Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

1. Code for calculating distance between Oxygen atoms:

```
1.  import sys
2.  import numpy as np
3.  data = np.loadtxt(sys.argv[1], skiprows=1, dtype=str)
4.  xvals = []
5.  yvals = []
6.  zvals = []
7.  for i in range(data.shape[0]):
8.      if data[i][0] == 'O':
9.          #making 3 lists of the 2 values for each cartesian coordinate of the Oxygen
    coordinates
10.         xvals.append(float(data[i][1]))
11.         yvals.append(float(data[i][2]))
12.         zvals.append(float(data[i][3]))
13. #print(xvals)
14. #print(yvals)
15. #print(zvals)
16.
17. dx = xvals[1] - xvals[0]
18. #print('dx: {}'.format(dx))
19. dy = yvals[1] - yvals[0]
20. #print('dy: {}'.format(dy))
21. dz = zvals[1] - zvals[0]
22. #print('dz: {}'.format(dz))
23.
24. distance = np.sqrt((dx**2 + dy**2 + dz**2))
25. print('The distance between oxygen atoms for the optimized structure in angstroms is:
    {}'.format(distance))
```

Q1 part a: Dimer

Q1 part a)i: E = -152.06328857476336 Hartree. Using 1 Hartree = 2625.5 KJ/mol, E = -399242.164 KJ/mol

The distance between oxygen atoms for the optimized structure is: 2.984121410099132 Angstroms.

Terminal output is subsequently highlighted in cyan:

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python optimizeHF.py dimer ccpvdz
dimer.xyz

Geometry optimization cycle 1
Cartesian coordinates (Angstrom)
 Atom        New coordinates              dX        dY        dZ
   H  -1.958940  -0.032063   0.725554    0.000000  0.000000  0.000000
   H  -0.607485   0.010955   0.056172    0.000000  0.000000  0.000000
   O  -1.538963   0.004548  -0.117331    0.000000  0.000000  0.000000
   H   1.727607   0.762122  -0.351887    0.000000  0.000000  0.000000
   H   1.704312  -0.747744  -0.399151    0.000000  0.000000  0.000000
   O   1.430776  -0.003706   0.113495    0.000000  0.000000  0.000000
converged SCF energy = -152.063106503991
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H    -0.0004238490     0.0001338854    -0.0038257059
1 H    -0.0022492883     0.0001426363    -0.0023536285
2 O     0.0027470697    -0.0002438499     0.0061707182
3 H    -0.0020874146    -0.0015053383     0.0031207283
4 H    -0.0020251779     0.0013787906     0.0032136445
5 O     0.0040386601     0.0000938759    -0.0063257566
----------------------------------------------
cycle 1: E = -152.063106504  dE = -152.063  norm(grad) = 0.0126556
***skipping down to the last cycle for the sake of brevity***
Geometry optimization cycle 16
Cartesian coordinates (Angstrom)
```

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```
 Atom        New coordinates             dX        dY        dZ
   H  -1.910063  -0.023700   0.777761   -0.000496  0.000078 -0.000380
   H  -0.647337   0.001836  -0.028233    0.000320 -0.000017  0.000650
   O  -1.593907   0.005593  -0.113180    0.000389 -0.000023 -0.000044
   H   1.766523   0.759469  -0.320254   -0.000409 -0.000028 -0.000311
   H   1.758571  -0.743298  -0.375264   -0.000214  0.000066 -0.000364
   O   1.383520  -0.005787   0.086021    0.000410 -0.000076  0.000449
converged SCF energy = -152.063288574763
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H     0.0000043756     0.0000005544     0.0000035556
1 H     0.0000181742    -0.0000231442     0.0000114243
2 O     0.0000028752     0.0000086476    -0.0000114966
3 H     0.0000147805    -0.0000070162     0.0000002374
4 H    -0.0000114972     0.0000083745    -0.0000002371
5 O    -0.0000287084     0.0000125839    -0.0000034834
----------------------------------------------
cycle 16: E = -152.063288575  dE = -2.76013e-08  norm(grad) = 5.20439e-05
converged SCF energy = -152.063288574763


************************************************************
For the optimized structure, E(HF) =  -152.06328857476336  in hartree
The optimized coordinates (in Angstroms) were outputted to  dimer.xyz

(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python distance_eval.py dimer.xyz
The distance between oxygen atoms for the optimized structure in angstroms is: 2.984121410099132
```

Q1 part a)ii: E = -152.1226374794083 Hartree. 1 Hartree = 2625.5 KJ/mol, so E = -399397.985 KJ/mol
The distance between oxygen atoms for the optimized structure in angstroms is: 3.0302632213725738

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python optimizeHF.py dimer ccpvtz
dimer_ccpvtz.xyz
Geometry optimization cycle 1
Cartesian coordinates (Angstrom)
 Atom        New coordinates             dX        dY        dZ
   H  -1.958940  -0.032063   0.725554    0.000000  0.000000  0.000000
   H  -0.607485   0.010955   0.056172    0.000000  0.000000  0.000000
   O  -1.538963   0.004548  -0.117331    0.000000  0.000000  0.000000
   H   1.727607   0.762122  -0.351887    0.000000  0.000000  0.000000
   H   1.704312  -0.747744  -0.399151    0.000000  0.000000  0.000000
   O   1.430776  -0.003706   0.113495    0.000000  0.000000  0.000000
converged SCF energy = -152.122484578778
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H    -0.0011832892    -0.0001212034     0.0026563177
1 H     0.0035131635     0.0001094257     0.0004817249
2 O    -0.0015071634     0.0000491243    -0.0033090564
3 H     0.0004351139     0.0024437048    -0.0013638617
4 H     0.0003809489    -0.0023575713    -0.0015047694
5 O    -0.0016387737    -0.0001234801     0.0030396450
----------------------------------------------
cycle 1: E = -152.122484579  dE = -152.122  norm(grad) = 0.00788733
***skipping down to the last cycle for the sake of brevity***
Geometry optimization cycle 19
Cartesian coordinates (Angstrom)
 Atom        New coordinates             dX        dY        dZ
   H  -1.955608  -0.024520   0.777526    0.001134 -0.000056  0.000585
   H  -0.678650   0.002560  -0.016540   -0.000067  0.000084 -0.001220
   O  -1.619421   0.005649  -0.099736   -0.000189  0.000247  0.000112
   H   1.804670   0.760884  -0.319134   -0.000345 -0.000050  0.000562
   H   1.799543  -0.745454  -0.371847    0.000630 -0.000008  0.000640
   O   1.406773  -0.005007   0.056584   -0.001163 -0.000216 -0.000679
converged SCF energy = -152.122637479403
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H     0.0000150348    -0.0000010658     0.0000303214
1 H     0.0000094215     0.0000112523     0.0000179934
```

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```
2 O    -0.0000408352    -0.0000054483    -0.0000522393
3 H    -0.0000120712     0.0000077897     0.0000087702
4 H    -0.0000079009    -0.0000095231     0.0000072248
5 O     0.0000363510    -0.0000030049    -0.0000120704
-----------------------------------------------
cycle 19: E = -152.122637479  dE = -5.34536e-08  norm(grad) = 8.98699e-05
converged SCF energy = -152.122637479408
***************************************************************
For the optimized structure, E(HF) =  -152.1226374794083  in hartree
The optimized coordinates (in Angstroms) were outputted to  dimer_ccpvtz.xyz
***************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python distance_eval.py
dimer_ccpvtz.xyz
The distance between oxygen atoms for the optimized structure in angstroms is: 3.0302632213725738
```

Q1 part a)iii: The CCPVTZ basis set yields a larger distance between oxygen atoms, and a more negative Hartree-Fock energy. The CCPVTZ basis set, as a Triple-Zeta basis set, means there are three basis functions for each valence orbital. For example, when comparing just a Hydrogen atom between cc-pVDZ and cc-pVTZ, the former has just the 2s and 1p orbitals, while the latter adds the 3s, 2p and 1d orbitals (the next 3 highest orbitals). Having these high energy valence polarization functions provides a more informative description of the molecule, resulting in a larger distance between the oxygen atoms, and a larger absolute energy (more stable optimized structure).

Q1 part a)iv:

In evalHF_energy.py I changed the “dimer” string to the new optimized geometry, and created two separate strings (one for each optimized monomer). The “elif” statements were also updated. Code is included at the end of the document for reference.

Interaction Energy in its own basis:

E_monomer1 = -76.02703420494112 hartree E_monomer2 = -76.02704455380736 hartree
E_dimer= -152.063288575318 hartree
Interaction energy = -0.00920981656 hartree, or -24.1803734033 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py
monomer_from_optimized_dimer  ccpvdz
converged SCF energy = -76.0270342049411
***************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02703420494112  in hartree
***************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py
monomer_from_optimized_dimer_2  ccpvdz
converged SCF energy = -76.0270445538074
***************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02704455380736  in Hartree
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py dimer ccpvdz
converged SCF energy = -152.063106503991
***************************************************************
For the current structure, E(HF( ccpvdz )) =  -152.063288575318 in hartree
***************************************************************
```

Interaction energy in the basis of the dimer using ghost atoms

In evalHF_energy.py in addition to the changes above, I created 2 strings variables, one for each monomer, in which the 3 atoms (the 2 H’s and O belonging to the other monomer) were denoted ghost-H, ghost-H, ghost-O.

E_monomer1 = -76.02737564711428 hartree E_monomomer2 = -76.02973060499913 hartree
E_dimer = -152.063288575318 hartree
Interaction Energy = -0.0061823232 hartree, or -16.2316895737 KJ/mol

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```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py
monomer_from_optimized_dimer_in_dimer_basis ccpvdz
converged SCF energy = -76.0273756471143
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02737564711428  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py
monomer_from_optimized_dimer_in_dimer_basis_2 ccpvdz
converged SCF energy = -76.0297306049991
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02973060499913  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy.py dimer ccpvdz
converged SCF energy = -152.063106503991
************************************************************
For the current structure, E(HF( ccpvdz )) =  -152.063288575318 in hartree
************************************************************
```

Q1 part b: Cage Isomer

Q1 part b)i: E = -456.24183025309077 hartree. Using 1 Hartree = 2625.5 KJ/mol, E = -1197862.92533 KJ/mol. Optimization was performed using terminal in a manner similar to Q1 part a)i.

Q1 part b)ii: Code used for this is included at the end of the document.

Interaction Energy in its own basis:

E_cage = -456.24183025215945 Ha

E_monomer1 = -76.0269342077347 Ha

E_monomer2 = -76.02697438917919 Ha

E_monomer3 = -76.02690536657963 Ha

E_monomer4 = -76.02681714556823 Ha

E_monomer5 = -76.02694572234081 Ha

E_monomer6 = -76.02666439604323 Ha

Interaction energy = -0.0805890247134471 Ha or -211.5864844 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py cage
ccpvdz
converged SCF energy = -456.241830252159
************************************************************
For the current structure, E(HF( ccpvdz )) =  -456.24183025215945  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage ccpvdz
converged SCF energy = -76.0269342077347
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.0269342077347  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage_2 ccpvdz
converged SCF energy = -76.0269743891792
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02697438917919  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage_3 ccpvdz
converged SCF energy = -76.0269053665796
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02690536657963  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage_4 ccpvdz
converged SCF energy = -76.0268171455682
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02681714556823  in hartree
************************************************************
```

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```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage_5 ccpvdz
converged SCF energy = -76.0269457223408
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02694572234081  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage.py
monomer_from_optimized_cage_6 ccpvdz
converged SCF energy = -76.0266643960432
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02666439604323  in hartree
************************************************************
```

Interaction Energy in full basis of the hexamer:

