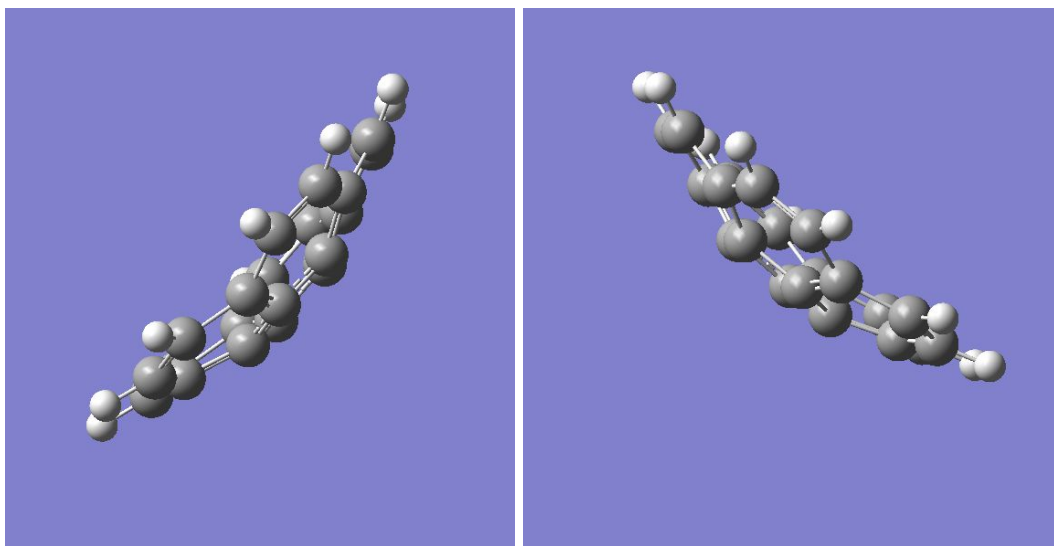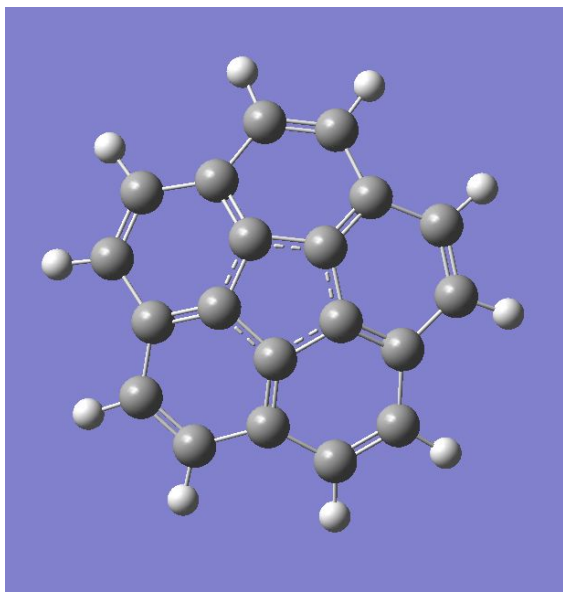# Kushagra Agarwal 2018113012 CND LAB EXAM END SEMESTER

Q1) Corranulene $C_{20}H_{10}$ bowl inversion and cation pi interactions

Corranulene Bowl Shape Shown in both directions

Corranulene Bowl Inversion Transition State Shown

a) Now for calculation of bowl depth we will resort to trigonometry. We first calculated the dihedral angle between carbons in pentane ring and outermost carbons of benzene. Then we

calculated the distance between the atoms. Now applying simple trigonometry (sin(dihed)*length) we found out the bowl depth.

Dihedral angle = 160.29312 degrees

Length= 2.366 A

So final bowl depth came out to be = 0.79783486146 A

b) To calculate the energy barrier we first calculated energy of transition and then energy of bowl, their difference will give the inversion barrier

Bowl Energy= -753.8912534 Hartrees

Transition State Energy = -753.8776189 Hartrees

Barrier = (TSE-BOWLE)= 0.0136345 Hartrees

c)

The following 4 photos represent the Lithium ion showing cation pi interaction with the molecule.

The concave and convex side have been shown for the bowl as well.

