

## 1 Bowl inversion of Corranulene

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

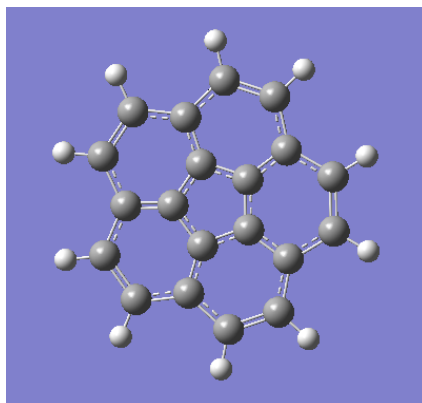


Figure 1: TS

### 1.1 (a) Bowl depth

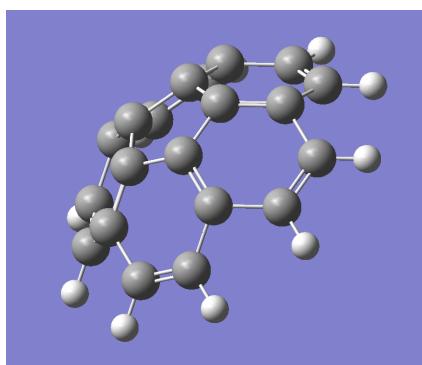
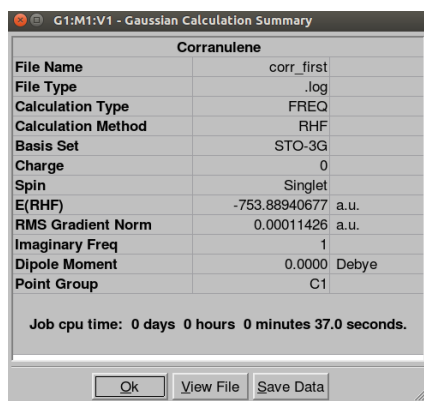


Figure 2: Final Bowl Structure

Bond length = 2.5500 A      Bond angle = 160.29 degrees       $\sin(\text{Bond Angle}) = 0.33725957$

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

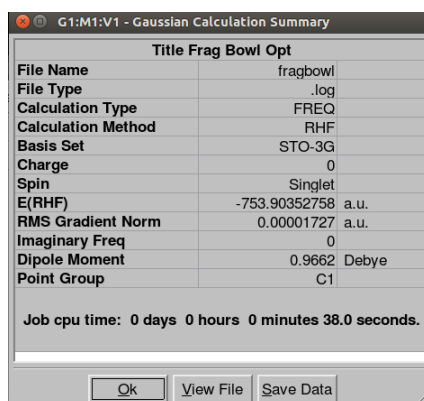
## 1.2 (b) Energy Barrier



A screenshot of a Gaussian Calculation Summary window titled 'G1:M1:V1 - Gaussian Calculation Summary'. The window displays a table of calculation parameters for a molecule named 'Corranulene'. The parameters include File Name, File Type, Calculation Type, Calculation Method, Basis Set, Charge, Spin, E(RHF), RMS Gradient Norm, Imaginary Freq, Dipole Moment, and Point Group. At the bottom, it shows the job CPU time and buttons for 'Ok', 'View File', and 'Save Data'.

Corranulene	
File Name	corr_first
File Type	.log
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
E(RHF)	-753.88940677 a.u.
RMS Gradient Norm	0.00011426 a.u.
Imaginary Freq	1
Dipole Moment	0.0000 Debye
Point Group	C1
Job cpu time: 0 days 0 hours 0 minutes 37.0 seconds.	

Figure 3: Summary of TS



A screenshot of a Gaussian Calculation Summary window titled 'G1:M1:V1 - Gaussian Calculation Summary'. The window displays a table of calculation parameters for a molecule named 'Title Frag Bowl Opt'. The parameters include File Name, File Type, Calculation Type, Calculation Method, Basis Set, Charge, Spin, E(RHF), RMS Gradient Norm, Imaginary Freq, Dipole Moment, and Point Group. At the bottom, it shows the job CPU time and buttons for 'Ok', 'View File', and 'Save Data'.

Title Frag Bowl Opt	
File Name	fragbowl
File Type	.log
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
E(RHF)	-753.90352758 a.u.
RMS Gradient Norm	0.00001727 a.u.
Imaginary Freq	0
Dipole Moment	0.9662 Debye
Point Group	C1
Job cpu time: 0 days 0 hours 0 minutes 38.0 seconds.	

Figure 4: Summary of Bowl Structure

$$\Delta Energy_{\text{barrier}} = Energy_{\text{bowl}} - Energy_{\text{TS}} = 0.01412081 \text{ Hartrees} \quad (2)$$

## 1.3 (c)

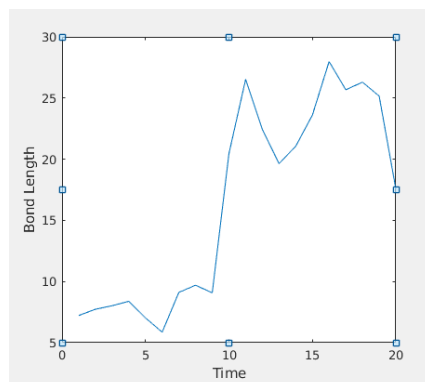
There are 5 possible structures.

## 1.4 (d)

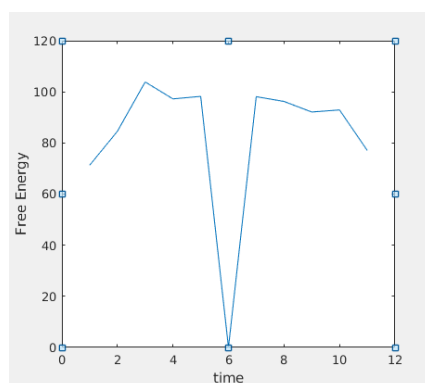
No, Inversion does not take place due to pi-pi interactions.

## 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).