E_cage = -456.24183025215945 Ha

E_monomer1 = -76.03202749704155 Ha

E_monomer2 = -76.03195346568955 Ha

E_monomer3 = -76.03019384169043 Ha

E_monomer4 = -76.03151537627886 Ha

E_monomer5 = -76.03089701764661 Ha

E_monomer6 = -76.03182311025395 Ha

Interaction Energy = -0.0534199435583673 Ha, or -140.2540618 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis ccpvdz
converged SCF energy = -76.0320274970416
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03202749704155  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis_2 ccpvdz
converged SCF energy = -76.0319534656896
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03195346568955  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis_3 ccpvdz
converged SCF energy = -76.0301938416904
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03019384169043  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis_4 ccpvdz
converged SCF energy = -76.0315153762789
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03151537627886  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis_5 ccpvdz
converged SCF energy = -76.0308970176466
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03089701764661  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_cage_full.py
monomer_from_optimized_cage_in_cage_basis_6 ccpvdz
converged SCF energy = -76.031823110254
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03182311025395  in hartree
************************************************************
```

Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

Q1 part c: Prism Isomer

Q1 part c)i: E = –456.2436802296074 Ha, or -1197867.78244 KJ/mol. Optimization was performed using terminal in a manner similar to Q1 part a)i.

Q1 part c)ii:

Interaction Energy in its own basis:

E_prism = -456.2436802279798 Ha
E_monomer1 = -76.02666153550385 Ha
E_monomer2 = -76.02692549663814 Ha
E_monomer3 = -76.02686872424016 Ha
E_monomer4 = -76.02683812876518 Ha
E_monomer5 = -76.02699891966354 Ha
E_monomer6 = -76.02679719887885 Ha
Interaction Energy = -0.0825902242896177 Ha or -216.8406339 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
prism  ccpvdz
converged SCF energy = -456.24368022798
************************************************************
For the current structure, E(HF( ccpvdz )) =  -456.2436802279798  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism ccpvdz
converged SCF energy = -76.0266615355038
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02666153550385  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_2 ccpvdz
converged SCF energy = -76.0269254966381
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02692549663814  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_3 ccpvdz
converged SCF energy = -76.0268687242402
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02686872424016  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_4 ccpvdz
converged SCF energy = -76.0268381287652
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02683812876518  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_5 ccpvdz
converged SCF energy = -76.0269989196635
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02699891966354  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_6 ccpvdz
converged SCF energy = -76.0267971988789
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.02679719887885  in hartree
************************************************************
```

Interaction Energy in full basis of the hexamer:

E_prism = -456.2436802279798 Ha
E_monomer1 = -76.0313848272428 Ha

E_monomer2 = -76.03209492550015 Ha
E_monomer3 = -76.03161197051098 Ha
E_monomer4 = -76.03104778163367 Ha
E_monomer5 = -76.03144875333318 Ha
E_monomer6 = -76.03219199661227 Ha
Interaction energy = -0.0538999731462582 Ha, or -141.5143795 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis ccpvdz
converged SCF energy = -76.0313848272428
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03138482724276  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis_2 ccpvdz
converged SCF energy = -76.0320949255001
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03209492550015  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis_3 ccpvdz
converged SCF energy = -76.031611970511
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03161197051098  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis_4 ccpvdz
converged SCF energy = -76.0310477816337
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03104778163367  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis_5 ccpvdz
converged SCF energy = -76.0314487533332
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03144875333318  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalHF_energy_prism_full.py
monomer_from_optimized_prism_in_prism_basis_6 ccpvdz
converged SCF energy = -76.0321919966123
************************************************************
For the current structure, E(HF( ccpvdz )) =  -76.03219199661227  in hartree
************************************************************
```

Q1 part d):

The prism has the larger absolute (or more negative) E_HF and interaction energy for both evaluations (in the basis of the monomer and in the full basis of the hexamer), indicating that this is the more stable conformation. This is confirmed by Wang et al., JACS 2012 (DOI: 10.1021/ja304528m) where a CCSD(T) theory was used to yield a cage isomer structure 1.046KJ/mol above the prism isomer. This is similar to the .75 KJ/mol difference seen in the full basis interaction energy calculations between parts b)ii and c)ii. Intriguing is that the evaluation in the full basis of the hexamer decreases the E_HF by more than 70KJ/mol in both the prism and cage isomer instances, highlighting the importance of evaluating in the full basis of the hexamer.

2. DFT Calculations (NOTE: the same code for evaluating the distance between oxygen atoms is used here, just a different filename supplied).

Q2 part a: Dimer

Q2 part a)i:

E_HF = -152.78013197280234 Ha, or -401124.236495 KJ/mol

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The distance between oxygen atoms for the optimized structure in angstroms is: 2.8824509825254925

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python optimizeDFT.py dimer ccpvdz
b3lyp dimer_dftccpvdz.xyz
Geometry optimization cycle 1
Cartesian coordinates (Angstrom)
 Atom        New coordinates             dX        dY        dZ
   H  -1.958940  -0.032063   0.725554    0.000000  0.000000  0.000000
   H  -0.607485   0.010955   0.056172    0.000000  0.000000  0.000000
   O  -1.538963   0.004548  -0.117331    0.000000  0.000000  0.000000
   H   1.727607   0.762122  -0.351887    0.000000  0.000000  0.000000
   H   1.704312  -0.747744  -0.399151    0.000000  0.000000  0.000000
   O   1.430776  -0.003706   0.113495    0.000000  0.000000  0.000000
converged SCF energy = -152.776878987922
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H     0.0084697506     0.0010198988    -0.0244471124
1 H    -0.0269018875     0.0000103325    -0.0071139061
2 O     0.0159980415    -0.0010022518     0.0319533609
3 H    -0.0087584626    -0.0190972570     0.0148793119
4 H    -0.0081511015     0.0183970005     0.0160435294
5 O     0.0193350674     0.0006722992    -0.0313116057
-----------------------------------------------
cycle 1: E = -152.776878988  dE = -152.777  norm(grad) = 0.0735019
***skipping down to the last cycle for the sake of brevity***
Geometry optimization cycle 23
Cartesian coordinates (Angstrom)
 Atom        New coordinates             dX        dY        dZ
   H  -1.871152  -0.042177   0.724929   -0.000357 -0.002125 -0.001114
   H  -0.514243   0.016612   0.045582    0.000629  0.001530  0.001601
   O  -1.469850   0.010591  -0.154795    0.000980  0.001309 -0.000289
   H   1.626166   0.766953  -0.364120   -0.001509 -0.000516 -0.001451
   H   1.593118  -0.754526  -0.402809   -0.001604 -0.000340  0.000368
   O   1.393268  -0.003342   0.178066    0.001861  0.000142  0.000885
converged SCF energy = -152.780131972772
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 H    -0.0000569265    -0.0000021591     0.0000338650
1 H    -0.0000322600    -0.0000016637    -0.0000309906
2 O     0.0001071142     0.0000029260     0.0000075062
3 H     0.0000041214     0.0000655921    -0.0000073857
4 H     0.0000131310    -0.0000765500    -0.0000183833
5 O    -0.0000346489     0.0000060667     0.0000201102
-----------------------------------------------
cycle 23: E = -152.780131973  dE = -2.3648e-07  norm(grad) = 0.000174127
converged SCF energy = -152.780131972802
************************************************************
For the optimized structure, E(HF) =  -152.78013197280234  in hartree
The optimized coordinates (in Angstroms) were outputted to  dimer_dftccpvdz.xyz
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python distance_eval.py
dimer_dftccpvdz.xyz
The distance between oxygen atoms for the optimized structure in angstroms is: 2.8824509825254925
```

Q2 part a)ii:

E_HF = -152.85514622272578 Ha, -401321.186408 KJ/mol

The distance between oxygen atoms for the optimized structure in angstroms is: 2.911214724642932

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python optimizeDFT.py dimer ccpvtz
b3lyp dimer_dftccpvtz.xyz
Geometry optimization cycle 1
Cartesian coordinates (Angstrom)
 Atom        New coordinates             dX        dY        dZ
   H  -1.958940  -0.032063   0.725554    0.000000  0.000000  0.000000
   H  -0.607485   0.010955   0.056172    0.000000  0.000000  0.000000
```

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```
   O  -1.538963   0.004548  -0.117331    0.000000  0.000000  0.000000
   H   1.727607   0.762122  -0.351887    0.000000  0.000000  0.000000
   H   1.704312  -0.747744  -0.399151    0.000000  0.000000  0.000000
   O   1.430776  -0.003706   0.113495    0.000000  0.000000  0.000000
converged SCF energy = -152.853640088906
--------------- SCF_Scanner gradients ---------------
        x               y               z
0 H     0.0077265573     0.0007341931    -0.0172231391
1 H    -0.0203753406    -0.0000304369    -0.0040780794
2 O     0.0113989436    -0.0006692657     0.0214014086
3 H    -0.0061494966    -0.0147746674     0.0098949029
4 H    -0.0056738944     0.0143157826     0.0108067532
5 O     0.0130690720     0.0004256933    -0.0207993276
----------------------------------------------
cycle 1: E = -152.853640089  dE = -152.854  norm(grad) = 0.0518517
***skipping down to the last cycle for the sake of brevity***
Geometry optimization cycle 14
Cartesian coordinates (Angstrom)
 Atom        New coordinates              dX        dY        dZ
   H  -1.911665  -0.026834   0.741182    0.001689  0.000045  0.000042
   H  -0.560606   0.004350   0.028940    0.000403 -0.000098  0.000079
   O  -1.515895   0.006528  -0.133572    0.000427  0.000085 -0.000674
   H   1.687675   0.771777  -0.345238   -0.000974 -0.000045  0.000151
   H   1.674718  -0.755357  -0.397088   -0.000781  0.000070  0.000146
   O   1.383080  -0.006352   0.132628   -0.000764 -0.000057  0.000257
converged SCF energy = -152.855146222667
--------------- SCF_Scanner gradients ---------------
        x               y               z
0 H    -0.0000356492    -0.0000008346    -0.0000320743
1 H    -0.0000071414     0.0000202574    -0.0000461329
2 O     0.0000421374    -0.0000146292     0.0000920454
3 H     0.0000384435     0.0000124150    -0.0000085844
4 H     0.0000391492    -0.0000188816    -0.0000140279
5 O    -0.0000778740     0.0000016693     0.0000101968
----------------------------------------------
cycle 14: E = -152.855146223  dE = -6.74955e-07  norm(grad) = 0.000159106
converged SCF energy = -152.855146222726
************************************************************
For the optimized structure, E(HF) =  -152.85514622272578  in hartree
The optimized coordinates (in Angstroms) were outputted to  dimer_dftccpvtz.xyz
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python distance_eval.py
dimer_dftccpvtz.xyz
The distance between oxygen atoms for the optimized structure in angstroms is: 2.911214724642932
```

Q2 part a)iii:

Just as seen in the Hartree-Fock section, the CCPVTZ basis set yields a larger distance between oxygen atoms, and a more negative Hartree-Fock energy (almost 200 KJ/mol). This is because of the additional basis functions included for each higher energy valence orbital for an atom, compared to only the lower energy valence orbitals being accounted for in CCPVDZ.

Q2 part a)iv:

Interaction Energy in its own basis:

E_dimer = -152.7801319718138 Ha

E_monomer1 = -76.38343170668335 Ha

E_monomer2 = -76.38346792580269 Ha

Interaction Energy = -0.0132323393271179 Ha, or -34.7415069 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py dimer ccpvdz
b3lyp
converged SCF energy = -152.780131971814
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -152.7801319718138  in hartree
```

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```
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_dimer ccpvdz b3lyp
converged SCF energy = -76.3834317066834
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38343170668335  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_dimer_2 ccpvdz b3lyp
converged SCF energy = -76.3834679258027
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38346792580269  in hartree
************************************************************
```

Interaction Energy in full basis of the dimer:

E_dimer = -152.7801319718138 Ha

E_monomer1 = -76.3841416289346 Ha

E_monomer2 = -76.38922920261312 Ha

Interaction Energy = -0.0067611402652972 Ha, or -17.75137377 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_dimer_in_dimer_basis ccpvdz b3lyp
converged SCF energy = -76.3841416289346
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3841416289346  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_dimer_in_dimer_basis_2 ccpvdz b3lyp
converged SCF energy = -76.3892292026131
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38922920261312  in hartree
************************************************************
```

Q2 part b: Cage Isomer

Q2 part b)i: -458.42411308302513 Ha, or -1203592.5089 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python optimizeDFT.py cage ccpvdz
b3lyp cage_dftccpvdz.xyz
Geometry optimization cycle 1
Cartesian coordinates (Angstrom)
 Atom        New coordinates              dX        dY        dZ
   O   0.803889   0.381762  -1.685143    0.000000  0.000000  0.000000
   H   0.362572  -0.448201  -1.556674    0.000000  0.000000  0.000000
   H   1.668734   0.275528  -1.301550    0.000000  0.000000  0.000000
   O   0.666169  -0.420958   1.707749    0.000000  0.000000  0.000000
   H   0.236843   0.404385   1.523931    0.000000  0.000000  0.000000
   H   0.226003  -1.053183   1.153395    0.000000  0.000000  0.000000
   O   2.996112   0.001740   0.125207    0.000000  0.000000  0.000000
   H   2.356345  -0.159970   0.813642    0.000000  0.000000  0.000000
   H   3.662033  -0.660038   0.206711    0.000000  0.000000  0.000000
   O  -0.847903  -1.777751  -0.469278    0.000000  0.000000  0.000000
   H  -1.654759  -1.281222  -0.344427    0.000000  0.000000  0.000000
   H  -1.091666  -2.653858  -0.718356    0.000000  0.000000  0.000000
   O  -2.898828   0.065636   0.089967    0.000000  0.000000  0.000000
   H  -3.306527   0.037245   0.940083    0.000000  0.000000  0.000000
   H  -2.312757   0.817025   0.097526    0.000000  0.000000  0.000000
   O  -0.655160   1.814997   0.176741    0.000000  0.000000  0.000000
   H  -0.134384   1.449649  -0.543456    0.000000  0.000000  0.000000
   H  -0.526672   2.749233   0.167243    0.000000  0.000000  0.000000
converged SCF energy = -458.407765358838
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 O     0.0144520566    -0.0306337189     0.0154258388
1 H     0.0116934963     0.0246903147    -0.0067838199
```