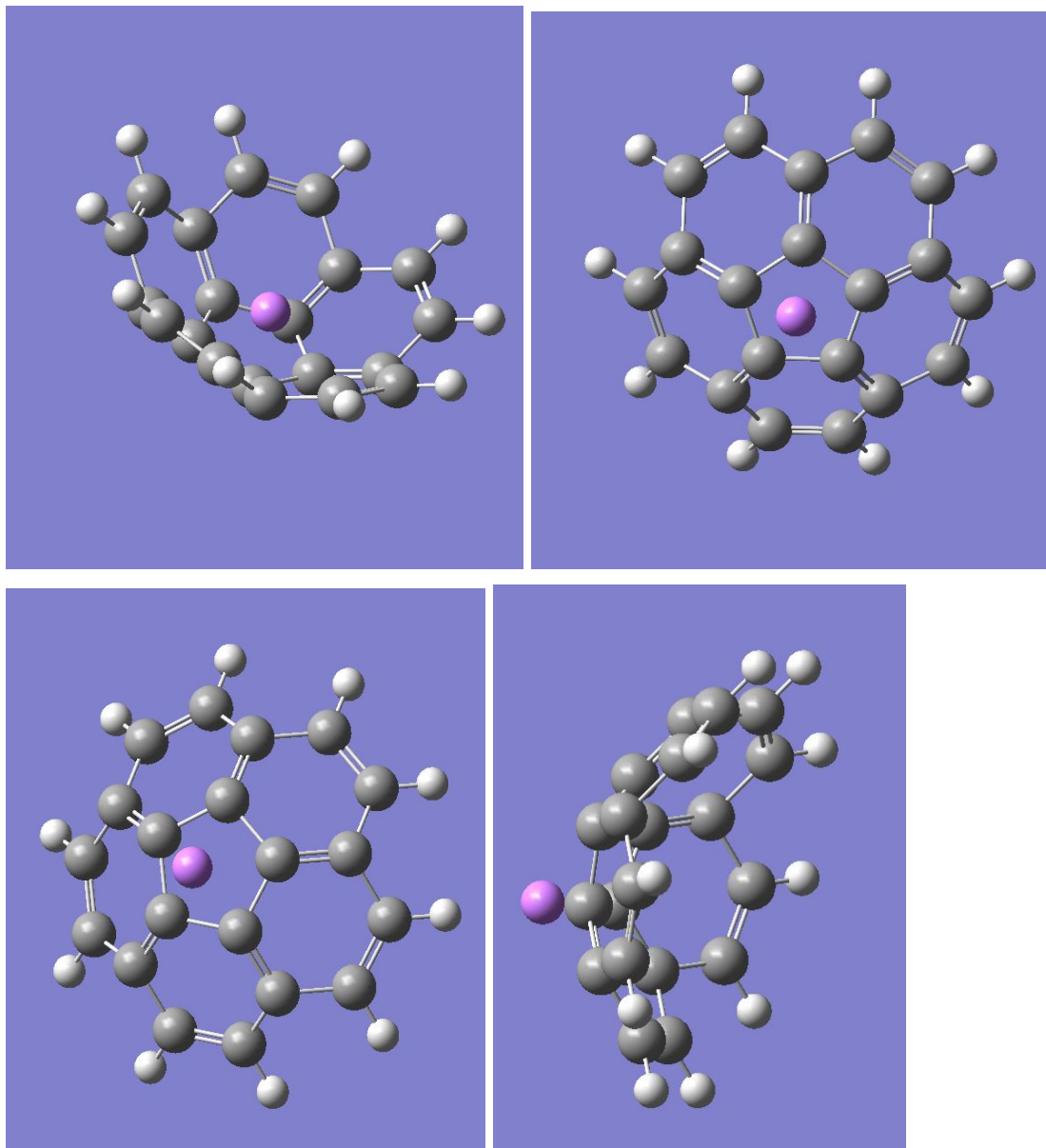The enrgies as follows- in hartrees

1) -760.8745632
2) -760.8735467
3) -761.1288304
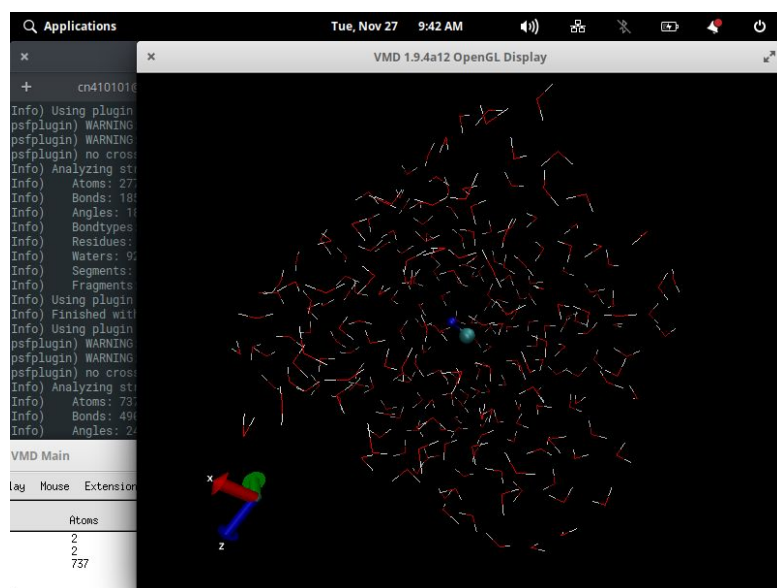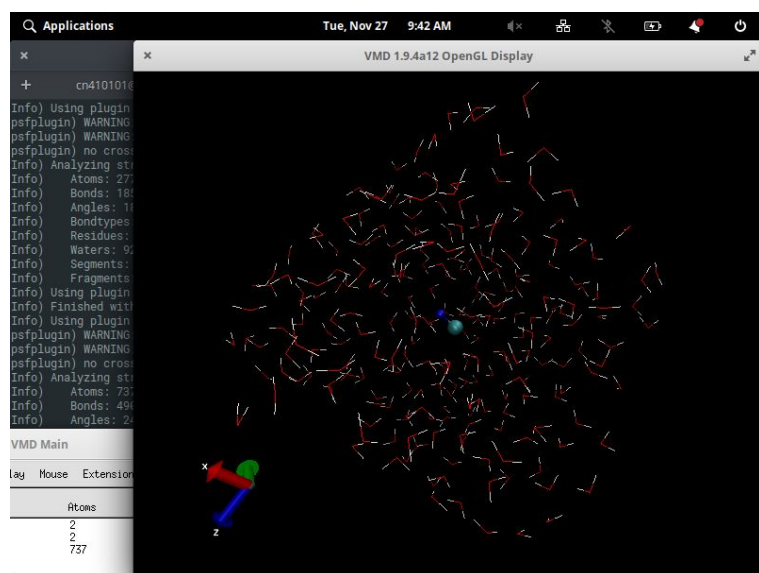4) -760.3571937

 Most stable is 3

Photos in order are

3 1

d)No, Corranulene does not undergo bowl to bowl inversion barrier.

Q2) Performing Umbrella Sampling.

     a) Solvated NaCl has been shown below

To create this, first we loaded NaCl pdb molecule. Did an Auto PSF then added Solvation box and NaClSolvated.psf was created.