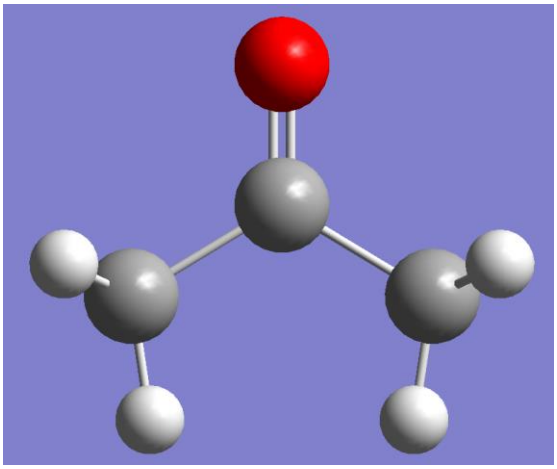
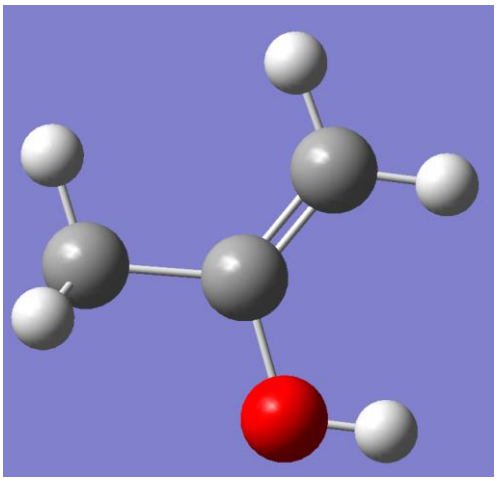
Gaussian Software

Problem 1:

Reactant and product are acetone and propenal

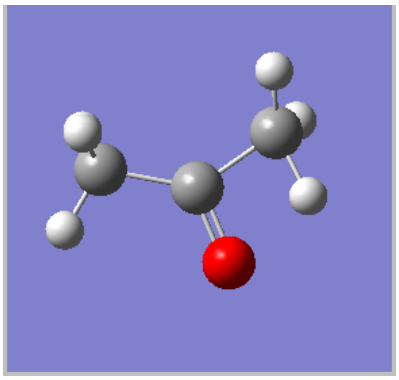


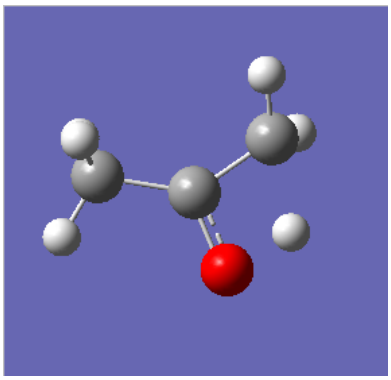
Acetone

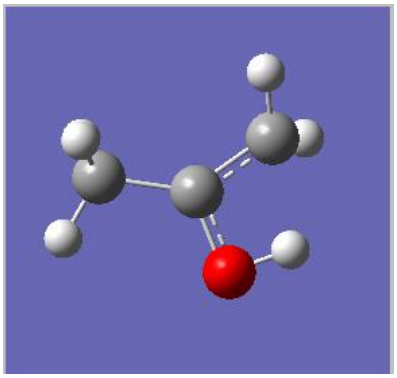


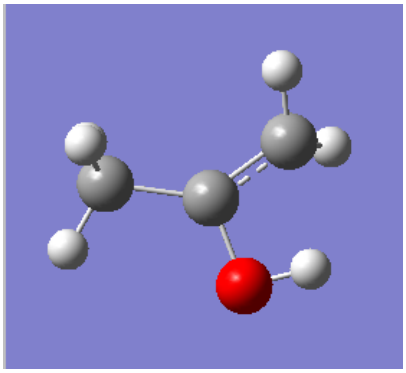
Propenal

Steps:

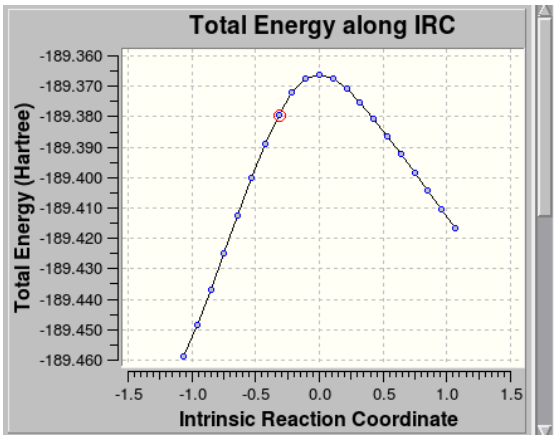
1. 

2. 

3. 

4. 

Graph:



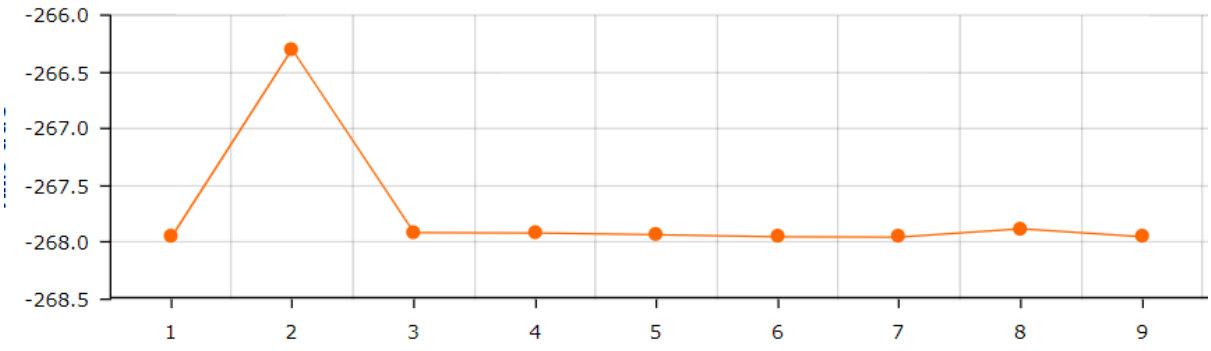
The difference between energies of reactants and products is 0.04 Hartree or 25.1004 kcal per mole.

The energy of transition state is 118,831.5687 kcal per mole.

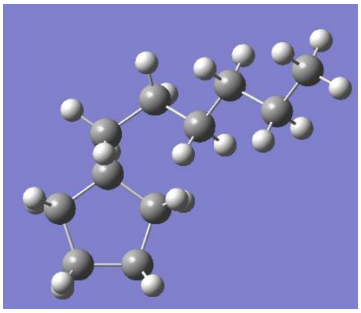
Here, acetone is more stable than propenal.

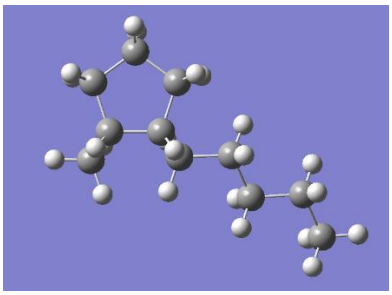
Problem 2:

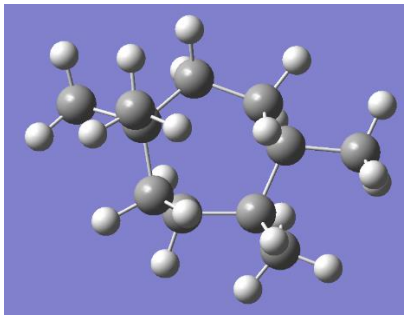
The energies of the 9 isomers of $c_{11}H_{22}$ are plotted in the following graph. It depicts that isomer 2 has more energy than the rest and that isomer 6 is most stable.