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```
2 H    -0.0248536095     0.0059439786    -0.0146905864
3 O    -0.0285072166     0.0058192924    -0.0226324909
4 H     0.0138290706    -0.0229511437     0.0089837173
5 H     0.0143412572     0.0159123350     0.0186805147
6 O     0.0018572765    -0.0268420607     0.0256774619
7 H     0.0199266912     0.0068633512    -0.0203468630
8 H    -0.0163730664     0.0194992044    -0.0036013875
9 O    -0.0352260457    -0.0135450329    -0.0041324554
10 H     0.0255760025    -0.0145735767    -0.0044746471
11 H     0.0085992181     0.0230900554     0.0065406702
12 O     0.0043079095     0.0237908338     0.0279996031
13 H     0.0089978836    -0.0007248788    -0.0241969350
14 H    -0.0183449677    -0.0223757669    -0.0026197686
15 O     0.0219279049     0.0197137183    -0.0240618288
16 H    -0.0175520906     0.0113311465     0.0225248547
17 H    -0.0046645472    -0.0250247751     0.0017002771
----------------------------------------------
cycle 1: E = -458.407765359  dE = -458.408  norm(grad) = 0.133473
***skipping down to the last cycle for the sake of brevity***
Geometry optimization cycle 41
Cartesian coordinates (Angstrom)
 Atom        New coordinates              dX        dY        dZ
   O   0.804482   0.440629  -1.648352    0.000058  0.000138  0.000006
   H   0.330822  -0.405965  -1.506660    0.000120  0.000051 -0.000307
   H   1.641032   0.308131  -1.131273   -0.000044  0.000025  0.000171
   O   0.552028  -0.350741   1.680167   -0.000373  0.000003 -0.000009
   H   0.144554   0.491103   1.383851   -0.000250  0.000001 -0.000199
   H   0.155393  -0.994495   1.055700   -0.000138 -0.000020 -0.000152
   O   2.786649   0.009090   0.171015   -0.000154 -0.000115  0.000197
   H   2.085235  -0.134430   0.860669   -0.000350  0.000017  0.000031
   H   3.239350  -0.845818   0.117067   -0.000368 -0.000229  0.000211
   O  -0.712042  -1.641399  -0.496259    0.000169 -0.000148 -0.000196
   H  -1.566677  -1.152272  -0.326862    0.000216 -0.000111  0.000037
   H  -0.969697  -2.544134  -0.732503    0.000020 -0.000119 -0.000162
   O  -2.727078  -0.004259   0.148778    0.000299 -0.000049  0.000424
   H  -2.872261  -0.107792   1.102356    0.000803 -0.000130  0.000493
   H  -2.122812   0.779135   0.098394    0.000130  0.000065  0.000113
   O  -0.630972   1.699546   0.131423    0.000009  0.000210 -0.000262
   H  -0.064872   1.334421  -0.630220   -0.000097  0.000198 -0.000236
   H  -0.523088   2.661268   0.106021   -0.000050  0.000212 -0.000159
converged SCF energy = -458.424113083035
--------------- SCF_Scanner gradients ---------------
         x                y                z
0 O     0.0000202030    -0.0000173421     0.0000080070
1 H     0.0000018392     0.0000104207     0.0000123606
2 H    -0.0000082343     0.0000017547     0.0000025565
3 O    -0.0000210064     0.0000034062    -0.0000284651
4 H     0.0000185836     0.0000040712     0.0000092226
5 H     0.0000143511     0.0000014589     0.0000190186
6 O    -0.0000058909    -0.0000009055    -0.0000045766
7 H     0.0000069225     0.0000068258    -0.0000148431
8 H    -0.0000038858    -0.0000025107     0.0000067635
9 O     0.0000036552     0.0000132056    -0.0000046059
10 H     0.0000018137    -0.0000262753    -0.0000018147
11 H    -0.0000106296     0.0000009806    -0.0000007920
12 O    -0.0000021304     0.0000077877    -0.0000011407
13 H     0.0000037027    -0.0000039477    -0.0000032889
14 H    -0.0000067298     0.0000037778     0.0000037103
15 O    -0.0000151291     0.0000001964     0.0000259489
16 H     0.0000038396    -0.0000128093    -0.0000174617
17 H     0.0000013500    -0.0000021696    -0.0000031298
----------------------------------------------
cycle 41: E = -458.424113083  dE = -4.63437e-08  norm(grad) = 8.02267e-05
converged SCF energy = -458.424113083025
************************************************************
For the optimized structure, E(HF) =  -458.42411308302513  in hartree
The optimized coordinates (in Angstroms) were outputted to  cage_dftccpvdz.xyz
```

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Q2 part b)ii:

Interaction Energy in its own basis:

E_cage = -458.424113083512 Ha
E_monomer1 = -76.38289505373156 Ha
E_monomer2 = -76.38322800430892 Ha
E_monomer3 = -76.38285824098992 Ha
E_monomer4 = -76.38238052168681 Ha
E_monomer5 = -76.38305542602583 Ha
E_monomer6 = -76.38115531533391 Ha
Interaction energy = -0.1285405214351840 Ha or -337.483139 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage ccpvdz b3lyp
converged SCF energy = -76.3828950537316
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38289505373156  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_2 ccpvdz b3lyp
converged SCF energy = -76.3832280043089
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38322800430892  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_3 ccpvdz b3lyp
converged SCF energy = -76.3828582409899
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38285824098992  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_4 ccpvdz b3lyp
converged SCF energy = -76.3823805216868
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38238052168681  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_5 ccpvdz b3lyp
converged SCF energy = -76.3830554260258
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38305542602583  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_6 ccpvdz b3lyp
converged SCF energy = -76.3811553153339
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38115531533391  in hartree
************************************************************
```

Interaction Energy in full basis of the hexamer:

E_cage = -458.424113083512 Ha
E_monomer1 = -76.39306060169139 Ha
E_monomer2 = -76.39293642268254 Ha
E_monomer3 = -76.3901028292451 Ha
E_monomer4 = -76.3917674474688 Ha
E_monomer5 = -76.39153246324155 Ha
E_monomer6 = -76.39156072907431 Ha
Interaction energy = -0.0731525901085206 Ha, or -192.0621253 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis ccpvdz b3lyp
```

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```
converged SCF energy = -76.3930606016914
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39306060169139  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis_2 ccpvdz b3lyp
converged SCF energy = -76.3929364226825
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39293642268254  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis_3 ccpvdz b3lyp
converged SCF energy = -76.3901028292451
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3901028292451  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis_4 ccpvdz b3lyp
converged SCF energy = -76.3917674474688
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3917674474688  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis_5 ccpvdz b3lyp
converged SCF energy = -76.3915324632415
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39153246324155  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_cage_in_cage_basis_6 ccpvdz b3lyp
converged SCF energy = -76.3915607290743
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39156072907431  in hartree
*************************************************************
```

Q2 part c: Prism Isomer

Q2 part c)i: E = -458.4266166987306 Ha, or -1203599.08214 KJ/mol

Q2 part c)ii:

Interaction Energy in its own basis:

E_cage = -458.42661669789516 Ha
E_monomer1 = -76.38111214477667 Ha
E_monomer2 = -76.3831553728805 Ha
E_monomer3 = -76.38269860604935 Ha
E_monomer4 = -76.38245584924707 Ha
E_monomer5 = -76.38328606607303 Ha
E_monomer6 = -76.38266129482503 Ha
Interaction energy = -0.1312473640436450 Ha, or -344.5899543 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py prism ccpvdz
b3lyp
converged SCF energy = -458.426616697895
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -458.42661669789516  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism ccpvdz b3lyp
converged SCF energy = -76.3811121447767
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38111214477667  in hartree
*************************************************************
```

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```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_2 ccpvdz b3lyp
converged SCF energy = -76.3831553728805
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3831553728805  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_3 ccpvdz b3lyp
converged SCF energy = -76.3826986060493
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38269860604935  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_4 ccpvdz b3lyp
converged SCF energy = -76.3824558492471
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38245584924707  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_5 ccpvdz b3lyp
converged SCF energy = -76.383286066073
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38328606607303  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_6 ccpvdz b3lyp
converged SCF energy = -76.382661294825
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.38266129482503  in hartree
```

Interaction Energy in full basis of the hexamer:

E_cage= −458.42661669789516 Ha
E_monomer1 = −76.39066866869578 Ha
E_monomer2 = −76.3935114123197 Ha
E_monomer3 = −76.39249710623638 Ha
E_monomer4 = −76.3911039639473 Ha
E_monomer5 = −76.39228310638224 Ha
E_monomer6 = −76.3935366235741 Ha
Interaction energy = -0.0730158167396553 Ha, or -191.7030268 KJ/mol

```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis ccpvdz b3lyp
converged SCF energy = -76.3906686686958
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39066866869578  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis_2 ccpvdz b3lyp
converged SCF energy = -76.3935114123197
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3935114123197  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis_3 ccpvdz b3lyp
converged SCF energy = -76.3924971062364
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39249710623638  in hartree
************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis_4 ccpvdz b3lyp
converged SCF energy = -76.3911039639473
************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3911039639473  in hartree
************************************************************
```

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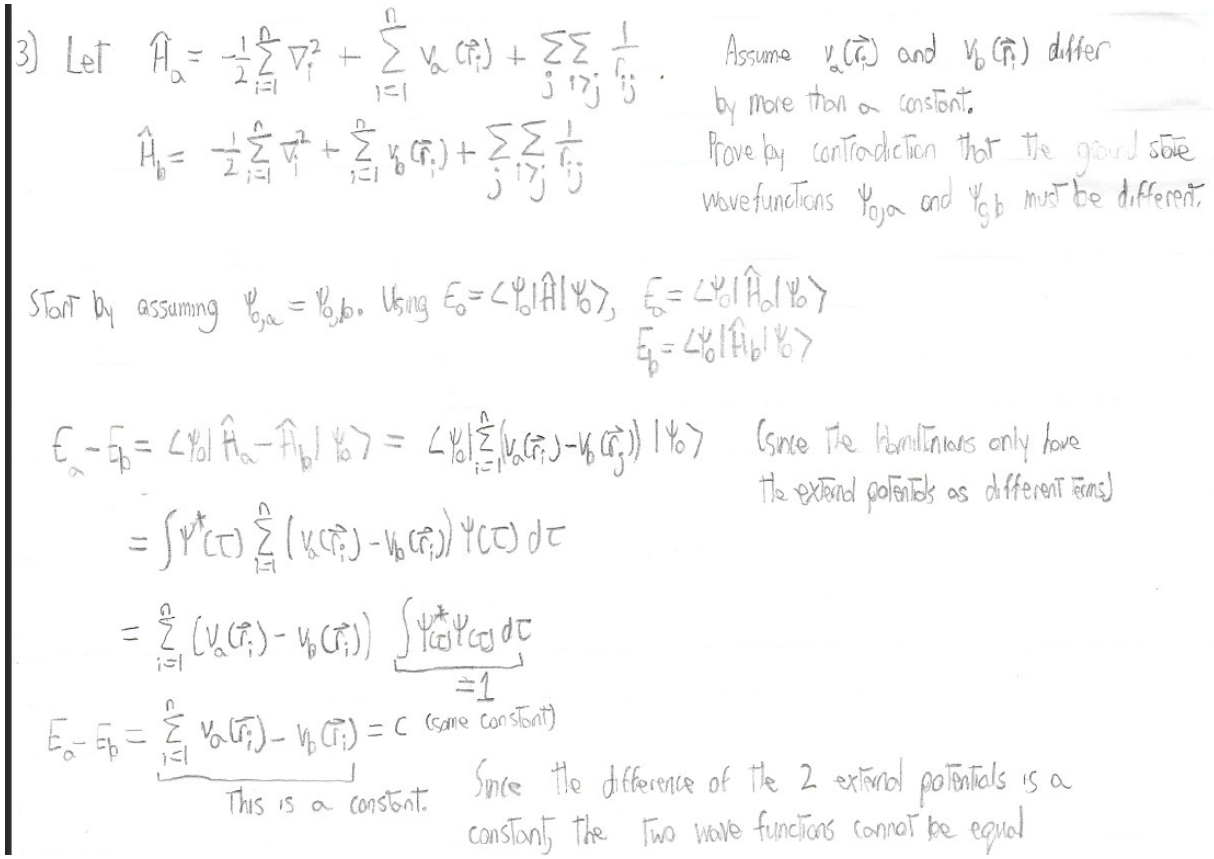
```
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis_5 ccpvdz b3lyp
converged SCF energy = -76.3922831063822


*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.39228310638224  in hartree
*************************************************************
(python.ne452) Sahad-Vasanjis-MacBook-Pro:a3_code Sahad_V$ python evalDFT_energy.py
monomer_from_optimized_prism_in_prism_basis_6 ccpvdz b3lyp
converged SCF energy = -76.3935366235741
*************************************************************
For the current structure, E( b3lyp , ccpvdz ) =  -76.3935366235741  in hartree
*************************************************************
```

