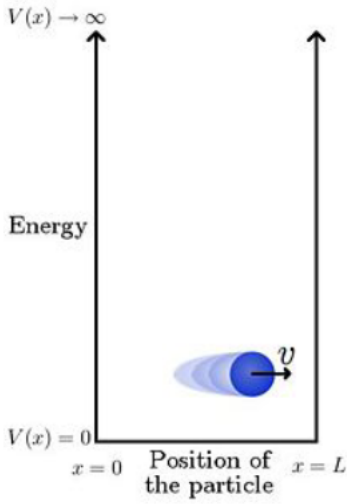
HW

1.particle in a box

The particle in a box is probably the most classic and analytically solvable system in quantum mechanics. By solving the Schrödinger equation of this system, we can understand the “weird” behavior of quantum effect. The particle in a box basically describes the translational motion of a single particle confined inside an infinitely deep well (0 to L) from which it cannot escape, as shown in the figure below. Please answer the question set below.



A

(a) The general form of the time-independent Schrödinger equation is:

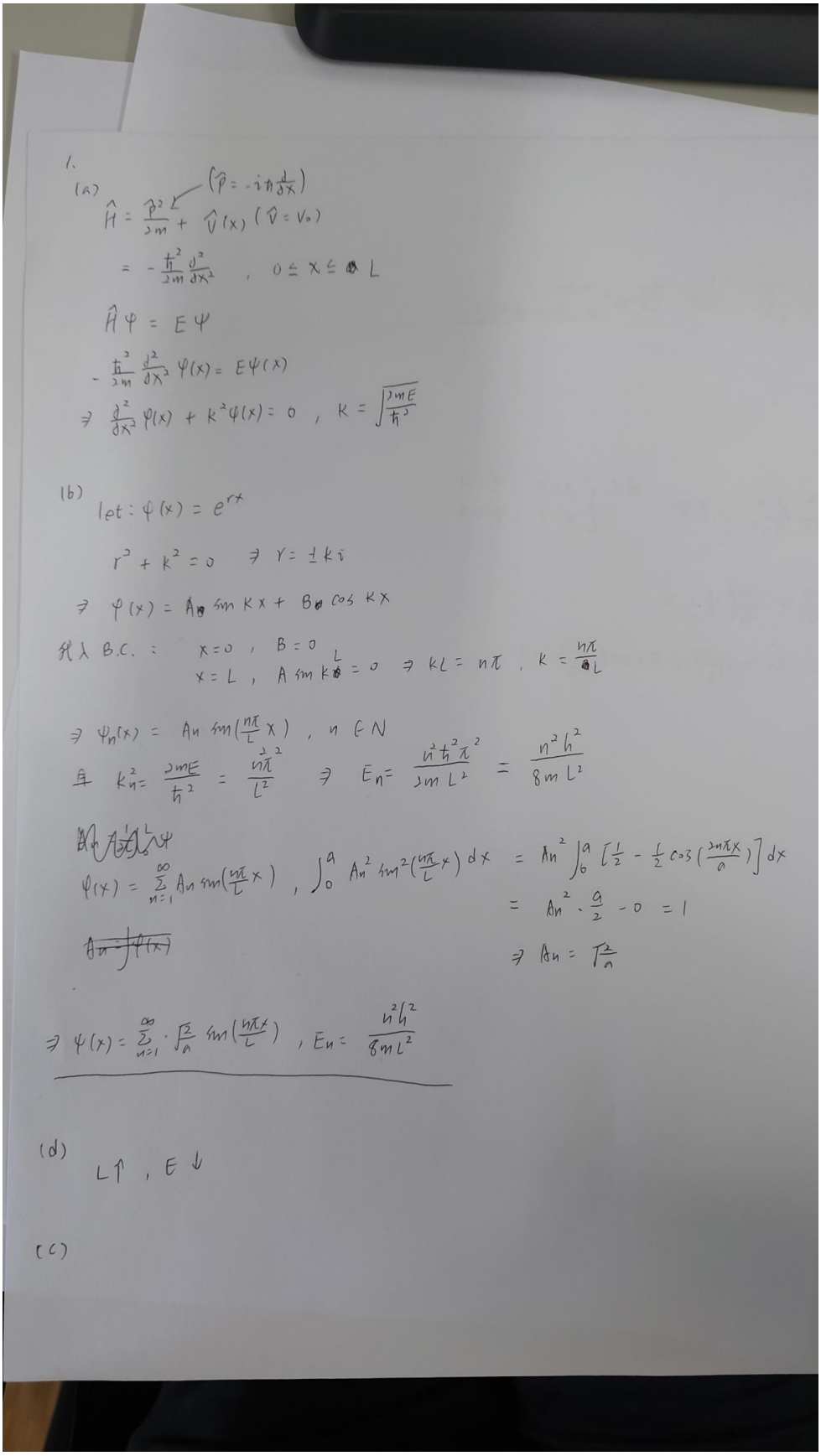
$$\hat{\mathrm{H}}\Psi = E\Psi$$

where $\hat{\mathrm{H}}$ is the Hamiltonian operator, Ψ is the wavefunction (eigen function) of the total system and E is the energy (eigen value) of the system. Please write down the Schrödinger equation of this 1-dimensional particle in a box system.

B

(b) Following Q1(a), please solve this equation. (*Hint: non-trivial solution of a 2nd order homogenous ODE*)

A,B Solution



ref

https://www.youtube.com/watch?v=1Ibrj02ope8&list=PL9EE7723EE2BE9102&index=5

(https://www.youtube.com/watch?v=1Ibrj02ope8&list=PL9EE7723EE2BE9102&index=5)

c

(c) Is the number of states between E and $E + \delta E$ (density of states) higher in high energy region or low energy region?

D

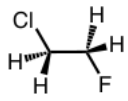
