```
pip install pyscf

-----------------------------------------------------------------

from pyscf import gto, dft


mol = gto.M(
    atom='''
    O 0  0  0
    H 0  0.77  0.58
    H 0  -0.77  0.58''',
    spin=0,
    charge=0,
    basis= 'ccpvdz',
    verbose=4)


mydft = dft.UKS(mol)
mydft.xc = 'b3lyp'
mydft.kernel()


mydft.analyze()

-----------------------------------------------------------------

from pyscf import gto, dft


bas='ccpvdz'
xc = 'b3lyp'


dim = gto.M(
```

```
    atom = '''
    O 0.000 0.000 0.000
    H -0.635 0.628 0.391
    H 0.869 0.421 0.090
    O -0.277 0.479 -2.567
    H -0.975 -0.048 -2.956
    H -0.230 0.212 -1.603''',
    spin=0,
    charge=0,
    basis = bas,
    verbose=0)

mydft = dft.RKS(dim)
mydft.xc = xc
e_dimer = mydft.kernel()
-----------------------------------------------------------------
mon1 = gto.M(
    atom = '''
    O 0.000 0.000 0.000
    H -0.635 0.628 0.391
    H 0.869 0.421 0.090''',
    spin=0,
    charge=0,
    basis = bas,
    verbose=0)
```

```
mydft = dft.RKS(mon1)
mydft.xc = xc
e_mon1 = mydft.kernel()
-----------------------------------------------------------------
mon2 = gto.M(
    atom = '''
    O -0.277 0.479 -2.567
    H -0.975 -0.048 -2.956
    H -0.230 0.212 -1.603''',
    spin=0,
    charge=0,
    basis = bas,
    verbose=0)

mydft = dft.RKS(mon2)
mydft.xc = xc
e_mon2 = mydft.kernel()
-----------------------------------------------------------------
Eint = (e_dimer - e_mon1 - e_mon2)*627.509
print(Eint)
print('B3LYP energy = %.3f' %Eint)
```