Q2 part d):

Using DFT calculations, we see that the cage has the more stable structure (larger absolute Energy, or more negative energy) when evaluated in the full basis of the hexamer. This is seen when comparing the -191.7KJ/mol to -192.06 KJ/mol, and is in contrast to the Hartree-Fock results in question 1. However, when evaluating only in the basis of the monomer, the prism is more stable than the cage (-344 KJ/mol vs. -337KJ/mol). It's also important to notice in the HF calculations of Question 1, the prism's optimized structure was the more stable isomer regardless of basis used, but here that's not the case. As well, DFT calculations present a much larger contrast between full basis evaluation versus monomer-basis evaluation when compared to HF calculations.

Question 3:



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Question 4:

4) Consider an individual water monomer with 2 internal energy expressions: $E_{oH\text{-}bond}(r) = k_r(r-r_{eq})^2$

$E_{HoH\text{-}angle}(\theta) = k_\theta(\theta-\theta_{eq})^2$

Where $k_r = 450\ \frac{kJ}{mol}$, $k_\theta = 55\ \frac{kJ}{mol/deg^2}$

$r_{eq} = .9572\text{Å}$ $\theta_{eq} = 104.52^\circ$

If you set the position of the oxygen atom at (0,0), what are possible coordinates for the Hydrogen atoms for the minimized structure in Å?

When $E_{bond} = 0$, $r = r_{eq} = .9572\text{Å}$ and $E_{angle} = 0$, $\theta = \theta_{eq} = 104.52^\circ$ } This bond angle and bond length elicit the minimum bond energy, and the minimum H-O-H angle energy.

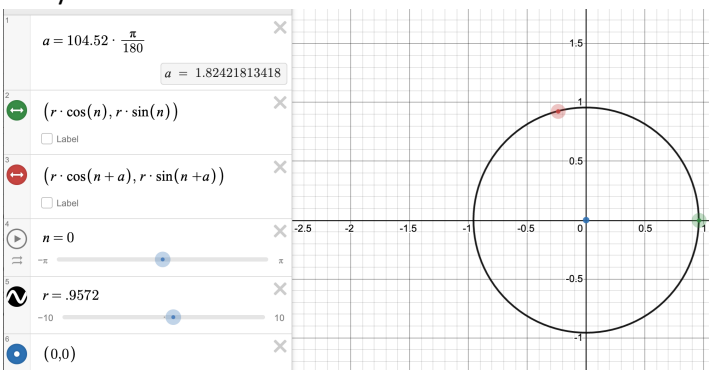
If this is a minimized energy structure, both O-H bond lengths must be the same, or equal .9572Å
As well, the angle between the two bonds must be constant, or stay at 104.52°

Denoting $\vec{v}_1 \equiv$ First oxygen-hydrogen bond
$\vec{v}_2 \equiv$ Second O-H bond

$||\vec{v}_1|| = ||\vec{v}_2|| = r_{eq}$ and $\theta = \cos^{-1}\left(\frac{\vec{v}_1 \cdot \vec{v}_2}{||\vec{v}_1||\,||\vec{v}_2||}\right) = 104.52^\circ$

If Oxygen is at the origin, and this is a 2D system (since the origin was given as (0,0)), both H's stay .9572Å away from the oxygen atom. This means the allowable coordinates for the H's, or hydrogen atoms, are along the circumference of a circle with radius .9572Å, provided the 2 H atoms have separation by arc length $s = r_{eq}\theta_{eq} = .9572\text{Å} \times 104.52^\circ \times \frac{\pi}{180^\circ} = 1.746142\text{ Å}$

If the protocol in the following image is observed in Desmos (an online graphing calculator), we can verify the above coordinates:



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Eval_HF Code for Question 1a)iv:

```
from pyscf import gto, scf
from pyscf.geomopt.berny_solver import optimize
from sys import argv, exit

#Cartesian coordinates in angstroms for water dimer
#dimer = '''
#H       -1.958940   -0.032063    0.725554
#H       -0.607485    0.010955    0.056172
#O       -1.538963    0.004548   -0.117331
#H        1.727607    0.762122   -0.351887
#H        1.704312   -0.747744   -0.399151
#O        1.430776   -0.003706    0.113495'''

dimer = '''
H -1.910073232120457 -0.023700616859325573 0.7777653730901837
H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
H 1.7665326391220741 0.759472532838855 -0.32025546132092003
H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
O 1.3835276501924945 -0.005786797280116391 0.08602171452506603'''

#Cartesian coordinates in angstroms for cage isomer of water hexamer
cage = '''
O         0.803889    0.381762   -1.685143
H         0.362572   -0.448201   -1.556674
H         1.668734    0.275528   -1.301550
O         0.666169   -0.420958    1.707749
H         0.236843    0.404385    1.523931
H         0.226003   -1.053183    1.153395
O         2.996112    0.001740    0.125207
H         2.356345   -0.159970    0.813642
H         3.662033   -0.660038    0.206711
O        -0.847903   -1.777751   -0.469278
H        -1.654759   -1.281222   -0.344427
H        -1.091666   -2.653858   -0.718356
O        -2.898828    0.065636    0.089967
H        -3.306527    0.037245    0.940083
H        -2.312757    0.817025    0.097526
O        -0.655160    1.814997    0.176741
H        -0.134384    1.449649   -0.543456
H        -0.526672    2.749233    0.167243'''

#Cartesian coordinates in angstroms for prism isomer of water hexamer
prism = '''
O                  1.526924   -0.407825    1.467087
H                  0.615293   -0.694811    1.569578
H                  2.001971   -0.712098    2.222674
O                  0.831994    2.016713   -0.073306
H                  1.169971    1.534473    0.670375
H                  1.181010    1.553886   -0.823001
O                  1.709464   -0.492590   -1.370853
H                  2.421392   -0.900609   -1.835542
H                  1.839304   -0.657788   -0.441680
O                 -1.891336    1.277844   -0.075746
H                 -1.013035    1.654737   -0.078267
H                 -2.500751    1.992871   -0.154652
O                 -1.172193   -1.306705   -1.416807
H                 -0.263214   -1.117130   -1.610277
H                 -1.591494   -0.462719   -1.314422
```

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```
O                  -1.135583   -1.129560    1.451997
H                  -1.200738   -1.536124    0.593247
H                  -1.613872   -0.317697    1.342986'''

#You will need to create these coordinates variables using the output of optimizeHF.py
#For example, if you only want to get E(HF) for a water monomer from the optimized water dimer
monomer_from_optimized_dimer = '''
H -1.910073232120457 -0.023700616859325573 0.7777653730901837
H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
'''

monomer_from_optimized_dimer_2 = '''
H 1.7665326391220741 0.759472532838855 -0.32025546132092003
H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
'''
#For example, if you want to get E(HF) for a water monomer from the optimized water dimer
#but in the basis of the full dimer, you need to 'ghost' the non-relevant atoms
#This allows for orbital mixing between monomers but removes the charges for the 2nd monomer
monomer_from_optimized_dimer_in_dimer_basis='''
H -1.910073232120457 -0.023700616859325573 0.7777653730901837
H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
ghost-H 1.7665326391220741 0.759472532838855 -0.32025546132092003
ghost-H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
ghost-O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
'''
monomer_from_optimized_dimer_in_dimer_basis_2='''
ghost-H -1.910073232120457 -0.023700616859325573 0.7777653730901837
ghost-H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
ghost-O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
H 1.7665326391220741 0.759472532838855 -0.32025546132092003
H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
'''
#Specify the molecule
clus = argv[1]
if clus == 'dimer':
    cluster = dimer
elif clus == 'cage':
    cluster = cage
elif clus == 'prism':
    cluster = prism
elif clus == 'monomer_from_optimized_dimer' :
    cluster = monomer_from_optimized_dimer
elif clus == 'monomer_from_optimized_dimer_2' :
    cluster = monomer_from_optimized_dimer_2
elif clus == 'monomer_from_optimized_dimer_in_dimer_basis':
    cluster = monomer_from_optimized_dimer_in_dimer_basis
elif clus == 'monomer_from_optimized_dimer_in_dimer_basis_2':
    cluster = monomer_from_optimized_dimer_in_dimer_basis_2
#Possible basis sets include:
#ccpvdz
#ccpvtz
#ccpvqz
basis = argv[2]

mol = gto.Mole()
#Set verbose to 3,4,5 depending on how much output you want to see from the calculation
mol.verbose = 3
```

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```
mol.atom = cluster
mol.basis = basis
mol.build()
mf = scf.RHF(mol)

HF_energy = mf.kernel()
print('\n\n************************************************************')

print('For the current structure, E(HF(',basis,')) = ', HF_energy, ' in hartree')


print('************************************************************')
```

Eval_HF Code used for Question 1b)ii in the monomer basis:

```
from pyscf import gto, scf
from pyscf.geomopt.berny_solver import optimize
from sys import argv, exit

#Cartesian coordinates in angstroms for optimized cage isomer of water hexamer
cage = '''
O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
O 0.6289918836743734 -0.39682689707154317 1.701783662513783
H 0.19869210273321308 0.4250933664954657 1.49006502670088
H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
O 2.996874626833252 -0.023210810895334923 0.13646764406951148
H 2.347256293497991 -0.16160099579680304 0.8246209926372199
H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
O -2.894141056494115 0.038057451027571014 0.14090464395327157
H -3.2497362664724694 0.01817386909810281 1.0182145178872812
H -2.321519085665555 0.8030719139507743 0.1224165566401051
O -0.6719074651628764 1.8308269660174914 0.15346584816264947
H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
H -0.5296403762327344 2.766445604416275 0.1447134753637766'''


#You will need to create these coordinates variables using the output of optimizeHF.py
#For example, if you only want to get E(HF) for a water monomer from the optimized water dimer
monomer_from_optimized_cage = '''
O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
'''

monomer_from_optimized_cage_2 = '''
O 0.6289918836743734 -0.39682689707154317 1.701783662513783
H 0.19869210273321308 0.4250933664954657 1.49006502670088
H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
'''

monomer_from_optimized_cage_3 = '''
O 2.996874626833252 -0.023210810895334923 0.13646764406951148
H 2.347256293497991 -0.16160099579680304 0.8246209926372199
H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
'''
```