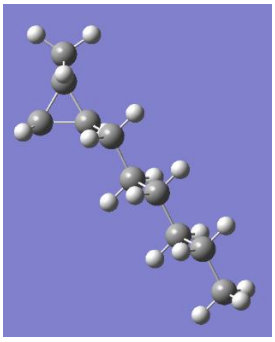


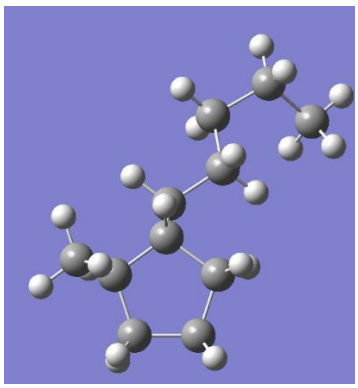
The structures of the 9 isomers are the following in order:

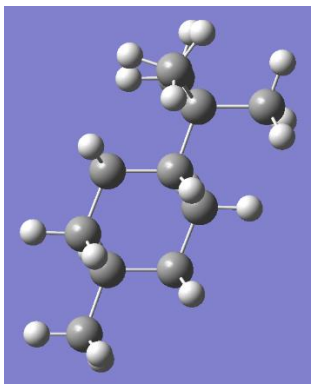
1. 

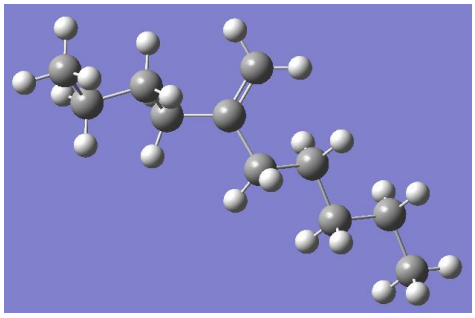
2. 

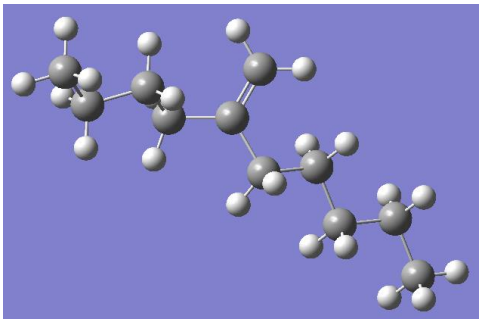
3. 

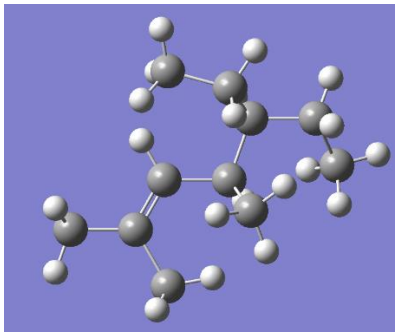
4. 

5. 

6. 

7. 

8. 

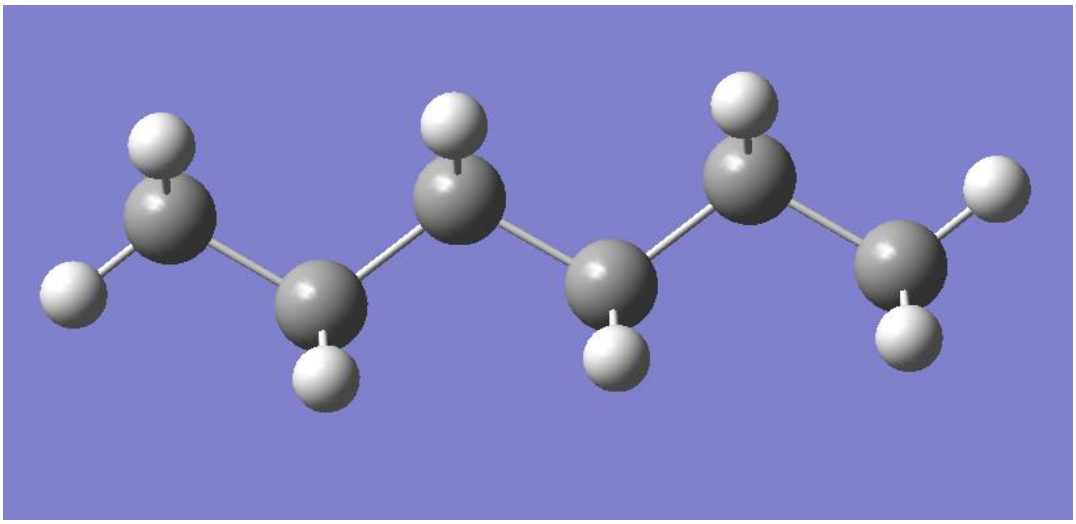
9. 

Problem 3:

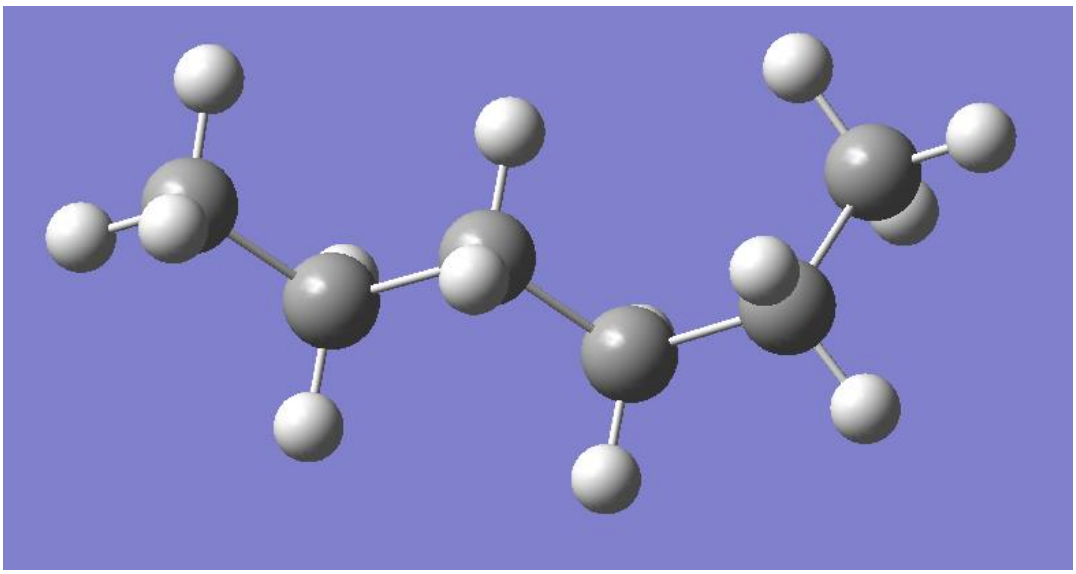
Dihedral scans of n hexane along different atoms as given

