Gaussian Software

Challenge 1:

Reactant and product are acetone and propenal

A picture containing indoor

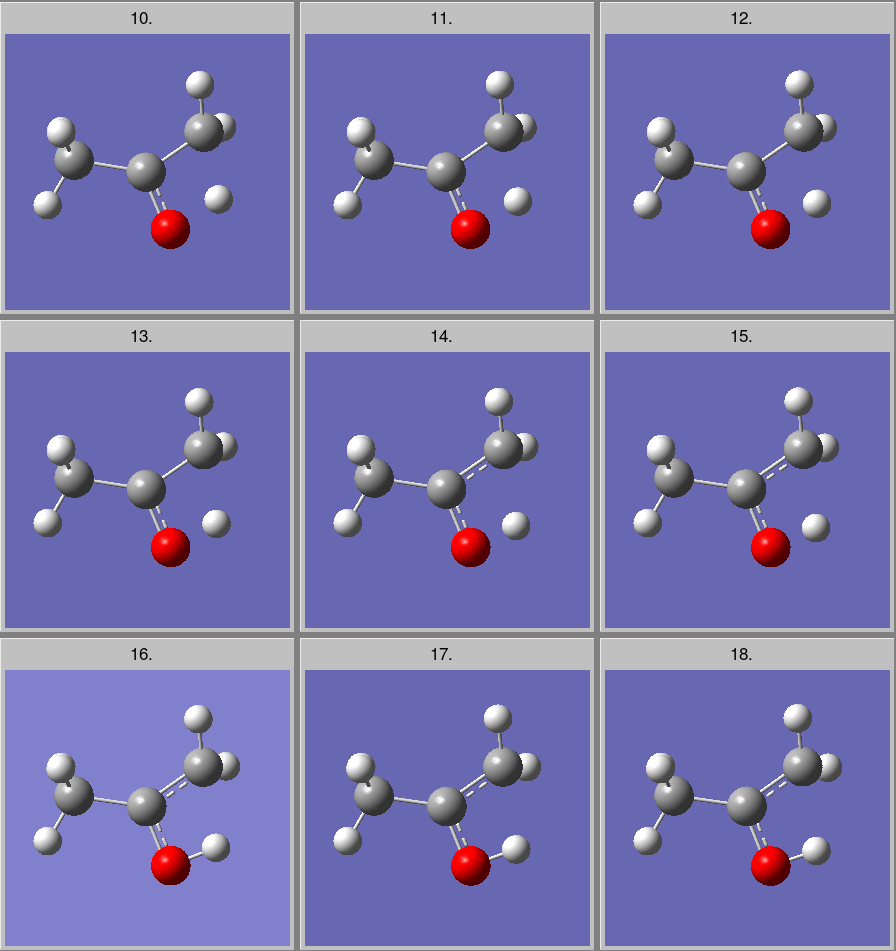
Description automatically generated A picture containing baseball, ball, indoor