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```
46.
47. monomer_from_optimized_cage_4 = '''
48. O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
49. H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
50. H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
51. '''
52.
53. monomer_from_optimized_cage_5 = '''
54. O -2.894141056494115 0.038057451027571014 0.14090464395327157
55. H -3.2497362664724694 0.01817386909810281 1.0182145178872812
56. H -2.321519085665555 0.8030719139507743 0.1224165566401051
57. '''
58.
59. monomer_from_optimized_cage_6 = '''
60. O -0.6719074651628764 1.8308269660174914 0.15346584816264947
61. H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
62. H -0.5296403762327344 2.766445604416275 0.1447134753637766
63. '''
64.
65. #For example, if you want to get E(HF) for a water monomer from the optimized water dimer
66. #but in the basis of the full dimer, you need to 'ghost' the non-relevant atoms
67. #This allows for orbital mixing between monomers but removes the charges for the 2nd monomer
68. monomer_from_optimized_dimer_in_dimer_basis='''
69. H -1.910073232120457 -0.023700616859325573 0.7777653730901837
70. H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
71. O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
72. ghost-H 1.7665326391220741 0.759472532838855 -0.32025546132092003
73. ghost-H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
74. ghost-O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
75. '''
76. monomer_from_optimized_dimer_in_dimer_basis_2='''
77. ghost-H -1.910073232120457 -0.023700616859325573 0.7777653730901837
78. ghost-H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
79. ghost-O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
80. H 1.7665326391220741 0.759472532838855 -0.32025546132092003
81. H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
82. O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
83. '''
84. #Specify the molecule
85. clus = argv[1]
86. if clus == 'cage':
87.     cluster = cage
88. elif clus == 'monomer_from_optimized_cage':
89.     cluster = monomer_from_optimized_cage
90. elif clus == 'monomer_from_optimized_cage_2' :
91.     cluster = monomer_from_optimized_cage_2
92. elif clus == 'monomer_from_optimized_cage_3' :
93.     cluster = monomer_from_optimized_cage_3
94. elif clus == 'monomer_from_optimized_cage_4':
95.     cluster = monomer_from_optimized_cage_4
96. elif clus == 'monomer_from_optimized_cage_5':
97.     cluster = monomer_from_optimized_cage_5
98. elif clus == 'monomer_from_optimized_cage_6':
99.     cluster = monomer_from_optimized_cage_6
100.
101.#Possible basis sets include:
102.#ccpvdz
103.#ccpvtz
104.#ccpvqz
105.basis = argv[2]
106.
```

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```
mol = gto.Mole()
#Set verbose to 3,4,5 depending on how much output you want to see from the calculation
mol.verbose = 3
mol.atom = cluster
mol.basis = basis
mol.build()
mf = scf.RHF(mol)

HF_energy = mf.kernel()
print('\n\n************************************************************')

print('For the current structure, E(HF(',basis,')) = ', HF_energy, ' in hartree')


print('************************************************************')
```

Eval_HF Code used for Question 1b)ii in the full basis:

```
from pyscf import gto, scf
from pyscf.geomopt.berny_solver import optimize
from sys import argv, exit

#Cartesian coordinates in angstroms for optimized cage isomer of water hexamer
cage = '''
O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
O 0.6289918836743734 -0.39682689707154317 1.701783662513783
H 0.19869210273321308 0.4250933664954657 1.49006502670088
H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
O 2.996874626833252 -0.023210810895334923 0.13646764406951148
H 2.347256293497991 -0.16160099579680304 0.8246209926372199
H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
O -2.894141056494115 0.038057451027571014 0.14090464395327157
H -3.2497362664724694 0.01817386909810281 1.0182145178872812
H -2.321519085665555 0.8030719139507743 0.1224165566401051
O -0.6719074651628764 1.8308269660174914 0.15346584816264947
H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
H -0.5296403762327344 2.766445604416275 0.1447134753637766'''


#You will need to create these coordinates variables using the output of optimizeHF.py
#For example, if you only want to get E(HF) for a water monomer from the optimized water dimer
monomer_from_optimized_cage = '''
O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
'''

monomer_from_optimized_cage_2 = '''
O 0.6289918836743734 -0.39682689707154317 1.701783662513783
H 0.19869210273321308 0.4250933664954657 1.49006502670088
H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
'''

monomer_from_optimized_cage_3 = '''
```

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```
O 2.996874626833252 -0.023210810895334923 0.13646764406951148
H 2.347256293497991 -0.16160099579680304 0.8246209926372199
H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
'''

monomer_from_optimized_cage_4 = '''
O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
'''

monomer_from_optimized_cage_5 = '''
O -2.894141056494115 0.038057451027571014 0.14090464395327157
H -3.2497362664724694 0.01817386909810281 1.0182145178872812
H -2.321519085665555 0.8030719139507743 0.1224165566401051
'''

monomer_from_optimized_cage_6 = '''
O -0.6719074651628764 1.8308269660174914 0.15346584816264947
H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
H -0.5296403762327344 2.766445604416275 0.1447134753637766
'''

#For example, if you want to get E(HF) for a water monomer from the optimized water dimer
#but in the basis of the full dimer, you need to 'ghost' the non-relevant atoms
#This allows for orbital mixing between monomers but removes the charges for the 2nd monomer
monomer_from_optimized_dimer_in_dimer_basis='''
H -1.910073232120457 -0.023700616859325573 0.7777653730901837
H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
ghost-H 1.7665326391220741 0.759472532838855 -0.32025546132092003
ghost-H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
ghost-O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
'''
monomer_from_optimized_dimer_in_dimer_basis_2='''
ghost-H -1.910073232120457 -0.023700616859325573 0.7777653730901837
ghost-H -0.64734003226218 0.0018357461631999196 -0.028233534328845417
ghost-O -1.5939158376833815 0.0055931900328505205 -0.1131800992375836
H 1.7665326391220741 0.759472532838855 -0.32025546132092003
H 1.7585798042116998 -0.7433020859287404 -0.3752658512018215
O 1.3835276501924945 -0.005786797280116391 0.08602171452506603
'''
monomer_from_optimized_cage_in_cage_basis = '''
O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
ghost-O 0.6289918836743734 -0.39682689707154317 1.701783662513783
ghost-H 0.19869210273321308 0.4250933664954657 1.49006502670088
ghost-H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
ghost-O 2.996874626833252 -0.023210810895334923 0.13646764406951148
ghost-H 2.347256293497991 -0.16160099579680304 0.8246209926372199
ghost-H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
ghost-O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
ghost-H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
ghost-H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
ghost-O -2.894141056494115 0.038057451027571014 0.14090464395327157
ghost-H -3.2497362664724694 0.01817386909810281 1.0182145178872812
ghost-H -2.321519085665555 0.8030719139507743 0.1224165566401051
ghost-O -0.6719074651628764 1.8308269660174914 0.15346584816264947
ghost-H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
ghost-H -0.5296403762327344 2.766445604416275 0.1447134753637766'''
```

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```
103.
104.monomer_from_optimized_cage_in_cage_basis_2 = '''
105.ghost-O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
106.ghost-H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
107.ghost-H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
108.O 0.6289918836743734 -0.39682689707154317 1.701783662513783
109.H 0.19869210273321308 0.4250933664954657 1.49006502670088
110.H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
111.ghost-O 2.996874626833252 -0.023210810895334923 0.13646764406951148
112.ghost-H 2.347256293497991 -0.16160099579680304 0.8246209926372199
113.ghost-H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
114.ghost-O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
115.ghost-H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
116.ghost-H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
117.ghost-O -2.894141056494115 0.038057451027571014 0.14090464395327157
118.ghost-H -3.2497362664724694 0.01817386909810281 1.0182145178872812
119.ghost-H -2.321519085665555 0.8030719139507743 0.1224165566401051
120.ghost-O -0.6719074651628764 1.8308269660174914 0.15346584816264947
121.ghost-H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
122.ghost-H -0.5296403762327344 2.766445604416275 0.1447134753637766'''
123.
124.monomer_from_optimized_cage_in_cage_basis_3 = '''
125.ghost-O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
126.ghost-H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
127.ghost-H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
128.ghost-O 0.6289918836743734 -0.39682689707154317 1.701783662513783
129.ghost-H 0.19869210273321308 0.4250933664954657 1.49006502670088
130.ghost-H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
131.O 2.996874626833252 -0.023210810895334923 0.13646764406951148
132.H 2.347256293497991 -0.16160099579680304 0.8246209926372199
133.H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
134.ghost-O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
135.ghost-H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
136.ghost-H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
137.ghost-O -2.894141056494115 0.038057451027571014 0.14090464395327157
138.ghost-H -3.2497362664724694 0.01817386909810281 1.0182145178872812
139.ghost-H -2.321519085665555 0.8030719139507743 0.1224165566401051
140.ghost-O -0.6719074651628764 1.8308269660174914 0.15346584816264947
141.ghost-H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
142.ghost-H -0.5296403762327344 2.766445604416275 0.1447134753637766'''
143.
144.monomer_from_optimized_cage_in_cage_basis_4 = '''
145.ghost-O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
146.ghost-H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
147.ghost-H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
148.ghost-O 0.6289918836743734 -0.39682689707154317 1.701783662513783
149.ghost-H 0.19869210273321308 0.4250933664954657 1.49006502670088
150.ghost-H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
151.ghost-O 2.996874626833252 -0.023210810895334923 0.13646764406951148
152.ghost-H 2.347256293497991 -0.16160099579680304 0.8246209926372199
153.ghost-H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
154.O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
155.H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
156.H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
157.ghost-O -2.894141056494115 0.038057451027571014 0.14090464395327157
158.ghost-H -3.2497362664724694 0.01817386909810281 1.0182145178872812
159.ghost-H -2.321519085665555 0.8030719139507743 0.1224165566401051
160.ghost-O -0.6719074651628764 1.8308269660174914 0.15346584816264947
161.ghost-H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
162.ghost-H -0.5296403762327344 2.766445604416275 0.1447134753637766'''
163.
```

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```
monomer_from_optimized_cage_in_cage_basis_5 = '''
ghost-O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
ghost-H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
ghost-H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
ghost-O 0.6289918836743734 -0.39682689707154317 1.701783662513783
ghost-H 0.19869210273321308 0.4250933664954657 1.49006502670088
ghost-H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
ghost-O 2.996874626833252 -0.023210810895334923 0.13646764406951148
ghost-H 2.347256293497991 -0.16160099579680304 0.8246209926372199
ghost-H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
ghost-O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
ghost-H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
ghost-H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
O -2.894141056494115 0.038057451027571014 0.14090464395327157
H -3.2497362664724694 0.01817386909810281 1.0182145178872812
H -2.321519085665555 0.8030719139507743 0.1224165566401051
ghost-O -0.6719074651628764 1.8308269660174914 0.15346584816264947
ghost-H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
ghost-H -0.5296403762327344 2.766445604416275 0.1447134753637766'''

monomer_from_optimized_cage_in_cage_basis_6 = '''
ghost-O 0.8272369544936677 0.3977230528495672 -1.6967967876862162
ghost-H 0.38440597198841564 -0.43439651959093595 -1.5637936765080114
ghost-H 1.6853080309282906 0.27784055715415273 -1.2946240648768284
ghost-O 0.6289918836743734 -0.39682689707154317 1.701783662513783
ghost-H 0.19869210273321308 0.4250933664954657 1.49006502670088
ghost-H 0.20503682971195647 -1.0285781878515672 1.1292362079726266
ghost-O 2.996874626833252 -0.023210810895334923 0.13646764406951148
ghost-H 2.347256293497991 -0.16160099579680304 0.8246209926372199
ghost-H 3.6236027612807398 -0.7249016919008635 0.2333477295602606
ghost-O -0.8247308728284747 -1.7727528307523244 -0.49723845711948844
ghost-H -1.6437095350535371 -1.295586891040831 -0.35398428747523886
ghost-H -1.0740133085908488 -2.6527180579947482 -0.7399333783264129
ghost-O -2.894141056494115 0.038057451027571014 0.14090464395327157
ghost-H -3.2497362664724694 0.01817386909810281 1.0182145178872812
ghost-H -2.321519085665555 0.8030719139507743 0.1224165566401051
O -0.6719074651628764 1.8308269660174914 0.15346584816264947
H -0.13796586017817966 1.4753566880521185 -0.5655526331912395
H -0.5296403762327344 2.766445604416275 0.1447134753637766'''

#Specify the molecule
clus = argv[1]
if clus == 'cage':
    cluster = cage
elif clus == 'monomer_from_optimized_cage_in_cage_basis':
    cluster = monomer_from_optimized_cage_in_cage_basis
elif clus == 'monomer_from_optimized_cage_in_cage_basis_2' :
    cluster = monomer_from_optimized_cage_in_cage_basis_2
elif clus == 'monomer_from_optimized_cage_in_cage_basis_3' :
    cluster = monomer_from_optimized_cage_in_cage_basis_3
elif clus == 'monomer_from_optimized_cage_in_cage_basis_4':
    cluster = monomer_from_optimized_cage_in_cage_basis_4
elif clus == 'monomer_from_optimized_cage_in_cage_basis_5':
    cluster = monomer_from_optimized_cage_in_cage_basis_5
elif clus == 'monomer_from_optimized_cage_in_cage_basis_6':
    cluster = monomer_from_optimized_cage_in_cage_basis_6