Scan done for 180 degrees

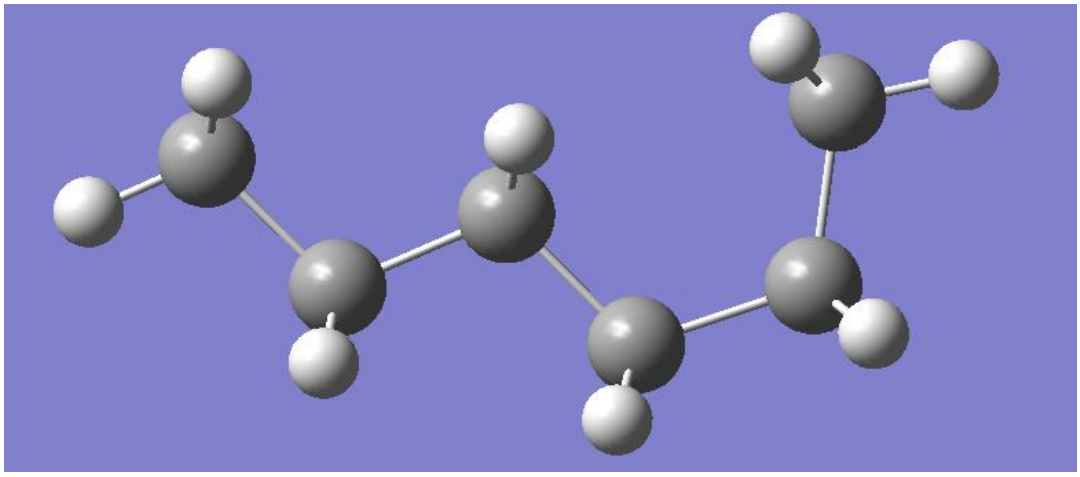
3. 1 .1: staggered form of the given scan



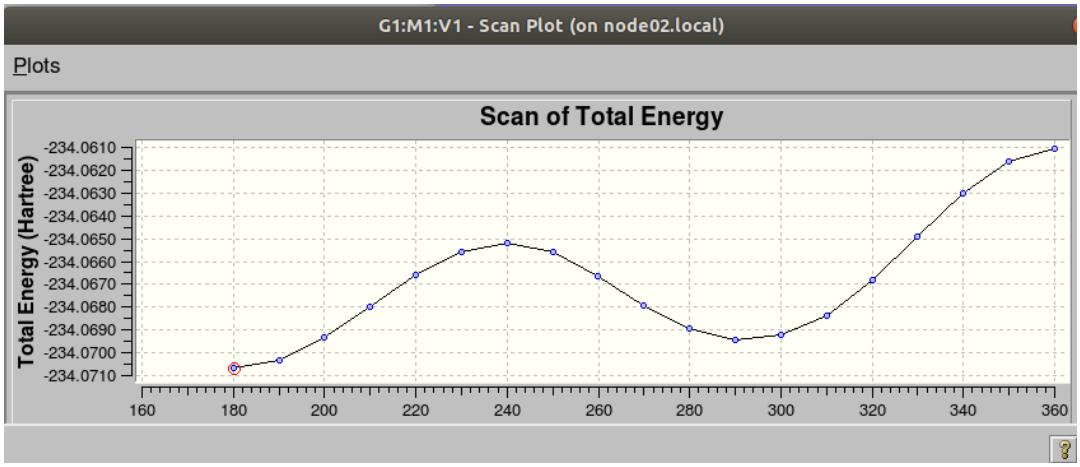
3.1 .2: Gauche form of given scan



3.1.3: Eclipsed form of the given scan



3.1: scan graph of energies

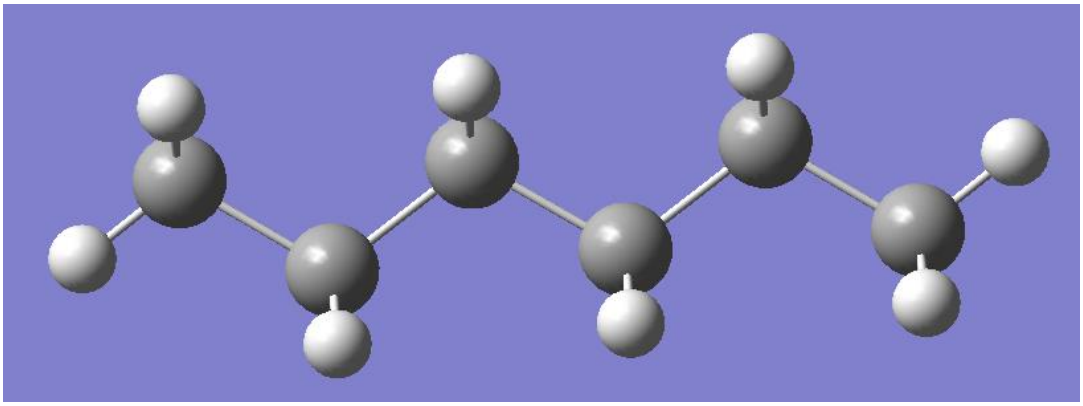


The staggered form is most stable form

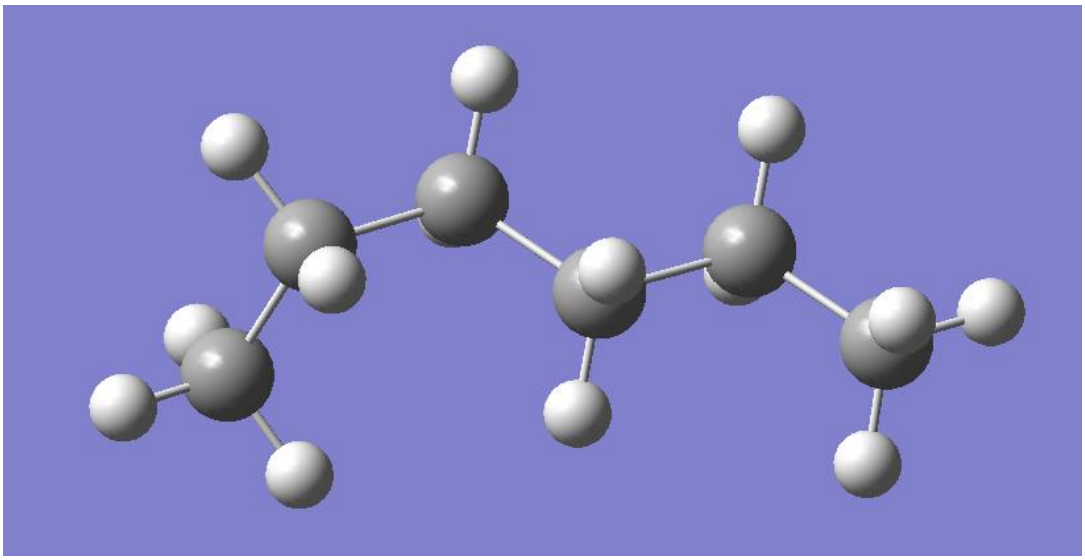
The gauche form is moderately stable

The eclipsed form is least stable out of the three

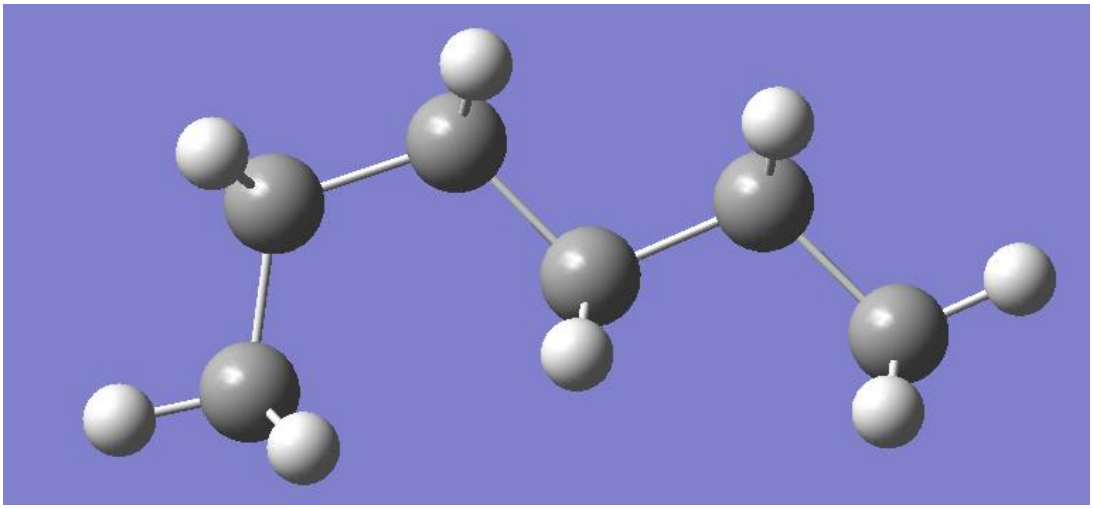
3. 2.1: staggered form of the given scan