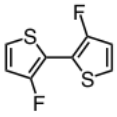
(d) How do the differences between energy levels change when we increase the box size (increase L)?

Solution

By \[E_{n} = \frac{n^{2}h^{2}}{8mL^{2}}\]
L ⬆️ En ⬇️

2.perform the ground-state geometry optimization

Following similar steps showing in the hands-on session, please perform the ground-state geometry optimization for the following molecules. Specify all the non-redundant internal coordinates (bond lengths, angles and dihedrals) according to symmetry. In addition, identify all possible conformational isomers for all compounds and specify their relative energies.

(a) O_2, (b) H_2O, (c) C_2H_6, (d)  and (e) 

Auto generate the output with molecular filename directory

```
export OMP_STACKSIZE=4G
ulimit -s unlimited
export OMP_NUM_THREADS=8,1
export MKL_NUM_THREADS=8

# loop every directory
for d in ./*/ ; do
    cd $d
    files=*.xyz
    for file in $files; do
        filename=$(basename -- "$file")
        extension="${filename##*.}"
        filename="${filename%.*}"
        mkdir "$filename"
        cp $file $filename
        cd "$filename"
        xtb -c 0 -u 0 "$filename".xyz --opt normal  > xtb.out
        cd ..
    done
    cd ..
done
```

1. O_2
   formal charge = 0
   unpaired electron = 2
   (u -0)->

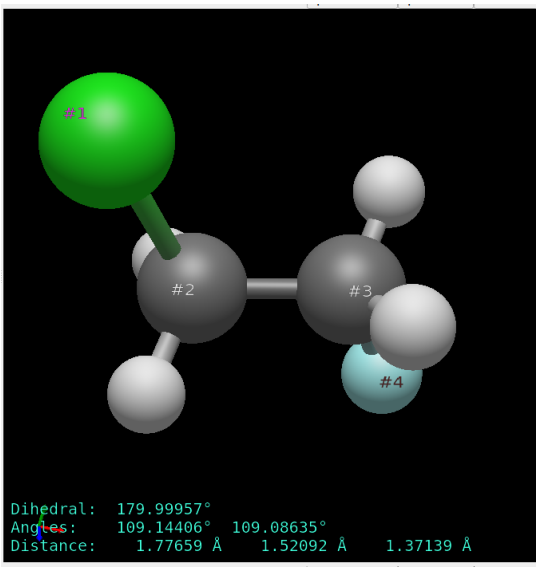
bond length : 1.2078 A
angles : 180 degree
dihedrals : x