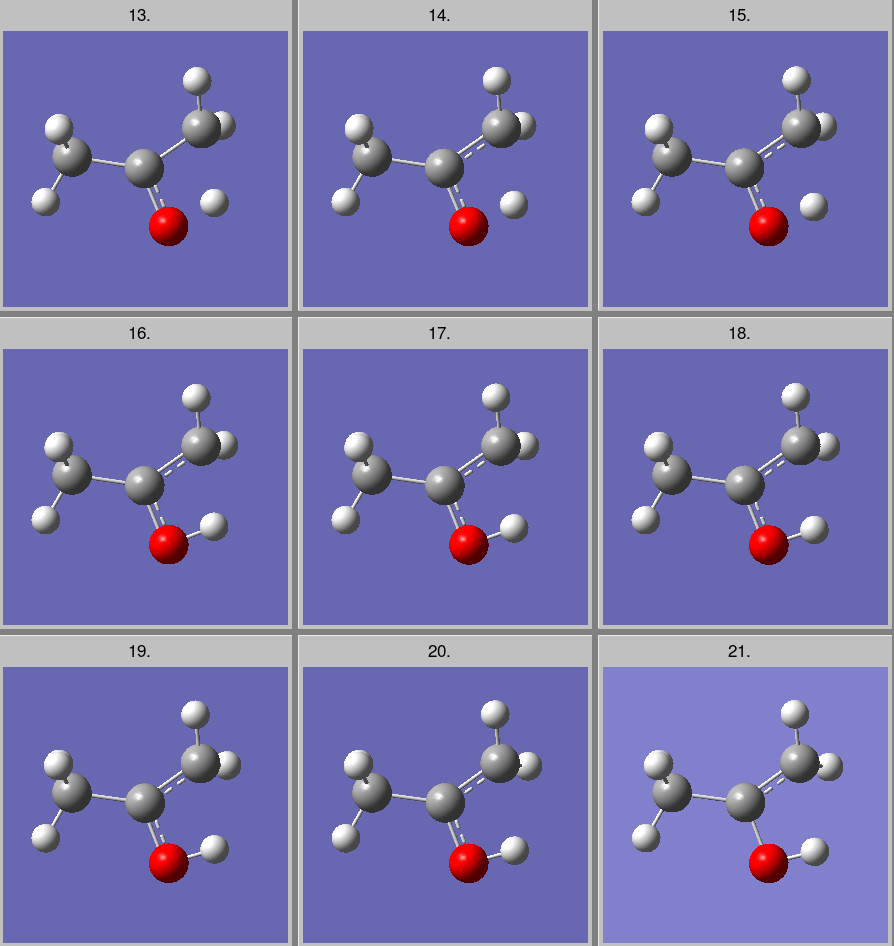
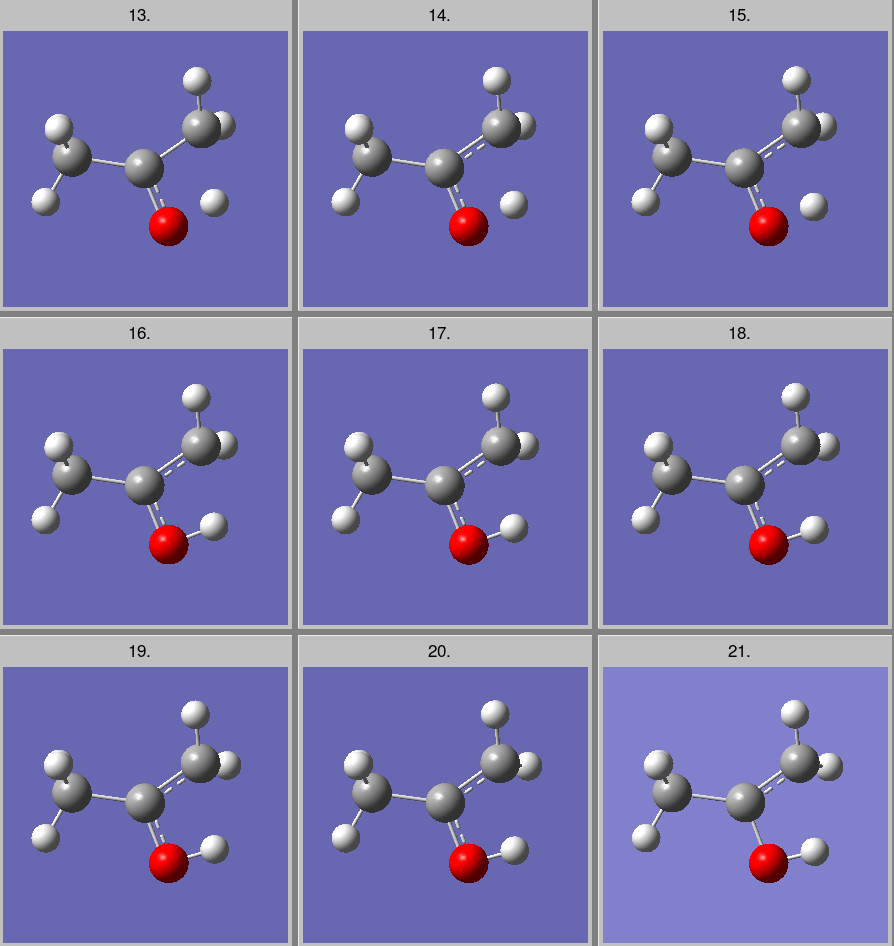
Description automatically generated

Acetone Propenal

Steps:

1. A picture containing sky, metal, bunch, table

   Description automatically generated 2. 