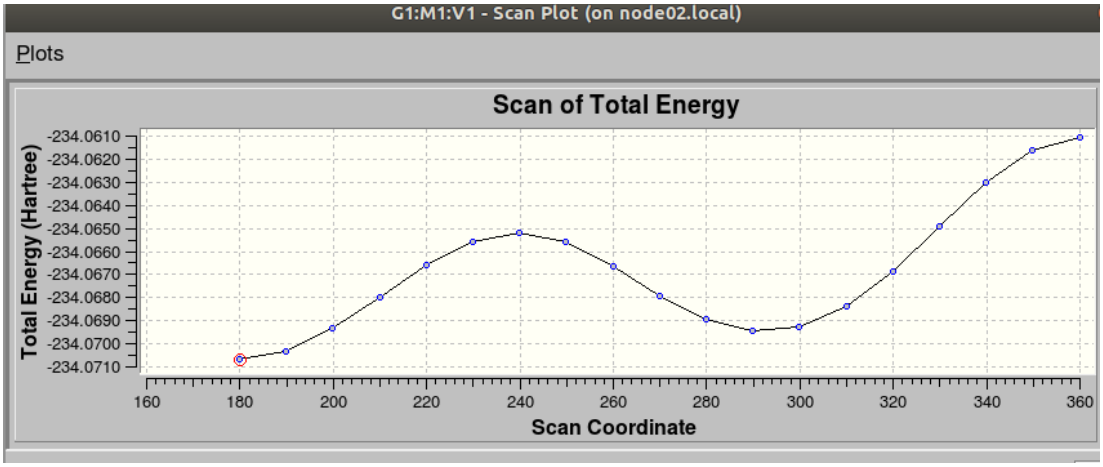
3.2.2: gauche form of the given scan



3.2.3: eclipsed form of the given scan



3.2: scan graph of energies

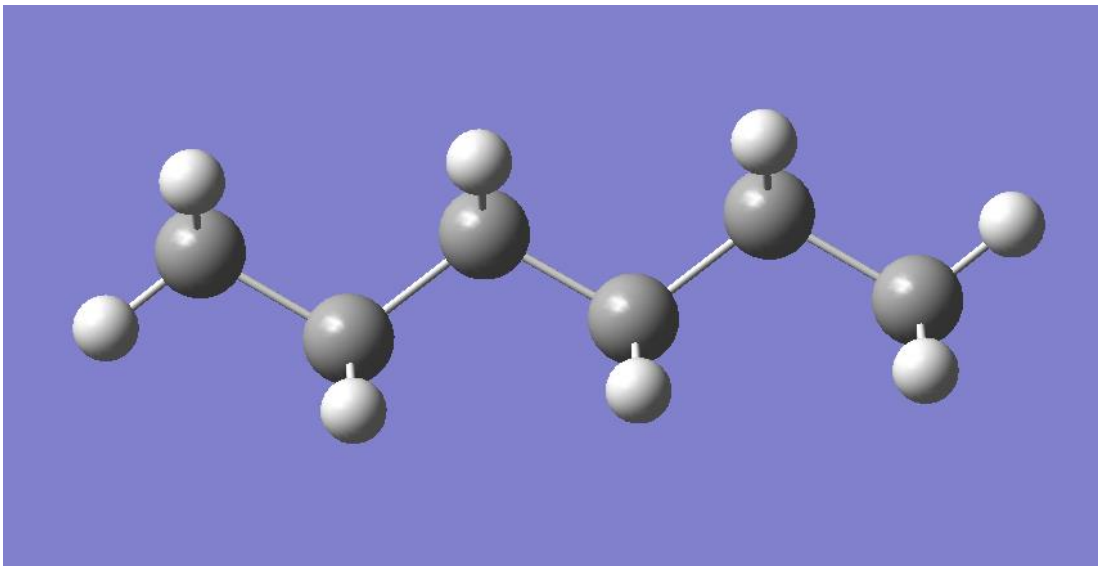


The staggered form is most stable

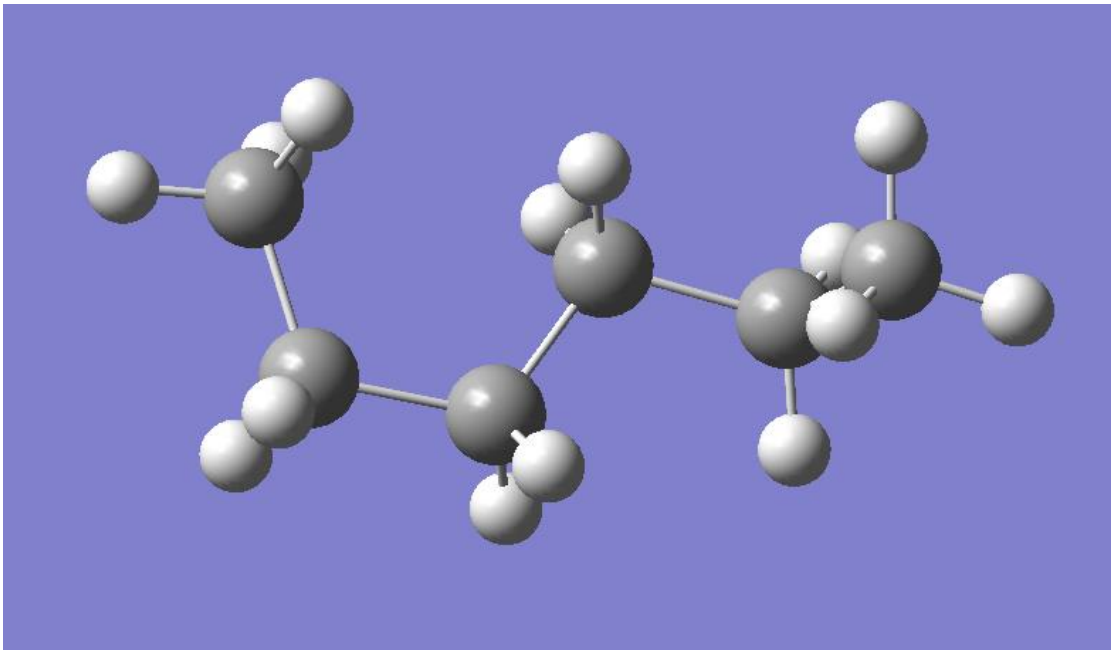
The gauche form is moderately stable

The eclipsed form is least stable

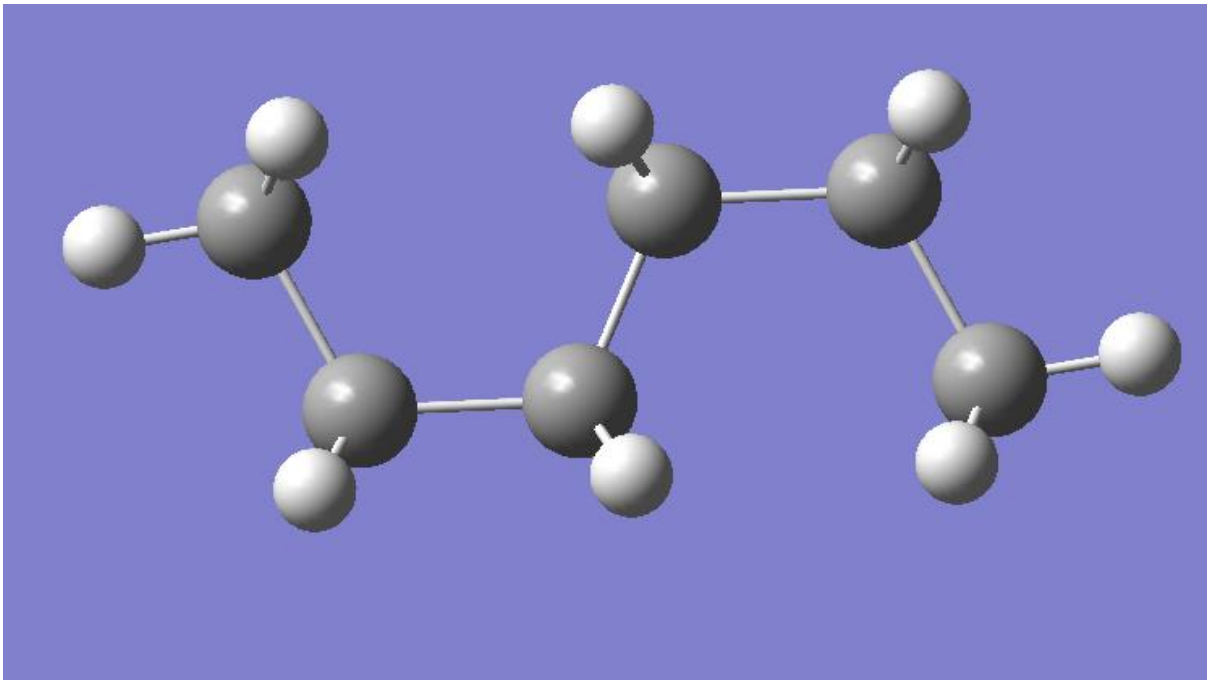
3.3.1: staggered form of the given scan



