CNS EndSem

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1 Bowl inversion of Corranulene

Run two optimizations on the TS and then IRC for maxpoints = 50

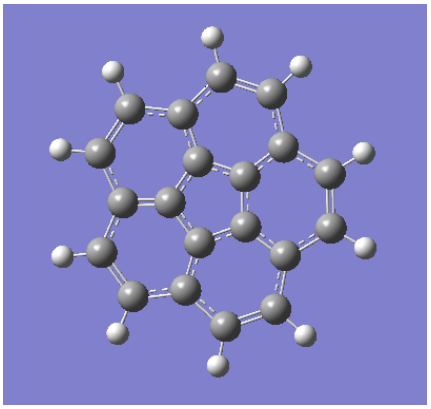


Figure 1: TS

1.1 (a) Bowl depth

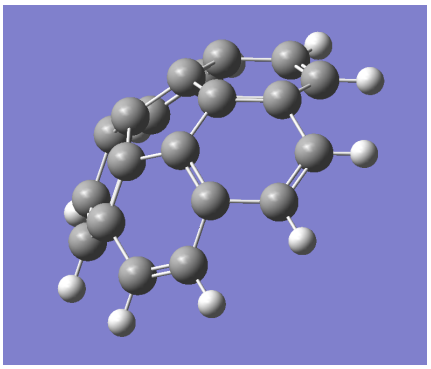


Figure 2: Final Bowl Structure

Bond length = 2.5500 A Bond angle = 160.29 degrees sin(Bond Angle) = 0.33725957

$$BowlDepth = Bondlength * sin(BondAngle) = 0.8600119035A \quad (1)$$

1.2 (b) Energy Barrier

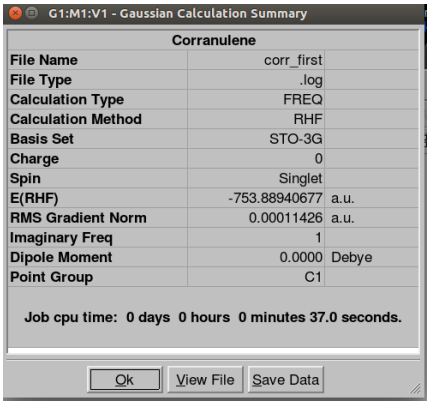


Figure 3: Summary of TS

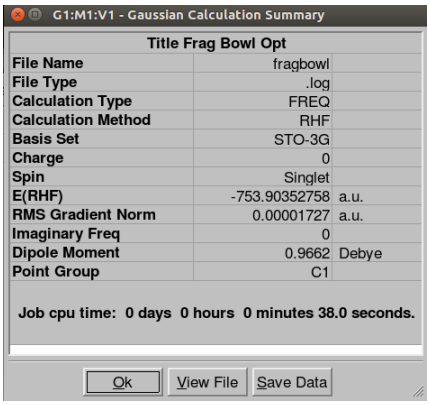


Figure 4: Summary of Bowl Structure

$$\Delta Energy_{\text{barrier}} = Energy_{\text{bowl}} - Energy_{\text{TS}} = 0.01412081 Hartrees \tag{2}$$

1.3 (c)

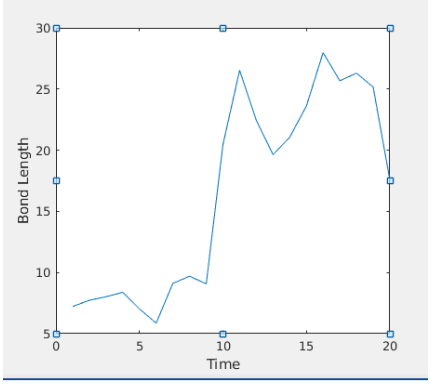
There are 5 possible structures.

1.4 (d)

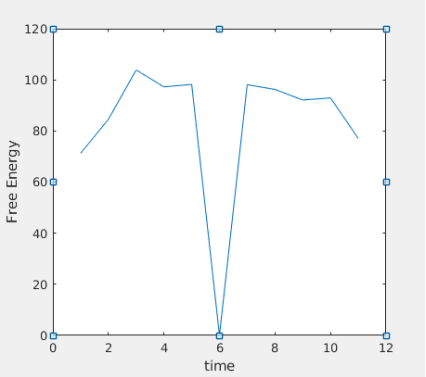
No, Inversion does not take place due to pi-pi interactions.

2 NaCl MD Simulation and Umbrella Sampling

2.1 (a)MD Simulation and Events of Association-Dissociation



2.2 (b)Umbrella Sampling at Room Temperature



2.3 (c)Umbrella Sampling at 500K

Due to high kinetic energy (on account of high temperature) molecules the umbrella sampling failed. Molecules were moving too fast.

However we can say due to high kinetic energy, randomness would be high implying that free energy of case (c) will be lesser than case (b).