3.  4. 

Graph:

A screenshot of a cell phone

Description automatically generated

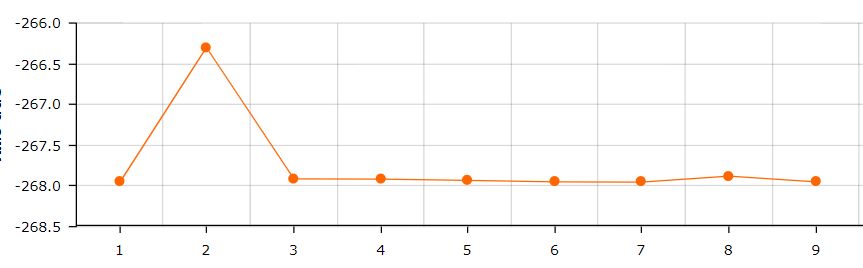
The difference between energies of reactants and products is 0.04 Hartree or 25.1004 kcal per mole.

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

Here, acetone is more stable than propenal.

Challenge 2:

The energies of the 9 isomers of c11H 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. A picture containing indoor, paper, metal, sky

Description automatically generated 2. A picture containing indoor, sky, top, small

Description automatically generated

3. A picture containing baseball, indoor, grass, metal

Description automatically generated 4. A picture containing indoor, metal, paper, small

Description automatically generated

5. A picture containing metal, sky, indoor, grass

Description automatically generated 6. A picture containing indoor, grass, baseball, metal

Description automatically generated

7. A close up of several top

Description automatically generated 8. A close up of several top

Description automatically generated

9. A picture containing indoor, metal, grass, paper

Description automatically generated

Challenge 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

A picture containing indoor, sitting, large, accessory

Description automatically generated

3.1 .2: Gauche form of given scan

A picture containing baseball, ball, indoor, grass

Description automatically generated

3.1.3: Eclipsed form of the given scan

A picture containing indoor, large, metal, ball

Description automatically generated

3.1: scan graph of energies

A screenshot of a cell phone

Description automatically generated

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

A picture containing indoor

Description automatically generated

3.2.2: gauche form of the given scan

A picture containing baseball, ball, indoor, grass

Description automatically generated

3.2.3: eclipsed form of the given scan

A picture containing indoor

Description automatically generated

3.2: scan graph of energies

A screenshot of a social media post

Description automatically generated

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

A picture containing baseball, grass, indoor, sitting

Description automatically generated

3.3.2: gauche form of the given scan

A picture containing baseball, ball, swinging, bat

Description automatically generated

3.3.3: eclipsed form of the given scan

A picture containing baseball, indoor, sitting

Description automatically generated

3.3: graph of the given scan/ potential energy diagram

A picture containing text

Description automatically generated

The staggered form is highly stable

The gauche form is moderately stable

The eclipsed form is least stable of all three

Challenge 4:

Ethanol structure:

A picture containing ball, indoor, device

Description automatically generated

The vibration IR spectrum

A screenshot of a social media post

Description automatically generated

Original spectrum:

A screenshot of a computer

Description automatically generated

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.

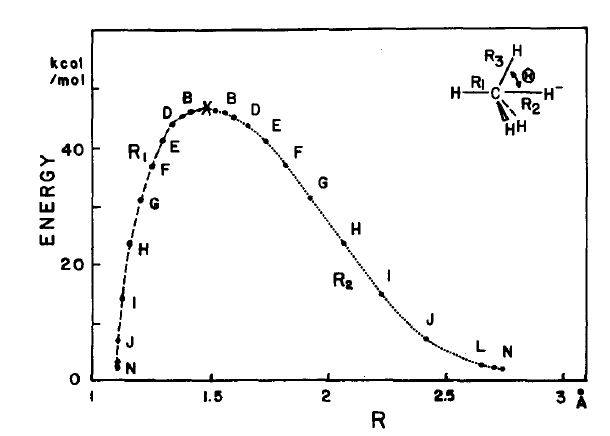
Challenge 5:

Energy diagram of **HNC-+HCN**

A screenshot of a cell phone

Description automatically generated

The referance graph

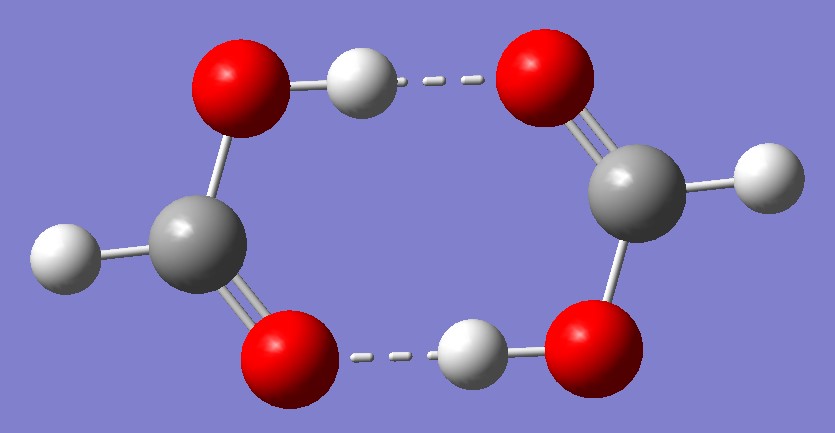


The position of the carbon atom moves only slightly during the reaction, and only the two extreme positions are shown. The position of the hydrogen atom at the transition state is shown by H. The hydrogen atom moves smoothly from the left-hand side, which corresponds to HNC, through the transition state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

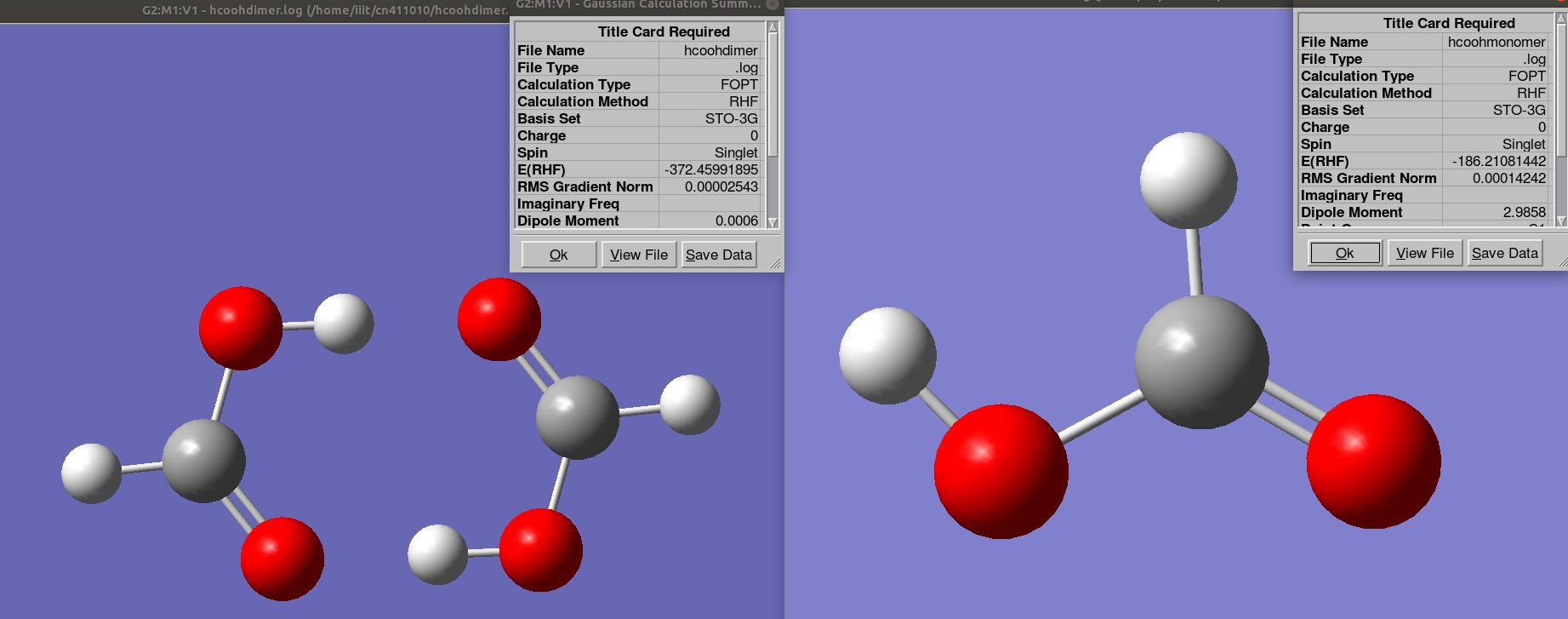
Problem 5

1. 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.