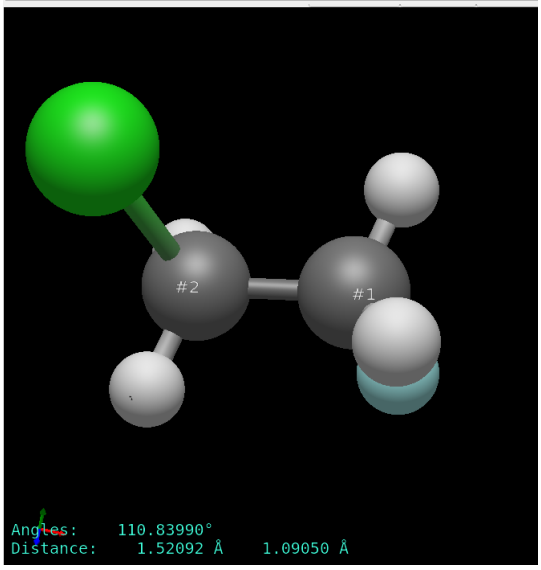
2. h2o
   formal charge = 0
   unpaired eletron = 2
   (u -0)->
   bond length : 0.95910 A
   angles : 107.22955

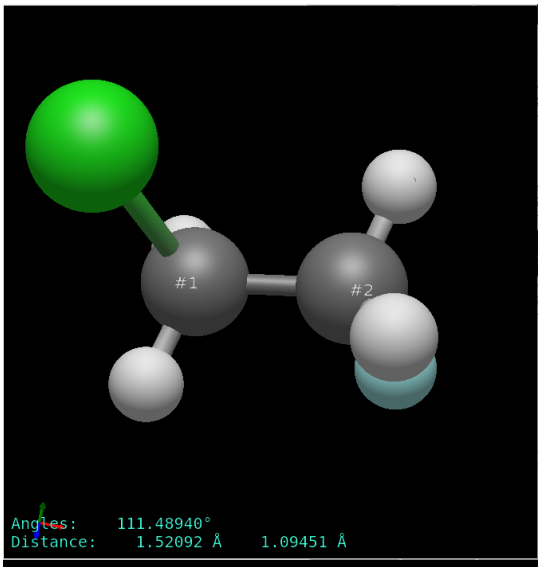
3. c2h6
   fornal charge = 0
   unpaired eletron = 0
   ->
   C-C bond length : 1.52126
   C-H bond length : 1.08775
   angle : 110.60739
   diheral : 59.99887

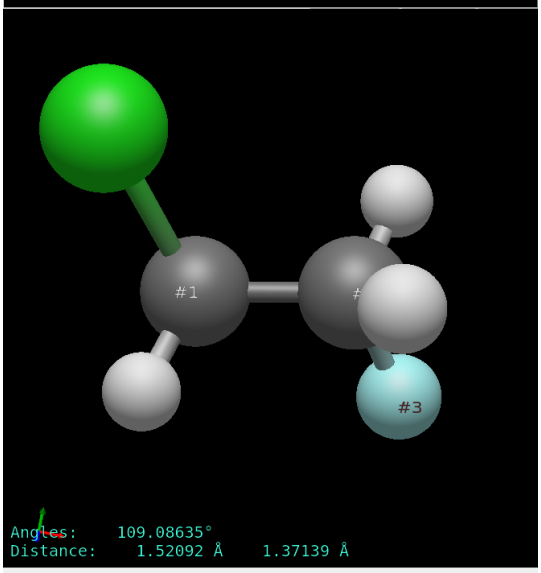
4. c2h4fcl
   formal charge = 0
   unpaired electron = ?
   ->