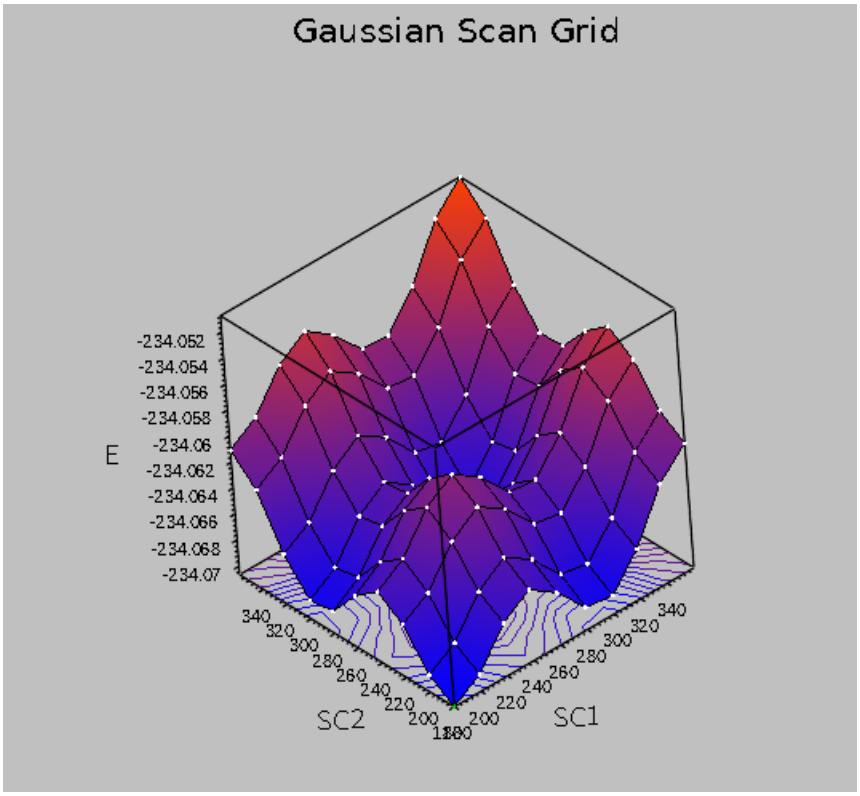
3.3.2: gauche form of the given scan



3.3.3: eclipsed form of the given scan



3.3: graph of the given scan/ potential energy diagram



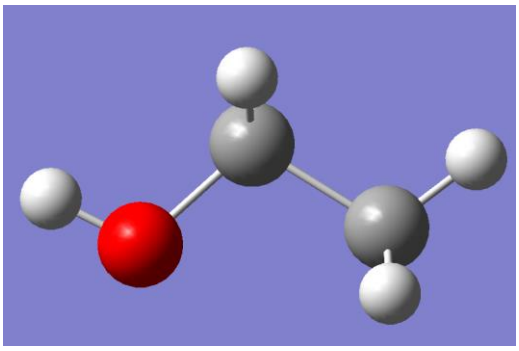
The staggered form is highly stable

The gauche form is moderately stable

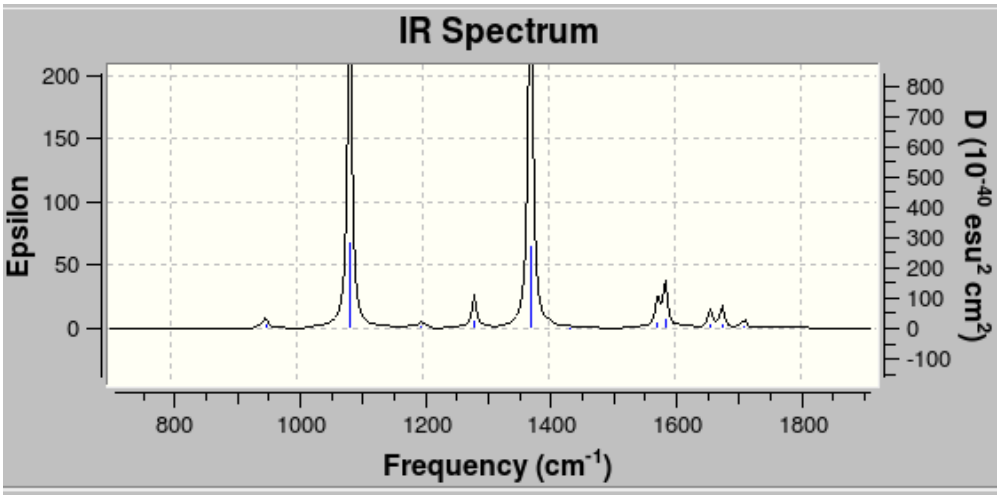
The eclipsed form is least stable of all three

Problem 4:

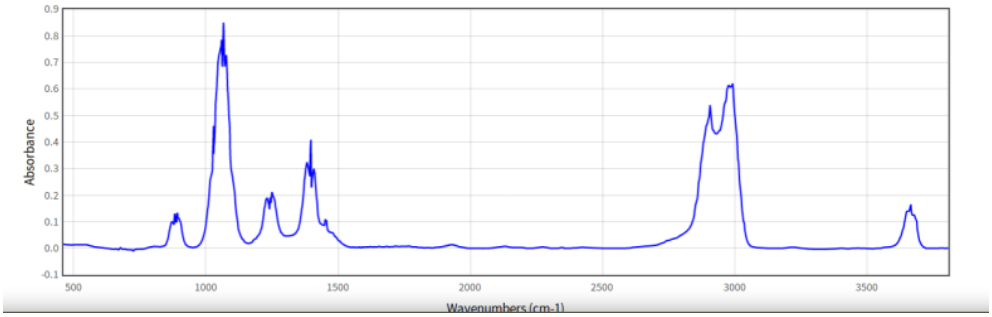
Ethanol structure:



The vibration IR spectrum



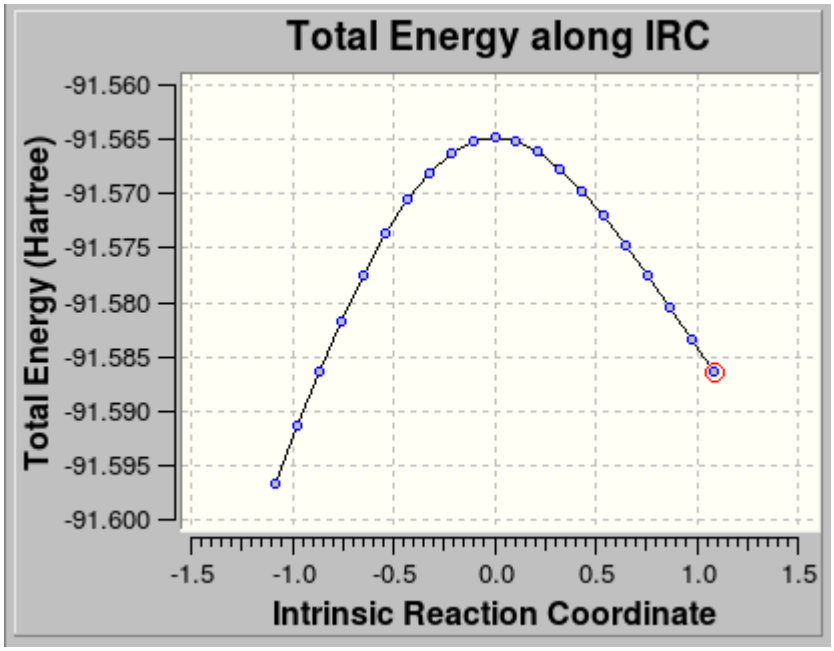
Original spectrum:



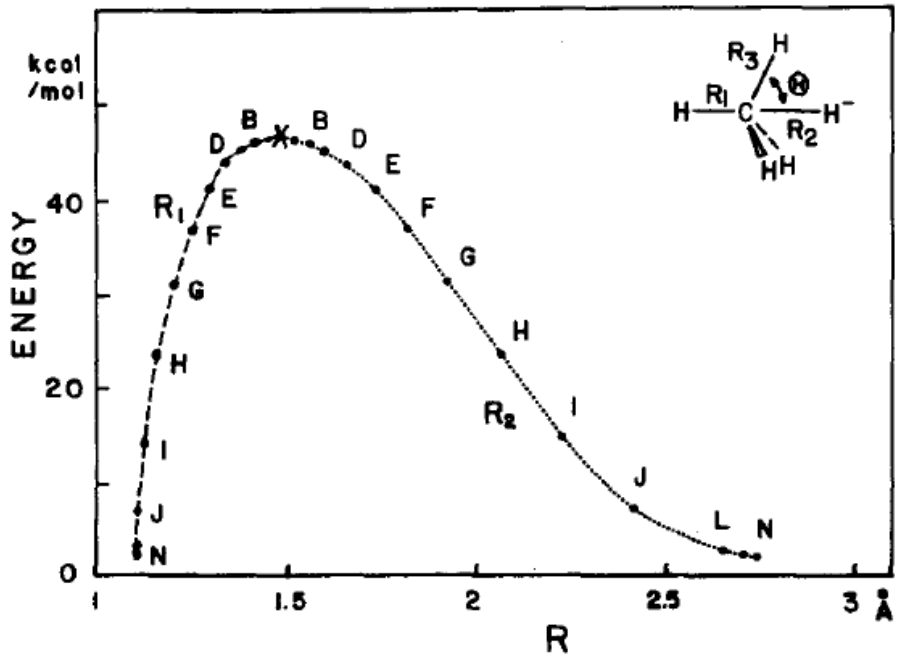
The peaks of this ethanol represent the respective vibrations that are with respect to the wavenumbers given in the graph. These are the vibrations that have maximum frequency. These are the vibrations that happen majorly with respect to hydrogens. Due to the less mass and more freedom of hydrogens, they have a higher frequency.

Problem 5:

Energy diagram of **HNC-+HCN**



The referance graph

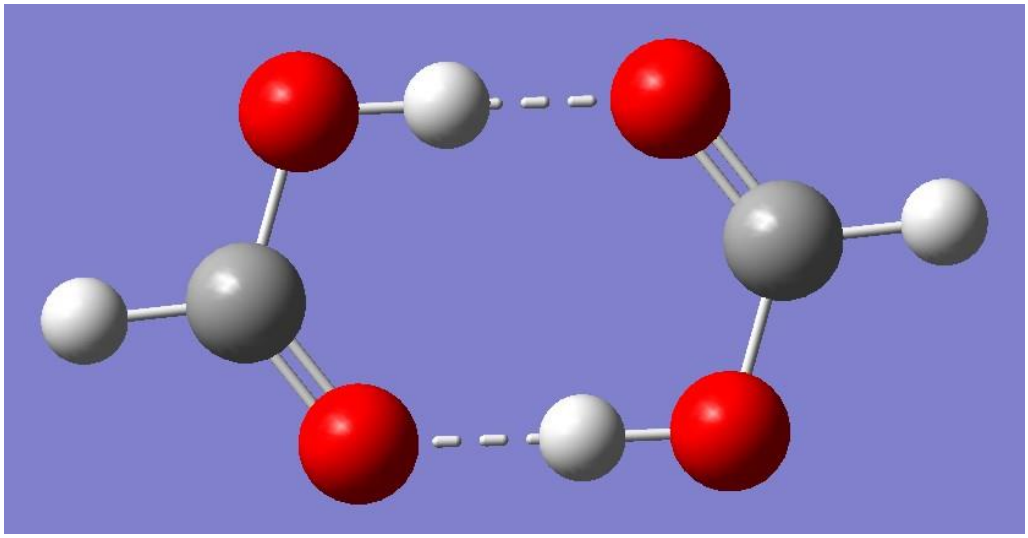


The position of the carbon atom moves only slightly during the reaction, and only the two extreme positions are shown. The position of the hydrogen atom at the transition state is shown by H. The hydrogen atom moves smoothly from the left-hand side, which corresponds to HNC, through the transition state to the right-hand side (HCN).

Here, the saddle point is the transition state. The hydrogen moves from the nitrogen atom to carbon atom across this transition state. The Activation energy of this reaction is approximately 91.565 RHF or 61,578.37815 kcal/mol.