1. 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.

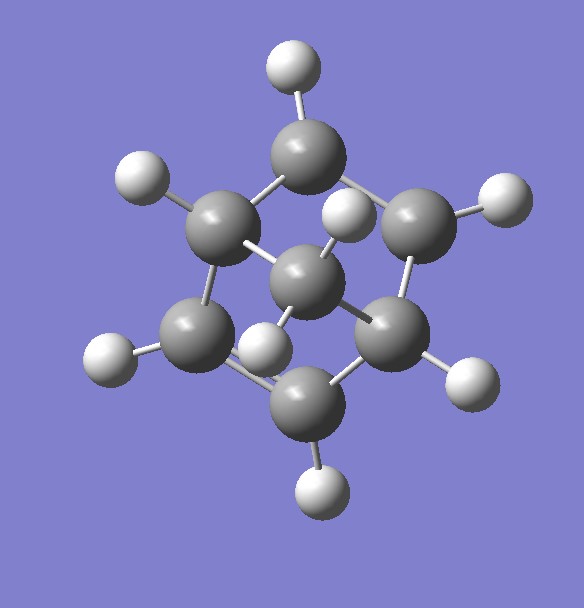
The energy difference b/w the dimer form and two monomers are −24.031191986 kJ/mol, i.e., the dimer form is more stable by having 24.031191986kJ/mol energy less than the monomeric form.



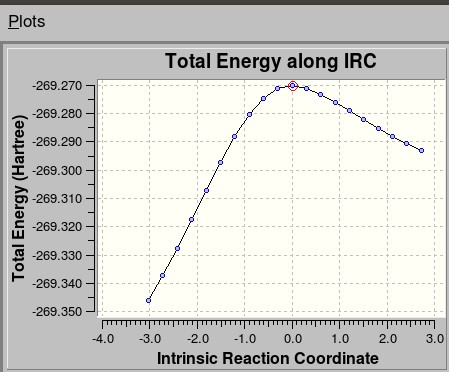
Problem 6.