- energy : -15.596100888091 Eh

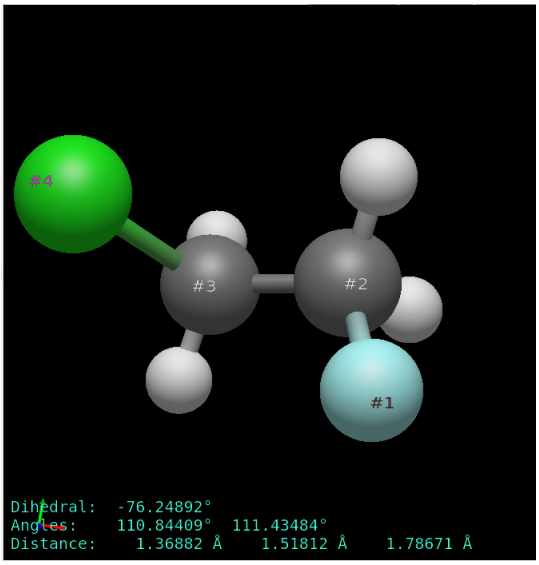






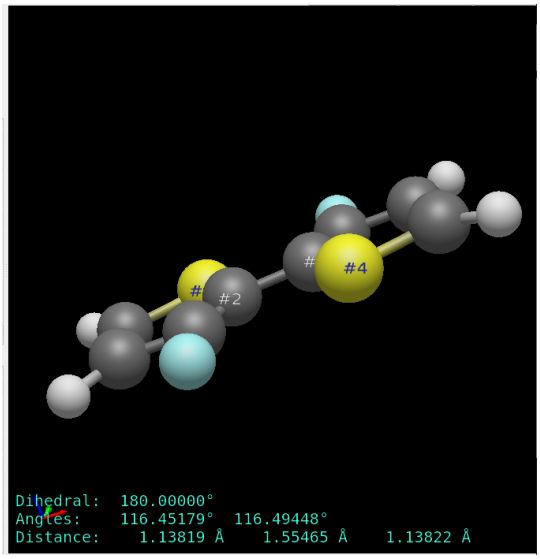


- energy : -15.593325040590 Eh

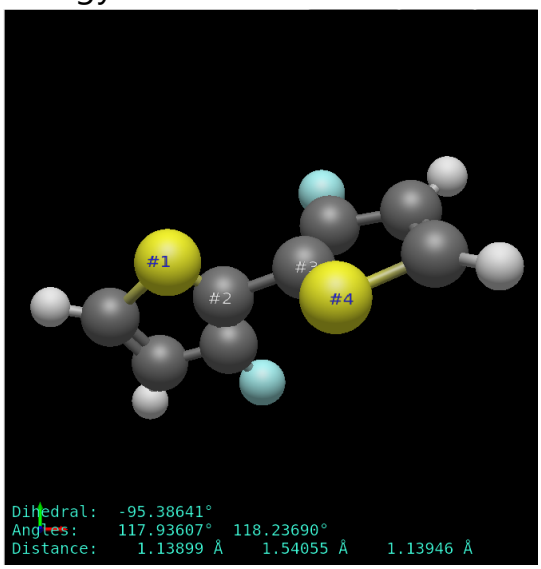


5. c8h4s2f2
   formal charge = 0
   unpaired electron = ?
   ->

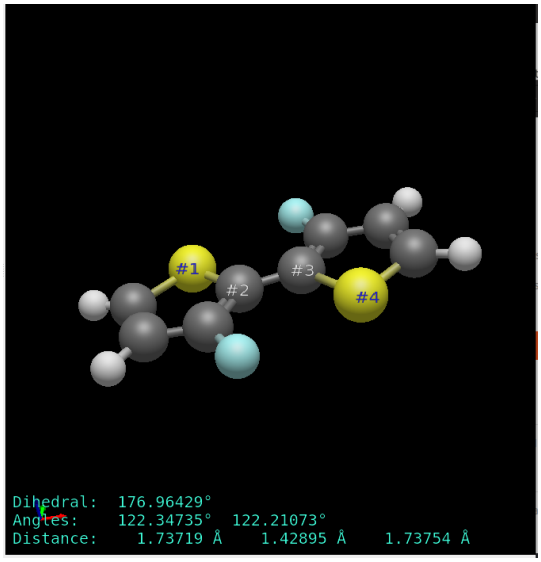
- Energy : -33.314732158128 Eh



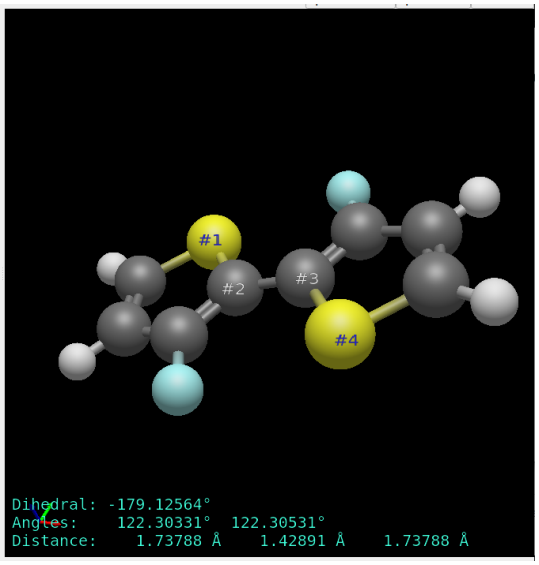
- Energy : -33.411759258290 Eh



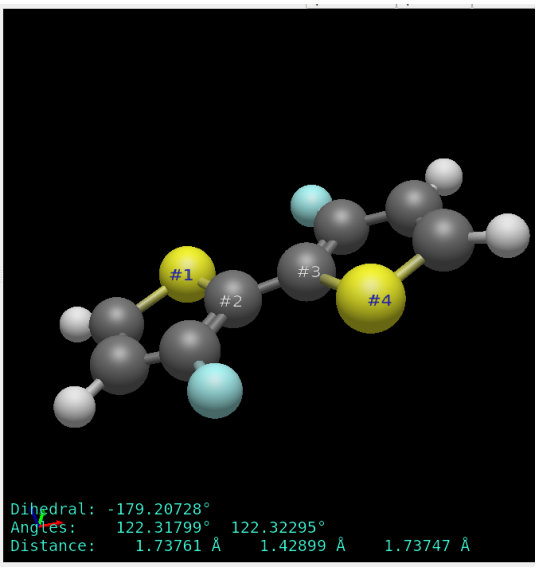
- Energy : -33.312569760068 Eh



- **Energy : -33.310644885065 Eh**



- Energy : -33.318542987727 Eh



3. please specify their molecular dipole moment

1. Inertia metrix

Moment of Inertia Matrix

Solid objects:

$$I = \begin{bmatrix} \int \rho(y^2+z^2)dV & -\int \rho xydV & -\int \rho xzdV \\ -\int \rho xydV & \int \rho(x^2+z^2)dV & -\int \rho yzdV \\ -\int \rho xzdV & -\int \rho yzdV & \int \rho(x^2+y^2)dV \end{bmatrix}$$

Symmetric Matrix:

- Matrix has real eigenvalues
- Matrix has orthogonal eigenvectors
- Can be rotated into diagonal form

2. How to define the molecular long axis? (Hint: moment of inertia matrix)
   解特徵值問題:$I\omega = \lambda\omega$

- λ=moment of inertail

- ω=long axis
  https://www.youtube.com/watch?v=oRrIL4P4lFI
  (https://www.youtube.com/watch?v=oRrIL4P4lFI)

3. how to allign the molecular

- calculate the molecular long axis