Problem 6

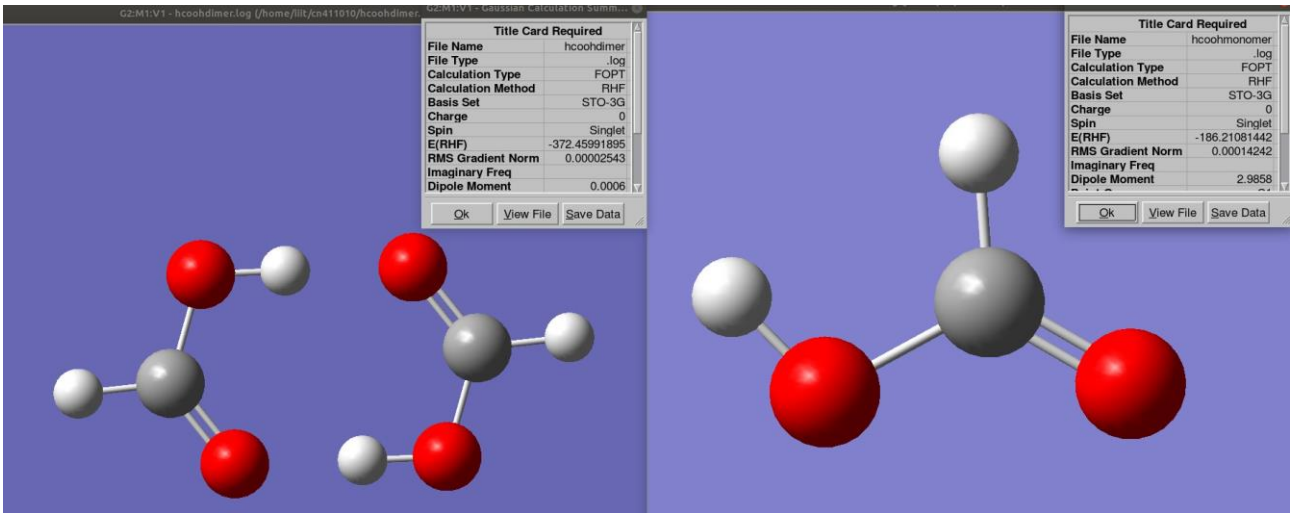
(a) Formic acid exists as a dimer in gas phase and the double bonded oxygen atoms of these molecules form a hydrogen bond with the other molecule's hydrogen atom linked with as a hydroxy group.



(b) The energy of two monomers of formaldehyde is higher than the energy of a formaldehyde dimer. Hence the dimer form is more stable enabling it prevail ore in the gaseous state instead of as monomers.

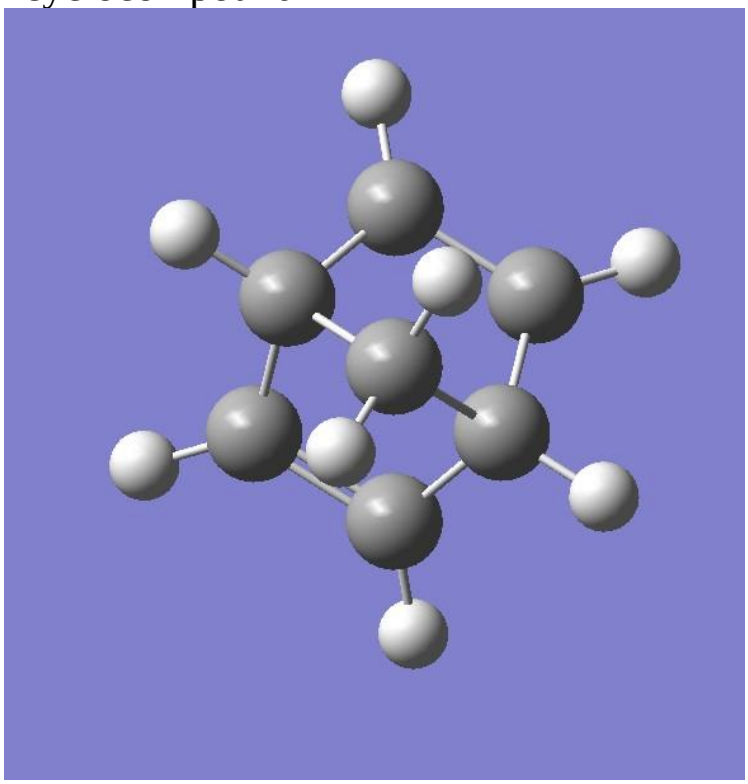
The energy difference b/w the dimer form and two monomers are −24.031191986 kJ/mol, i.e., the dimer form is more stable

by having 24.031191986kJ/mol energy less than the monomeric form.

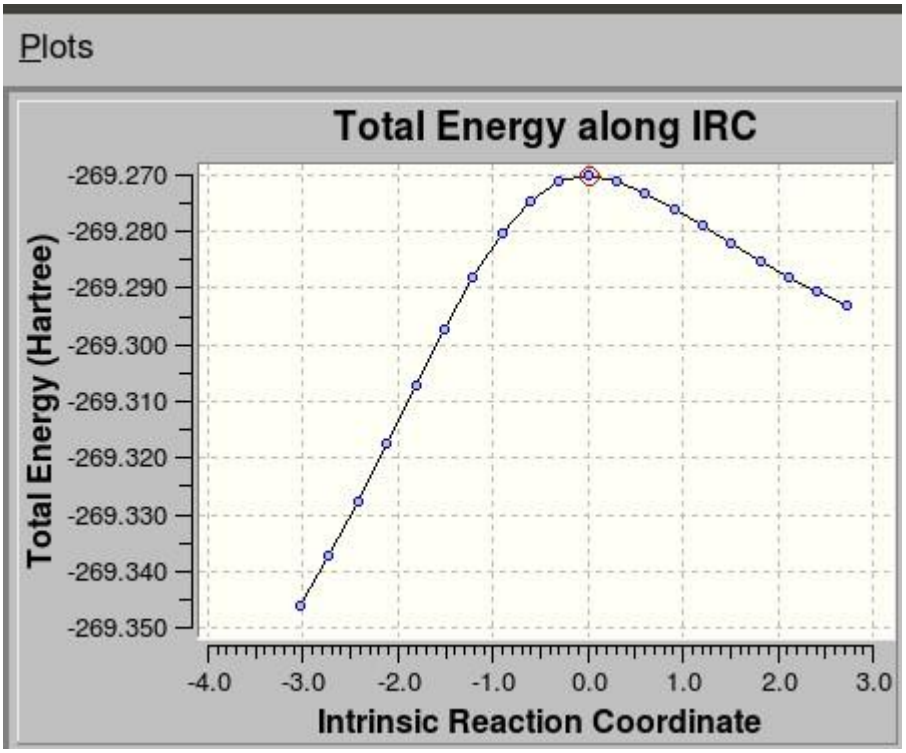


Problem 7

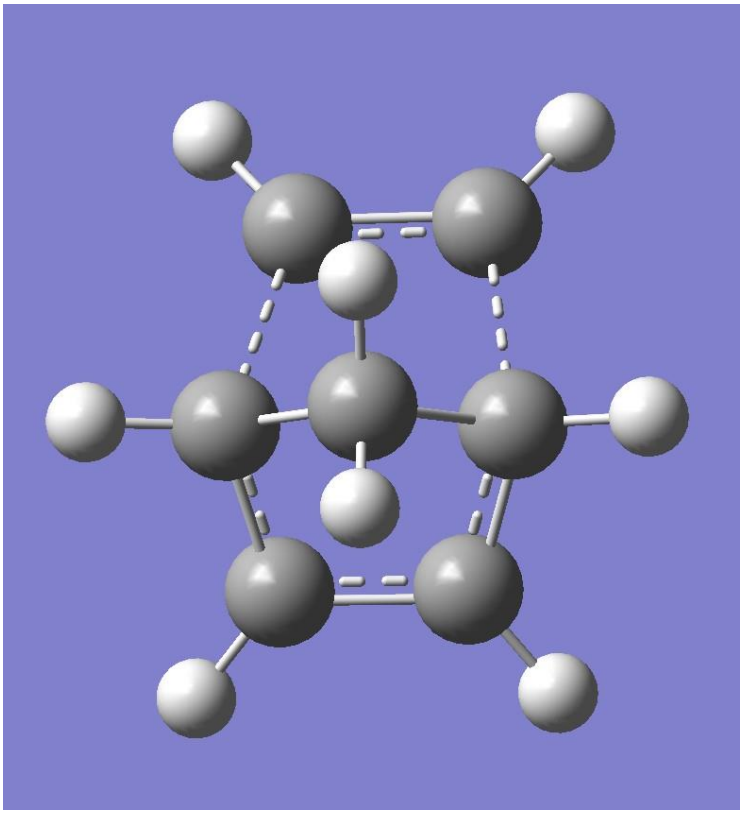
Reactants: cyclopent-1,3-ene and ethene
Product: Bicyclocompound