#Possible basis sets include:
#ccpvdz
#ccpvtz
#ccpvqz
```

```
225.basis = argv[2]
226.
227.mol = gto.Mole()
228.#Set verbose to 3,4,5 depending on how much output you want to see from the calculation
229.mol.verbose = 3
230.mol.atom = cluster
231.mol.basis = basis
232.mol.build()
233.mf = scf.RHF(mol)
234.
235.HF_energy = mf.kernel()
236.print('\n\n************************************************************')
237.
238.print('For the current structure, E(HF(',basis,')) = ', HF_energy, ' in hartree')
239.
240.
241.print('************************************************************')
```

Eval_HF Code used for Question 1c)ii (both monomer and full basis)

```
1.  from pyscf import gto, scf
2.  from pyscf.geomopt.berny_solver import optimize
3.  from sys import argv, exit
4.
5.  #Cartesian coordinates in angstroms for optimized cage isomer of water hexamer
6.  prism = '''
7.  O 1.5340130931301093 -0.40514158371241266 1.46814365331782
8.  H 0.6221755885635785 -0.6962543787274632 1.580367786088532
9.  H 1.9999223573838332 -0.7122370398608333 2.232343312507117
10. O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
11. H 1.181647349540349 1.531141791751101 0.6659171541600456
12. H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
13. O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
14. H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
15. H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
16. O -1.893798942309859 1.2674727267860049 -0.0759167196720318
17. H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
18. H -2.495134979307705 1.992894672814677 -0.161140526294898
19. O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
20. H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
21. H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
22. O -1.1455483849275396 -1.1338232944922193 1.457288744426707
23. H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
24. H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''
25.
26.
27. #You will need to create these coordinates variables using the output of optimizeHF.py
28. #For example, if you only want to get E(HF) for a water monomer from the optimized water dimer
29. monomer_from_optimized_prism = '''
30. O 1.5340130931301093 -0.40514158371241266 1.46814365331782
31. H 0.6221755885635785 -0.6962543787274632 1.580367786088532
32. H 1.9999223573838332 -0.7122370398608333 2.232343312507117
33. '''
34.
35. monomer_from_optimized_prism_2 = '''
36. O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
37. H 1.181647349540349 1.531141791751101 0.6659171541600456
38. H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
39. '''
```

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```
40.
41. monomer_from_optimized_prism_3 = '''
42. O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
43. H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
44. H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
45. '''
46.
47. monomer_from_optimized_prism_4 = '''
48. O -1.893798942309859 1.2674727267860049 -0.0759167196720318
49. H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
50. H -2.495134979307705 1.992894672814677 -0.161140526294898
51. '''
52.
53. monomer_from_optimized_prism_5 = '''
54. O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
55. H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
56. H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
57. '''
58.
59. monomer_from_optimized_prism_6 = '''
60. O -1.1455483849275396 -1.1338232944922193 1.457288744426707
61. H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
62. H -1.6218645344857052 -0.31941668465970346 1.3314186514719144
63. '''
64.
65. #For example, if you want to get E(HF) for a water monomer from the optimized water dimer
66. #but in the basis of the full dimer, you need to 'ghost' the non-relevant atoms
67. #This allows for orbital mixing between monomers but removes the charges for the 2nd monomer
68. monomer_from_optimized_prism_in_prism_basis = '''
69. O 1.5340130931301093 -0.40514158371241266 1.46814365331782
70. H 0.6221755885635785 -0.6962543787274632 1.580367786088532
71. H 1.9999223573838332 -0.7122370398608333 2.232343312507117
72. ghost-O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
73. ghost-H 1.181647349540349 1.531141791751101 0.6659171541600456
74. ghost-H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
75. ghost-O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
76. ghost-H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
77. ghost-H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
78. ghost-O -1.893798942309859 1.2674727267860049 -0.0759167196720318
79. ghost-H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
80. ghost-H -2.495134979307705 1.992894672814677 -0.161140526294898
81. ghost-O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
82. ghost-H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
83. ghost-H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
84. ghost-O -1.1455483849275396 -1.1338232944922193 1.457288744426707
85. ghost-H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
86. ghost-H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''
87.
88. monomer_from_optimized_prism_in_prism_basis_2 = '''
89. ghost-O 1.5340130931301093 -0.40514158371241266 1.46814365331782
90. ghost-H 0.6221755885635785 -0.6962543787274632 1.580367786088532
91. ghost-H 1.9999223573838332 -0.7122370398608333 2.232343312507117
92. O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
93. H 1.181647349540349 1.531141791751101 0.6659171541600456
94. H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
95. ghost-O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
96. ghost-H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
97. ghost-H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
98. ghost-O -1.893798942309859 1.2674727267860049 -0.0759167196720318
99. ghost-H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
100.ghost-H -2.495134979307705 1.992894672814677 -0.161140526294898
```

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```
ghost-O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
ghost-H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
ghost-H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
ghost-O -1.1455483849275396 -1.1338232944922193 1.457288744426707
ghost-H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
ghost-H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''

monomer_from_optimized_prism_in_prism_basis_3 = '''
ghost-O 1.5340130931301093 -0.40514158371241266 1.46814365331782
ghost-H 0.6221755885635785 -0.6962543787274632 1.580367786088532
ghost-H 1.9999223573838332 -0.7122370398608333 2.232343312507117
ghost-O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
ghost-H 1.181647349540349 1.531141791751101 0.6659171541600456
ghost-H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
ghost-O -1.893798942309859 1.2674727267860049 -0.0759167196720318
ghost-H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
ghost-H -2.495134979307705 1.992894672814677 -0.161140526294898
ghost-O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
ghost-H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
ghost-H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
ghost-O -1.1455483849275396 -1.1338232944922193 1.457288744426707
ghost-H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
ghost-H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''

monomer_from_optimized_prism_in_prism_basis_4 = '''
ghost-O 1.5340130931301093 -0.40514158371241266 1.46814365331782
ghost-H 0.6221755885635785 -0.6962543787274632 1.580367786088532
ghost-H 1.9999223573838332 -0.7122370398608333 2.232343312507117
ghost-O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
ghost-H 1.181647349540349 1.531141791751101 0.6659171541600456
ghost-H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
ghost-O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
ghost-H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
ghost-H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
O -1.893798942309859 1.2674727267860049 -0.0759167196720318
H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
H -2.495134979307705 1.992894672814677 -0.161140526294898
ghost-O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
ghost-H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
ghost-H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
ghost-O -1.1455483849275396 -1.1338232944922193 1.457288744426707
ghost-H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
ghost-H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''

monomer_from_optimized_prism_in_prism_basis_5 = '''
ghost-O 1.5340130931301093 -0.40514158371241266 1.46814365331782
ghost-H 0.6221755885635785 -0.6962543787274632 1.580367786088532
ghost-H 1.9999223573838332 -0.7122370398608333 2.232343312507117
ghost-O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
ghost-H 1.181647349540349 1.531141791751101 0.6659171541600456
ghost-H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
ghost-O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
ghost-H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
ghost-H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
ghost-O -1.893798942309859 1.2674727267860049 -0.0759167196720318
ghost-H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
ghost-H -2.495134979307705 1.992894672814677 -0.161140526294898
O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
```

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```
H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
ghost-O -1.1455483849275396 -1.1338232944922193 1.457288744426707
ghost-H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
ghost-H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''

monomer_from_optimized_prism_in_prism_basis_6 = '''
ghost-O 1.5340130931301093 -0.40514158371241266 1.46814365331782
ghost-H 0.6221755885635785 -0.6962543787274632 1.580367786088532
ghost-H 1.9999223573838332 -0.7122370398608333 2.232343312507117
ghost-O 0.8421006269128294 2.0217718273527794 -0.07564509372587898
ghost-H 1.181647349540349 1.531141791751101 0.6659171541600456
ghost-H 1.1888319046816782 1.5442076039849635 -0.8214165478580276
ghost-O 1.698366269569407 -0.48285525847917965 -1.3792480145312291
ghost-H 2.4225153260241914 -0.8873838524541354 -1.834821691516117
ghost-H 1.8399461739969982 -0.651370502203515 -0.4492134474378227
ghost-O -1.893798942309859 1.2674727267860049 -0.0759167196720318
ghost-H -1.0165925047426139 1.6539248698461904 -0.07977100279308681
ghost-H -2.495134979307705 1.992894672814677 -0.161140526294898
ghost-O -1.1786840097782552 -1.3128386746341376 -1.4188327193201777
ghost-H -0.2674902830568773 -1.114505310752413 -1.6081085921794562
ghost-H -1.5858185522941484 -0.4611963720120828 -1.3026698150827614
O -1.1455483849275396 -1.1338232944922193 1.457288744426707
H -1.2094746757397614 -1.5395209864171289 0.5946965187836248
H -1.6218645344857052 -0.31941668465970346 1.3314186514719144'''

#Specify the molecule
clus = argv[1]
if clus == 'prism':
    cluster = prism
elif clus == 'monomer_from_optimized_prism':
        cluster = monomer_from_optimized_prism
elif clus == 'monomer_from_optimized_prism_2':
        cluster = monomer_from_optimized_prism_2
elif clus == 'monomer_from_optimized_prism_3':
        cluster = monomer_from_optimized_prism_3
elif clus == 'monomer_from_optimized_prism_4':
        cluster = monomer_from_optimized_prism_4
elif clus == 'monomer_from_optimized_prism_5':
        cluster = monomer_from_optimized_prism_5
elif clus == 'monomer_from_optimized_prism_6':
        cluster = monomer_from_optimized_prism_6
elif clus == 'monomer_from_optimized_prism_in_prism_basis':
    cluster = monomer_from_optimized_prism_in_prism_basis
elif clus == 'monomer_from_optimized_prism_in_prism_basis_2' :
    cluster = monomer_from_optimized_prism_in_prism_basis_2
elif clus == 'monomer_from_optimized_prism_in_prism_basis_3' :
    cluster = monomer_from_optimized_prism_in_prism_basis_3
elif clus == 'monomer_from_optimized_prism_in_prism_basis_4':
    cluster = monomer_from_optimized_prism_in_prism_basis_4
elif clus == 'monomer_from_optimized_prism_in_prism_basis_5':
    cluster = monomer_from_optimized_prism_in_prism_basis_5
elif clus == 'monomer_from_optimized_prism_in_prism_basis_6':
    cluster = monomer_from_optimized_prism_in_prism_basis_6

#Possible basis sets include:
#ccpvdz
#ccpvtz
#ccpvqz
basis = argv[2]

```

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```
223.mol = gto.Mole()
224.#Set verbose to 3,4,5 depending on how much output you want to see from the calculation
225.mol.verbose = 3
226.mol.atom = cluster
227.mol.basis = basis
228.mol.build()
229.mf = scf.RHF(mol)
230.
231.HF_energy = mf.kernel()
232.print('\n\n*****************************************************************')
233.
234.print('For the current structure, E(HF(',basis,')) = ', HF_energy, ' in hartree')
235.
236.
237.print('*****************************************************************')
```

Eval_DFT Code used for all parts of Q2:

```
1.  from pyscf import gto, scf
2.  from pyscf.geomopt.berny_solver import optimize
3.  from sys import argv, exit
4.
5.  #Cartesian coordinates in angstroms for water dimer
6.  dimer = '''
7.  H -1.8711617490092503 -0.0421773760749265 0.724932670013913
8.  H -0.5142453830768674 0.016612368947530237 0.045581760149181874
9.  O -1.4698577423298251 0.010591039015758053 -0.15479617034030688
10. H 1.626174286244376 0.7669570797608419 -0.36412233419563794
11. H 1.5931261343134393 -0.7545295464830589 -0.40281079605279535
12. O 1.3932754453183782 -0.0033415961994219226 0.17806701195172442'''
13.
14. #Cartesian coordinates in angstroms for cage isomer of water hexamer
15. cage = '''
16. O 0.8044863808010561 0.4406317031074396 -1.6483607715383553
17. H 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
18. H 1.6410405254197464 0.3081322428904229 -1.1312788174771033
19. O 0.5520308305797719 -0.3507424818530152 1.6801755654291477
20. H 0.1445543499038291 0.4911060704843157 1.3838578268611876
21. H 0.1553933872965244 -0.9945003084717347 1.0557059280274026
22. O 2.78666390553782 0.009090341322986488 0.17101546050801425
23. H 2.085245989336808 -0.1344307050263977 0.8606730658308939
24. H 3.239366696035082 -0.8458227504818738 0.11706786884159348
25. O -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
26. H -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
27. H -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
28. O -2.727092216994081 -0.004259057955005899 0.14877911599480753
29. H -2.872275921822681 -0.10779242961088266 1.1023613558120058
30. H -2.1228236313558466 0.779139325283839 0.09839466573208608
31. O -0.6309758207807158 1.6995550021019497 0.13142377600032795
32. H -0.0648722876426901 1.3344279567168447 -0.6302234839956955
33. H -0.5230908624989717 2.6612823941816828 0.1060216658902553'''
34.
35. #Cartesian coordinates in angstroms for prism isomer of water hexamer
36. prism = '''
37. O 1.4136844197486191 -0.334097605354089 1.3547662678017625
38. H 0.4605050736243326 -0.6726829971748395 1.469553763183331
39. H 1.9119159112830295 -0.696161234018871 2.1013086498504117
40. O 0.8137235216877469 1.980883752569092 -0.07893565212013333
```

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```
H 1.1227176221180697 1.4495906203128666 0.6851061915784674
H 1.1474954736416885 1.43090633437145 -0.8170503586675695
O 1.5544950548144403 -0.42244940883164267 -1.327489602775074
H 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
H 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
O -1.7446453886474453 1.1543356239668419 -0.05951064357252846
H -0.8361836483831954 1.5698659973103715 -0.08215361364938012
H -2.363883483022787 1.8932054595626004 -0.14557820368794216
O -1.143109956669111 -1.31531167732704 -1.310025957079486
H -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
H -1.5235447208608675 -0.4225204001105232 -1.178353686497679
O -1.073726804002462 -1.1081228056254713 1.4076330012564242
H -1.123318927284131 -1.474476749288519 0.48594852833897445
H -1.520852300802837 -0.24854674234533952 1.2575394238996975'''

#You will need to create these coordinates variables using the output of optimizeHF.py
#For example, if you only want to get E(HF) for a water monomer from the optimized water dimer
monomer_from_optimized_dimer = '''
H -1.8711617490092503 -0.0421773760749265 0.724932670013913
H -0.5142453830768674 0.016612368947530237 0.045581760149181874
O -1.4698577423298251 0.010591039015758053 -0.15479617034030688
'''
monomer_from_optimized_dimer_2 = '''
H 1.626174286244376 0.7669570797608419 -0.36412233419563794
H 1.5931261343134393 -0.7545295464830589 -0.40281079605279535
O 1.3932754453183782 -0.0033415961994219226 0.17806701195172442
'''
#For example, if you want to get E(HF) for a water monomer from the optimized water dimer
#but in the basis of the full dimer, you need to 'ghost' the non-relevant atoms
#This allows for orbital mixing between monomers but removes the charges for the 2nd monomer
#I seem to be seeing a bug where ghost-H, no longer works as it did for HF, instead I use X1
#and X2 here and specify these basis functions in the mol.basis line below
monomer_from_optimized_dimer_in_dimer_basis='''
H -1.8711617490092503 -0.0421773760749265 0.724932670013913
H -0.5142453830768674 0.016612368947530237 0.045581760149181874
O -1.4698577423298251 0.010591039015758053 -0.15479617034030688
X1 1.626174286244376 0.7669570797608419 -0.36412233419563794
X1 1.5931261343134393 -0.7545295464830589 -0.40281079605279535
X2 1.3932754453183782 -0.0033415961994219226 0.17806701195172442
'''
monomer_from_optimized_dimer_in_dimer_basis_2='''
X1 -1.8711617490092503 -0.0421773760749265 0.724932670013913
X1 -0.5142453830768674 0.016612368947530237 0.045581760149181874
X2 -1.4698577423298251 0.010591039015758053 -0.15479617034030688
H 1.626174286244376 0.7669570797608419 -0.36412233419563794
H 1.5931261343134393 -0.7545295464830589 -0.40281079605279535
O 1.3932754453183782 -0.0033415961994219226 0.17806701195172442
'''

monomer_from_optimized_cage = '''
O 0.8044863808010561 0.4406317031074396 -1.6483607715383553
H 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
H 1.6410405254197464 0.3081322428904229 -1.1312788174771033
'''
monomer_from_optimized_cage_2 = '''
O 0.5520308305797719 -0.3507424818530152 1.6801755654291477
H 0.1445543499038291 0.4911060704843157 1.3838578268611876
H 0.1553933872965244 -0.9945003084717347 1.0557059280274026
'''
monomer_from_optimized_cage_3 = '''
O 2.78666390553782 0.009090341322986488 0.17101546050801425
```

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```
H 2.085245989336808 -0.1344307050263977 0.8606730658308939
H 3.239366696035082 -0.8458227504818738 0.11706786884159348
'''
monomer_from_optimized_cage_4 = '''
O -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
H -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
H -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
'''
monomer_from_optimized_cage_5 = '''
O -2.727092216994081 -0.004259057955005899 0.14877911599480753
H -2.872275921822681 -0.10779242961088266 1.1023613558120058
H -2.1228236313558466 0.779139325283839 0.09839466573208608
'''
monomer_from_optimized_cage_6 = '''
O -0.6309758207807158 1.6995550021019497 0.13142377600032795
H -0.0648722876426901 1.3344279567168447 -0.6302234839956955
H -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis = '''
O 0.8044863808010561 0.4406317031074396 -1.6483607715383553
H 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
H 1.6410405254197464 0.3081322428904229 -1.1312788174771033
X2 0.5520308305797719 -0.3507424818530152 1.6801755654291477
X1 0.1445543499038291 0.4911060704843157 1.3838578268611876
X1 0.1553933872965244 -0.9945003084717347 1.0557059280274026
X2 2.78666390553782 0.009090341322986488 0.17101546050801425
X1 2.085245989336808 -0.1344307050263977 0.8606730658308939
X1 3.239366696035082 -0.8458227504818738 0.11706786884159348
X2 -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
X1 -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
X1 -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
X2 -2.727092216994081 -0.004259057955005899 0.14877911599480753
X1 -2.872275921822681 -0.10779242961088266 1.1023613558120058
X1 -2.1228236313558466 0.779139325283839 0.09839466573208608
X2 -0.6309758207807158 1.6995550021019497 0.13142377600032795
X1 -0.0648722876426901 1.3344279567168447 -0.6302234839956955
X1 -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis_2 = '''
X2 0.8044863808010561 0.4406317031074396 -1.6483607715383553
X1 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
X1 1.6410405254197464 0.3081322428904229 -1.1312788174771033
O 0.5520308305797719 -0.3507424818530152 1.6801755654291477
H 0.1445543499038291 0.4911060704843157 1.3838578268611876
H 0.1553933872965244 -0.9945003084717347 1.0557059280274026
X2 2.78666390553782 0.009090341322986488 0.17101546050801425
X1 2.085245989336808 -0.1344307050263977 0.8606730658308939
X1 3.239366696035082 -0.8458227504818738 0.11706786884159348
X2 -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
X1 -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
X1 -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
X2 -2.727092216994081 -0.004259057955005899 0.14877911599480753
X1 -2.872275921822681 -0.10779242961088266 1.1023613558120058
X1 -2.1228236313558466 0.779139325283839 0.09839466573208608
X2 -0.6309758207807158 1.6995550021019497 0.13142377600032795
X1 -0.0648722876426901 1.3344279567168447 -0.6302234839956955
X1 -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis_3 = '''
X2 0.8044863808010561 0.4406317031074396 -1.6483607715383553
X1 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
```

Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

```
X1 1.6410405254197464 0.3081322428904229 -1.1312788174771033
X2 0.5520308305797719 -0.3507424818530152 1.6801755654291477
X1 0.1445543499038291 0.4911060704843157 1.3838578268611876
X1 0.1553933872965244 -0.9945003084717347 1.0557059280274026
O 2.78666390553782 0.009090341322986488 0.17101546050801425
H 2.085245989336808 -0.1344307050263977 0.8606730658308939
H 3.239366696035082 -0.8458227504818738 0.11706786884159348
X2 -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
X1 -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
X1 -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
X2 -2.727092216994081 -0.004259057955005899 0.14877911599480753
X1 -2.872275921822681 -0.10779242961088266 1.1023613558120058
X1 -2.1228236313558466 0.779139325283839 0.09839466573208608
X2 -0.6309758207807158 1.6995550021019497 0.13142377600032795
X1 -0.0648722876426901 1.3344279567168447 -0.6302234839956955
X1 -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis_4 = '''
X2 0.8044863808010561 0.4406317031074396 -1.6483607715383553
X1 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
X1 1.6410405254197464 0.3081322428904229 -1.1312788174771033
X2 0.5520308305797719 -0.3507424818530152 1.6801755654291477
X1 0.1445543499038291 0.4911060704843157 1.3838578268611876
X1 0.1553933872965244 -0.9945003084717347 1.0557059280274026
X2 2.78666390553782 0.009090341322986488 0.17101546050801425
X1 2.085245989336808 -0.1344307050263977 0.8606730658308939
X1 3.239366696035082 -0.8458227504818738 0.11706786884159348
O -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
H -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
H -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
X2 -2.727092216994081 -0.004259057955005899 0.14877911599480753
X1 -2.872275921822681 -0.10779242961088266 1.1023613558120058
X1 -2.1228236313558466 0.779139325283839 0.09839466573208608
X2 -0.6309758207807158 1.6995550021019497 0.13142377600032795
X1 -0.0648722876426901 1.3344279567168447 -0.6302234839956955
X1 -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis_5 = '''
X2 0.8044863808010561 0.4406317031074396 -1.6483607715383553
X1 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
X1 1.6410405254197464 0.3081322428904229 -1.1312788174771033
X2 0.5520308305797719 -0.3507424818530152 1.6801755654291477
X1 0.1445543499038291 0.4911060704843157 1.3838578268611876
X1 0.1553933872965244 -0.9945003084717347 1.0557059280274026
X2 2.78666390553782 0.009090341322986488 0.17101546050801425
X1 2.085245989336808 -0.1344307050263977 0.8606730658308939
X1 3.239366696035082 -0.8458227504818738 0.11706786884159348
X2 -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
X1 -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
X1 -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
O -2.727092216994081 -0.004259057955005899 0.14877911599480753
H -2.872275921822681 -0.10779242961088266 1.1023613558120058
H -2.1228236313558466 0.779139325283839 0.09839466573208608
X2 -0.6309758207807158 1.6995550021019497 0.13142377600032795
X1 -0.0648722876426901 1.3344279567168447 -0.6302234839956955
X1 -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
monomer_from_optimized_cage_in_cage_basis_6 = '''
X2 0.8044863808010561 0.4406317031074396 -1.6483607715383553
X1 0.33082410751803776 -0.40596742165057437 -1.5066683840596242
X1 1.6410405254197464 0.3081322428904229 -1.1312788174771033
```

Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

```
X2 0.5520308305797719 -0.3507424818530152 1.6801755654291477
X1 0.1445543499038291 0.4911060704843157 1.3838578268611876
X1 0.1553933872965244 -0.9945003084717347 1.0557059280274026
X2 2.78666390553782 0.009090341322986488 0.17101546050801425
X1 2.085245989336808 -0.1344307050263977 0.8606730658308939
X1 3.239366696035082 -0.8458227504818738 0.11706786884159348
X2 -0.7120461541223444 -1.6414081190880145 -0.4962617326077966
X1 -1.5666856846541442 -1.1522776727510293 -0.32686368548546596
X1 -0.9697019640940905 -2.5441475030343907 -0.7325063994857454
X2 -2.727092216994081 -0.004259057955005899 0.14877911599480753
X1 -2.872275921822681 -0.10779242961088266 1.1023613558120058
X1 -2.1228236313558466 0.779139325283839 0.09839466573208608
O -0.6309758207807158 1.6995550021019497 0.13142377600032795
H -0.0648722876426901 1.3344279567168447 -0.6302234839956955
H -0.5230908624989717 2.6612823941816828 0.1060216658902553
'''
#~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
monomer_from_optimized_prism = '''
O 1.4136844197486191 -0.334097605354089 1.3547662678017625
H 0.4605050736243326 -0.6726829971748395 1.469553763183331
H 1.9119159112830295 -0.696161234018871 2.1013086498504117
'''
monomer_from_optimized_prism_2 = '''
O 0.8137235216877469 1.980883752569092 -0.07893565212013333
H 1.1227176221180697 1.4495906203128666 0.6851061915784674
H 1.1474954736416885 1.43090633437145 -0.8170503586675695
'''
monomer_from_optimized_prism_3 = '''
O 1.5544950548144403 -0.42244940883164267 -1.327489602775074
H 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
H 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
'''
monomer_from_optimized_prism_4 = '''
O -1.7446453886474453 1.1543356239668419 -0.05951064357252846
H -0.8361836483831954 1.5698659973103715 -0.08215361364938012
H -2.363883483022787 1.8932054595626004 -0.14557820368794216
'''
monomer_from_optimized_prism_5 = '''
O -1.143109956669111 -1.31531167732704 -1.310025957079486
H -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
H -1.5235447208608675 -0.4225204001105232 -1.178353686497679
'''
monomer_from_optimized_prism_6 = '''
O -1.073726804002462 -1.1081228056254713 1.4076330012564242
H -1.123318927284131 -1.474476749288519 0.48594852833897445
H -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''

monomer_from_optimized_prism_in_prism_basis = '''
O 1.4136844197486191 -0.334097605354089 1.3547662678017625
H 0.4605050736243326 -0.6726829971748395 1.469553763183331
H 1.9119159112830295 -0.696161234018871 2.1013086498504117
X2 0.8137235216877469 1.980883752569092 -0.07893565212013333
X1 1.1227176221180697 1.4495906203128666 0.6851061915784674
X1 1.1474954736416885 1.43090633437145 -0.8170503586675695
X2 1.5544950548144403 -0.42244940883164267 -1.327489602775074
X1 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
X1 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
X2 -1.7446453886474453 1.1543356239668419 -0.05951064357252846
X1 -0.8361836483831954 1.5698659973103715 -0.08215361364938012
X1 -2.363883483022787 1.8932054595626004 -0.14557820368794216
```

Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