- rotate the molecular by rotation metrix(3d) to z axis

4.Generate energy curve

Bash code

```
export OMP_STACKSIZE=8G
ulimit -s unlimited
export OMP_NUM_THREADS=16,1
export MKL_NUM_THREADS=8

for d in $(seq 80 10 200) 250 300 400 500;do
    mkdir $d
    D=$(python3 -c "print(0.74*$d/100)")
    cd $d
    echo -e "2\n\nH 0 0 0\nH $D 0 0" > h2_$d.xyz
    xtb -c 0 -u 0 h2_$d.xyz  > xtb.out
    cd ..
done
```

Create files

```
for d in $(seq 80 10 200) 250 300 400 500;do
    mkdir $d
done
```

float and varieable calculation

- Use python to calculate

```
D=$(python3 -c "print(0.74*$d/100)")
```

echo file with the Escape Character

- -e parameter will output the escape character without direct print it

```
echo -e "2\n\nH 0 0 0\nH $D 0 0" > h2_$d.xyz
```

https://www.twblogs.net/a/5b7ffe812b717767c6b2ca6b (https://www.twblogs.net/a/5b7ffe812b717767c6b2ca6b)

get the file list

```
#start 80, end 200, increse 10
seq 80 10 200
```

get energy word by grep

- find the total enrgy word from every out file

```
grep -Rw */*.out -e "total energy"
```

-R : recursive find the directory
-w : show the line have the word
-e : the certain string need to searched
https://www.tecmint.com/find-a-specific-string-or-word-in-files-and-directories/ (https://www.tecmint.com/find-a-specific-string-or-word-in-files-and-directories/)

Excel data analyze