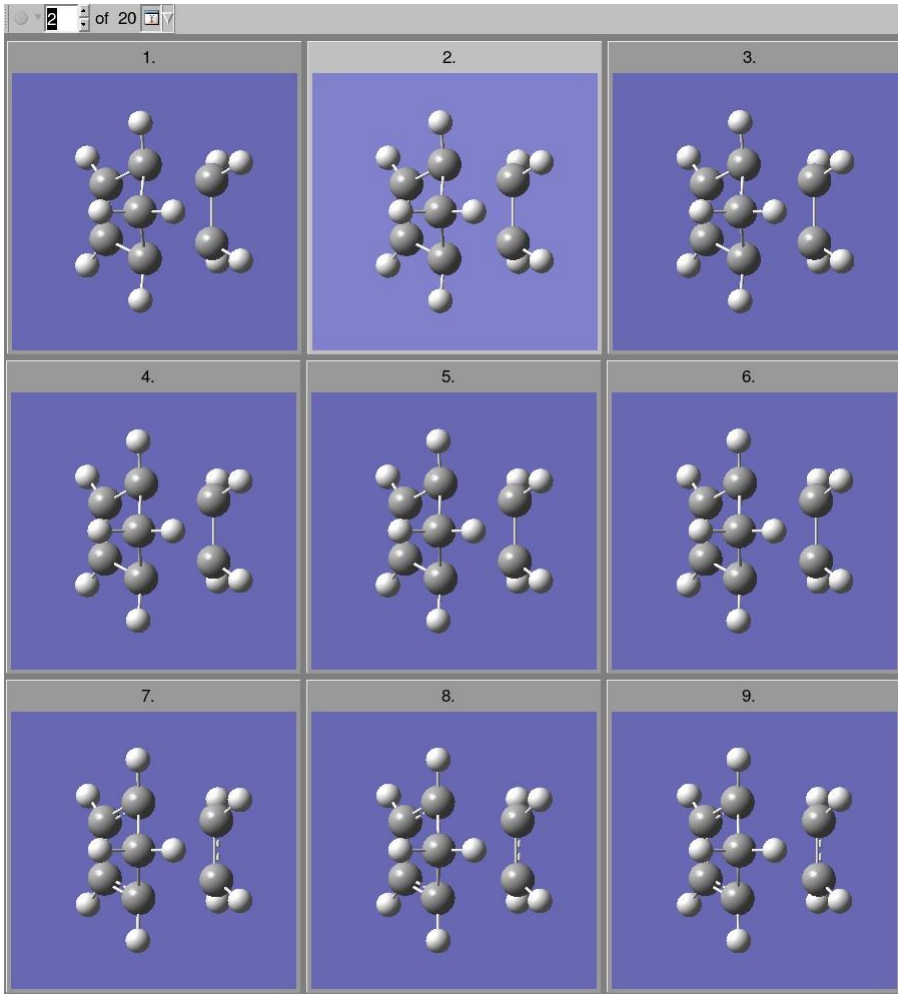
The IRC graphs

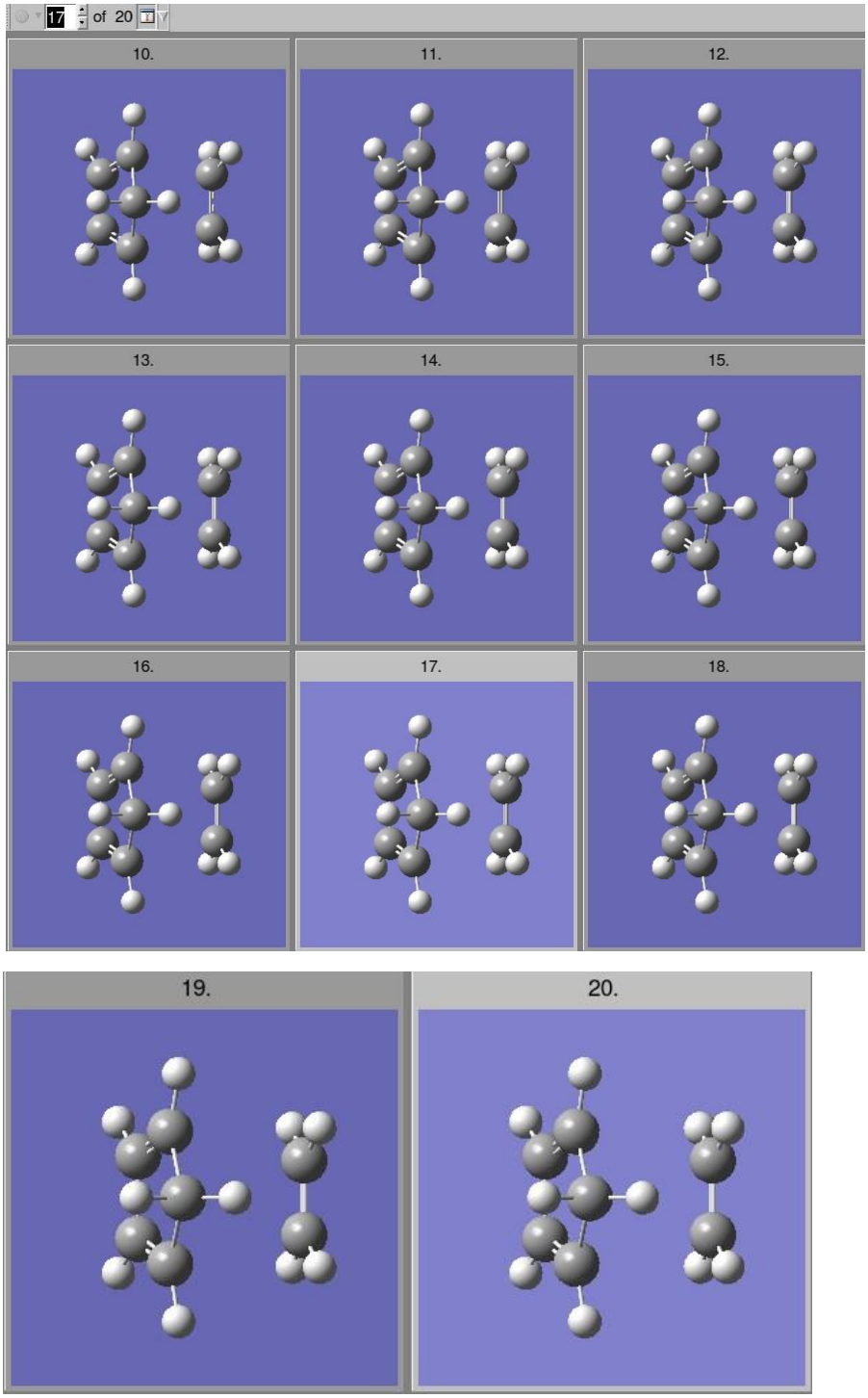


The transition states



The steps in IRC





In this reaction, there is a bond formed between two molecules, where the double bonds of both the molecules participate in the reaction. Here the formed product has only one double bond (there were three double bonds overall initially) and a bicyclo ring formed.