```
X2 -1.143109956669111 -1.31531167732704 -1.310025957079486
X1 -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
X1 -1.5235447208608675 -0.4225204001105232 -1.178353686497679
X2 -1.073726804002462 -1.1081228056254713 1.4076330012564242
X1 -1.123318927284131 -1.474476749288519 0.48594852833897445
X1 -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
monomer_from_optimized_prism_in_prism_basis_2 = '''
X2 1.4136844197486191 -0.334097605354089 1.3547662678017625
X1 0.4605050736243326 -0.6726829971748395 1.469553763183331
X1 1.9119159112830295 -0.696161234018871 2.1013086498504117
O 0.8137235216877469 1.980883752569092 -0.07893565212013333
H 1.1227176221180697 1.4495906203128666 0.6851061915784674
H 1.1474954736416885 1.43090633437145 -0.8170503586675695
X2 1.5544950548144403 -0.42244940883164267 -1.327489602775074
X1 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
X1 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
X2 -1.7446453886474453 1.1543356239668419 -0.05951064357252846
X1 -0.8361836483831954 1.5698659973103715 -0.08215361364938012
X1 -2.363883483022787 1.8932054595626004 -0.14557820368794216
X2 -1.143109956669111 -1.31531167732704 -1.310025957079486
X1 -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
X1 -1.5235447208608675 -0.4225204001105232 -1.178353686497679
X2 -1.073726804002462 -1.1081228056254713 1.4076330012564242
X1 -1.123318927284131 -1.474476749288519 0.48594852833897445
X1 -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
monomer_from_optimized_prism_in_prism_basis_3 = '''
X2 1.4136844197486191 -0.334097605354089 1.3547662678017625
X1 0.4605050736243326 -0.6726829971748395 1.469553763183331
X1 1.9119159112830295 -0.696161234018871 2.1013086498504117
X2 0.8137235216877469 1.980883752569092 -0.07893565212013333
X1 1.1227176221180697 1.4495906203128666 0.6851061915784674
X1 1.1474954736416885 1.43090633437145 -0.8170503586675695
O 1.5544950548144403 -0.42244940883164267 -1.327489602775074
H 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
H 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
X2 -1.7446453886474453 1.1543356239668419 -0.05951064357252846
X1 -0.8361836483831954 1.5698659973103715 -0.08215361364938012
X1 -2.363883483022787 1.8932054595626004 -0.14557820368794216
X2 -1.143109956669111 -1.31531167732704 -1.310025957079486
X1 -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
X1 -1.5235447208608675 -0.4225204001105232 -1.178353686497679
X2 -1.073726804002462 -1.1081228056254713 1.4076330012564242
X1 -1.123318927284131 -1.474476749288519 0.48594852833897445
X1 -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
monomer_from_optimized_prism_in_prism_basis_4 = '''
X2 1.4136844197486191 -0.334097605354089 1.3547662678017625
X1 0.4605050736243326 -0.6726829971748395 1.469553763183331
X1 1.9119159112830295 -0.696161234018871 2.1013086498504117
X2 0.8137235216877469 1.980883752569092 -0.07893565212013333
X1 1.1227176221180697 1.4495906203128666 0.6851061915784674
X1 1.1474954736416885 1.43090633437145 -0.8170503586675695
X2 1.5544950548144403 -0.42244940883164267 -1.327489602775074
X1 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
X1 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
O -1.7446453886474453 1.1543356239668419 -0.05951064357252846
H -0.8361836483831954 1.5698659973103715 -0.08215361364938012
H -2.363883483022787 1.8932054595626004 -0.14557820368794216
X2 -1.143109956669111 -1.31531167732704 -1.310025957079486
```

Sahad Vasanji Student ID#: 20603358. **The Terminal output will always follow the corresponding answers of the question. Different portions of a question are bolded or underlined**

```
X1 -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
X1 -1.5235447208608675 -0.4225204001105232 -1.178353686497679
X2 -1.073726804002462 -1.1081228056254713 1.4076330012564242
X1 -1.123318927284131 -1.474476749288519 0.48594852833897445
X1 -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
monomer_from_optimized_prism_in_prism_basis_5 = '''
X2 1.4136844197486191 -0.334097605354089 1.3547662678017625
X1 0.4605050736243326 -0.6726829971748395 1.469553763183331
X1 1.9119159112830295 -0.696161234018871 2.1013086498504117
X2 0.8137235216877469 1.980883752569092 -0.07893565212013333
X1 1.1227176221180697 1.4495906203128666 0.6851061915784674
X1 1.1474954736416885 1.43090633437145 -0.8170503586675695
X2 1.5544950548144403 -0.42244940883164267 -1.327489602775074
X1 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
X1 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
X2 -1.7446453886474453 1.1543356239668419 -0.05951064357252846
X1 -0.8361836483831954 1.5698659973103715 -0.08215361364938012
X1 -2.363883483022787 1.8932054595626004 -0.14557820368794216
O -1.143109956669111 -1.31531167732704 -1.310025957079486
H -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
H -1.5235447208608675 -0.4225204001105232 -1.178353686497679
X2 -1.073726804002462 -1.1081228056254713 1.4076330012564242
X1 -1.123318927284131 -1.474476749288519 0.48594852833897445
X1 -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
monomer_from_optimized_prism_in_prism_basis_6 = '''
X2 1.4136844197486191 -0.334097605354089 1.3547662678017625
X1 0.4605050736243326 -0.6726829971748395 1.469553763183331
X1 1.9119159112830295 -0.696161234018871 2.1013086498504117
X2 0.8137235216877469 1.980883752569092 -0.07893565212013333
X1 1.1227176221180697 1.4495906203128666 0.6851061915784674
X1 1.1474954736416885 1.43090633437145 -0.8170503586675695
X2 1.5544950548144403 -0.42244940883164267 -1.327489602775074
X1 2.3316893430558836 -0.7914371005201715 -1.7714237611143164
X1 1.6927489258118744 -0.5812165723735889 -0.3586648379319481
X2 -1.7446453886474453 1.1543356239668419 -0.05951064357252846
X1 -0.8361836483831954 1.5698659973103715 -0.08215361364938012
X1 -2.363883483022787 1.8932054595626004 -0.14557820368794216
X2 -1.143109956669111 -1.31531167732704 -1.310025957079486
X1 -0.20459829295233875 -1.1168949409926334 -1.5092778584687372
X1 -1.5235447208608675 -0.4225204001105232 -1.178353686497679
O -1.073726804002462 -1.1081228056254713 1.4076330012564242
H -1.123318927284131 -1.474476749288519 0.48594852833897445
H -1.520852300802837 -0.24854674234533952 1.2575394238996975
'''
#Specify the molecule
clus = argv[1]
if clus == 'dimer':
    cluster = dimer
elif clus == 'monomer_from_optimized_dimer' :
    cluster = monomer_from_optimized_dimer
elif clus == 'monomer_from_optimized_dimer_2' :
    cluster = monomer_from_optimized_dimer_2
elif clus == 'monomer_from_optimized_dimer_in_dimer_basis':
    cluster = monomer_from_optimized_dimer_in_dimer_basis
elif clus == 'monomer_from_optimized_dimer_in_dimer_basis_2':
    cluster = monomer_from_optimized_dimer_in_dimer_basis_2
elif clus == 'cage':
    cluster = cage
elif clus == 'monomer_from_optimized_cage':
```

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```
407.    cluster = monomer_from_optimized_cage
408.elif clus == 'monomer_from_optimized_cage_2' :
409.    cluster = monomer_from_optimized_cage_2
410.elif clus == 'monomer_from_optimized_cage_3' :
411.    cluster = monomer_from_optimized_cage_3
412.elif clus == 'monomer_from_optimized_cage_4':
413.    cluster = monomer_from_optimized_cage_4
414.elif clus == 'monomer_from_optimized_cage_5':
415.    cluster = monomer_from_optimized_cage_5
416.elif clus == 'monomer_from_optimized_cage_6':
417.    cluster = monomer_from_optimized_cage_6
418.elif clus == 'monomer_from_optimized_cage_in_cage_basis':
419.    cluster = monomer_from_optimized_cage_in_cage_basis
420.elif clus == 'monomer_from_optimized_cage_in_cage_basis_2' :
421.    cluster = monomer_from_optimized_cage_in_cage_basis_2
422.elif clus == 'monomer_from_optimized_cage_in_cage_basis_3' :
423.    cluster = monomer_from_optimized_cage_in_cage_basis_3
424.elif clus == 'monomer_from_optimized_cage_in_cage_basis_4':
425.    cluster = monomer_from_optimized_cage_in_cage_basis_4
426.elif clus == 'monomer_from_optimized_cage_in_cage_basis_5':
427.    cluster = monomer_from_optimized_cage_in_cage_basis_5
428.elif clus == 'monomer_from_optimized_cage_in_cage_basis_6':
429.    cluster = monomer_from_optimized_cage_in_cage_basis_6
430.elif clus == 'prism':
431.    cluster = prism
432.elif clus == 'monomer_from_optimized_prism':
433.        cluster = monomer_from_optimized_prism
434.elif clus == 'monomer_from_optimized_prism_2':
435.        cluster = monomer_from_optimized_prism_2
436.elif clus == 'monomer_from_optimized_prism_3':
437.        cluster = monomer_from_optimized_prism_3
438.elif clus == 'monomer_from_optimized_prism_4':
439.        cluster = monomer_from_optimized_prism_4
440.elif clus == 'monomer_from_optimized_prism_5':
441.        cluster = monomer_from_optimized_prism_5
442.elif clus == 'monomer_from_optimized_prism_6':
443.        cluster = monomer_from_optimized_prism_6
444.elif clus == 'monomer_from_optimized_prism_in_prism_basis':
445.    cluster = monomer_from_optimized_prism_in_prism_basis
446.elif clus == 'monomer_from_optimized_prism_in_prism_basis_2' :
447.    cluster = monomer_from_optimized_prism_in_prism_basis_2
448.elif clus == 'monomer_from_optimized_prism_in_prism_basis_3' :
449.    cluster = monomer_from_optimized_prism_in_prism_basis_3
450.elif clus == 'monomer_from_optimized_prism_in_prism_basis_4':
451.    cluster = monomer_from_optimized_prism_in_prism_basis_4
452.elif clus == 'monomer_from_optimized_prism_in_prism_basis_5':
453.    cluster = monomer_from_optimized_prism_in_prism_basis_5
454.elif clus == 'monomer_from_optimized_prism_in_prism_basis_6':
455.    cluster = monomer_from_optimized_prism_in_prism_basis_6
456.
457.#Possible basis sets include:
458.#ccpvdz
459.#ccpvtz
460.#ccpvqz
461.basis = argv[2]
462.
463.mol = gto.Mole()
464.#Set verbose to 3,4,5 depending on how much output you want to see from the calculation
465.mol.verbose = 3
466.mol.atom = cluster
467.mol.basis={'X1':gto.basis.load(basis, 'H'),
```

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```
468.         'X2':gto.basis.load(basis, 'O'),
469.                     'O':basis, 'H':basis}
470.mol.build()
471.mf = mol.KS()
472.#get the name of the exhange-correlation functional from user input
473.mf.xc = argv[3]
474.
475.DFT_energy = mf.kernel()
476.print('\n\n************************************************************')
477.
478.print('For the current structure, E(',argv[3],',',argv[2],') = ', DFT_energy, ' in hartree')
479.
480.
481.print('************************************************************')
```