8394e-02   2.5852e-02   1.9158e-02  -3.4745e-17  -3.2802e-01   1.7446e-01  -3.0473e-01  -3.1987e-16  -2.0930e-02  -1.5135e-03   1.2624e+00  -3.5047e-02
  -1.8394e-02   2.5852e-02  -1.9158e-02  -3.6949e-17  -3.2802e-01   1.7446e-01   3.0473e-01   9.3497e-17  -1.5135e-03  -2.0930e-02  -3.5047e-02   1.2624e+00
C: MO coefficients (C matrix)
   5.0765e-01   4.0457e-01   2.4641e-16  -1.5292e-15  -6.5277e-02   4.4737e-16   6.3580e-18   4.7335e-16  -1.6750e-01  -1.5682e-15   7.4300e-01  -1.2727e+00
  -3.0743e-02   1.7188e-01   6.8736e-16   1.9940e-14   5.0903e-01  -1.4182e-15   7.1499e-17  -9.8801e-16  -9.2904e-01  -1.2198e-15   5.0085e-01   6.9075e-01
  -3.9535e-16   7.3749e-16  -3.6732e-01  -3.8434e-01   1.4460e-14   6.1618e-17  -2.8239e-16  -7.2078e-01   2.1749e-16  -9.4758e-01  -2.0177e-15   1.4511e-15
  -2.7500e-17  -1.6015e-16   1.2818e-16  -9.1035e-16  -2.0578e-15  -6.3569e-01   8.0968e-01   6.2080e-18   1.2013e-16   1.0646e-16  -9.0597e-17   1.0435e-16
   5.0765e-01  -4.0457e-01   1.2453e-16  -2.3646e-15  -6.5277e-02   1.1662e-16  -8.9274e-17   5.8920e-16   1.6750e-01  -1.3181e-15   7.4300e-01   1.2727e+00
   3.0743e-02   1.7188e-01  -5.3615e-16  -1.9379e-14  -5.0903e-01   1.8813e-15   6.4822e-17  -1.5747e-15  -9.2904e-01   6.5576e-16  -5.0085e-01   6.9075e-01
  -4.1141e-16  -1.2910e-15  -3.6732e-01   3.8434e-01  -1.4261e-14  -1.0775e-15  -3.6179e-16  -7.2078e-01   1.0781e-15   9.4758e-01   3.1480e-15   1.8451e-15
   1.1913e-17   5.4530e-16   1.3132e-15  -9.1417e-16  -2.2583e-15  -6.3569e-01  -8.0968e-01   8.3484e-18   2.0887e-17   1.7093e-16   1.5913e-16   2.7920e-17
   9.0151e-02   2.3754e-01  -2.8099e-01  -3.5150e-01   2.1021e-01  -6.6999e-16   1.5448e-16   6.0842e-01   5.3310e-01   6.0204e-01  -6.1782e-01   3.4336e-01
   9.0151e-02   2.3754e-01   2.8099e-01   3.5150e-01   2.1021e-01  -1.0624e-15  -2.1056e-17  -6.0842e-01   5.3310e-01  -6.0204e-01  -6.1782e-01   3.4336e-01
   9.0151e-02  -2.3754e-01  -2.8099e-01   3.5150e-01   2.1021e-01  -1.2495e-15   1.5134e-16   6.0842e-01  -5.3310e-01  -6.0204e-01  -6.1782e-01  -3.4336e-01
   9.0151e-02  -2.3754e-01   2.8099e-01  -3.5150e-01   2.1021e-01  -6.7002e-17  -1.1278e-16  -6.0842e-01  -5.3310e-01   6.0204e-01  -6.1782e-01  -3.4336e-01
The molecule in file /Users/vittor/Documents/CLASSES/SPRING 2024/CHEM_179_HW3/sample_input/C2H4.txt has energy -211.48 eV(b(b(b(bas(ba(ba(b(((base(b((b(((
```