Reactants: cyclopent-1,3-ene and ethene

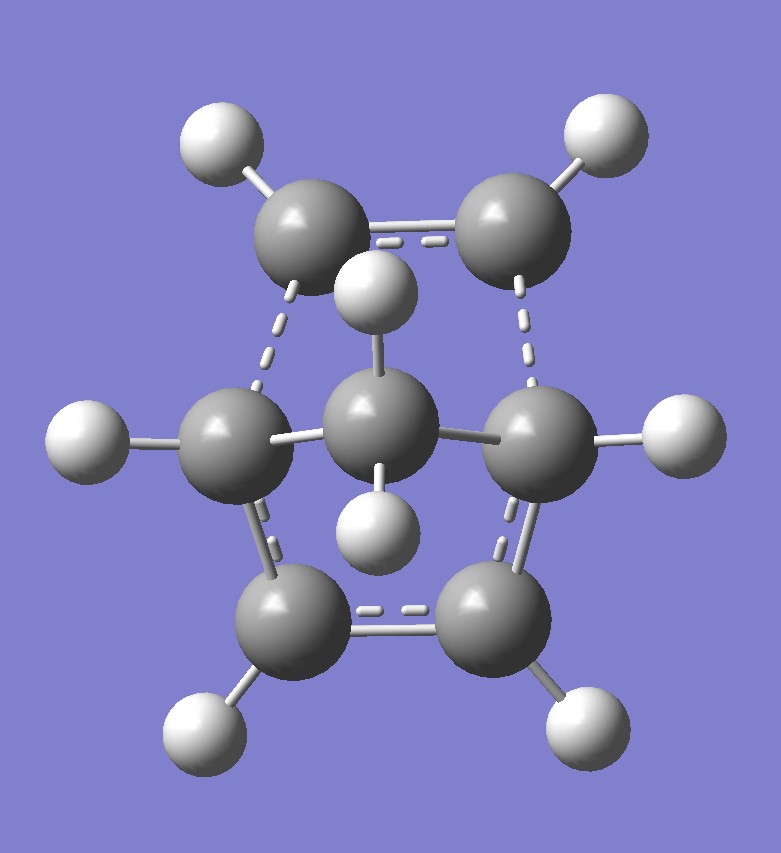
Product: Bicyclocompound



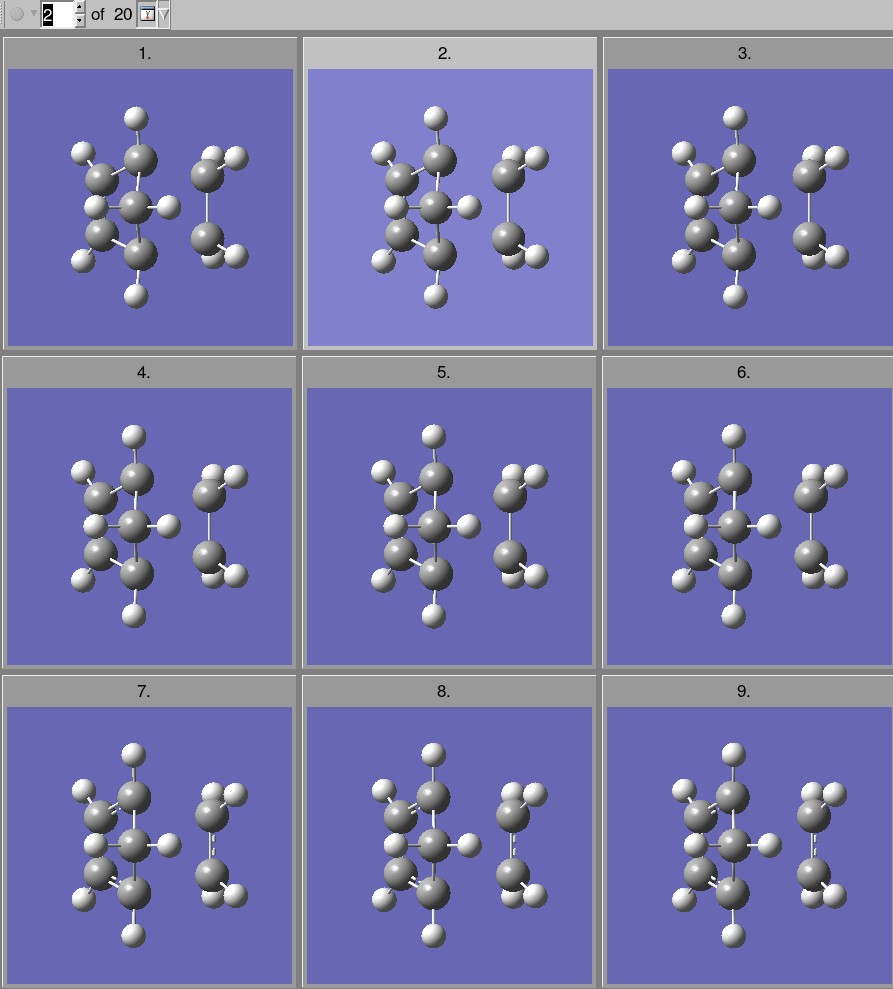
The IRC graphs

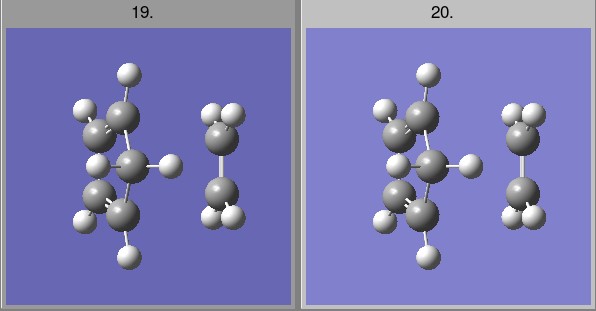
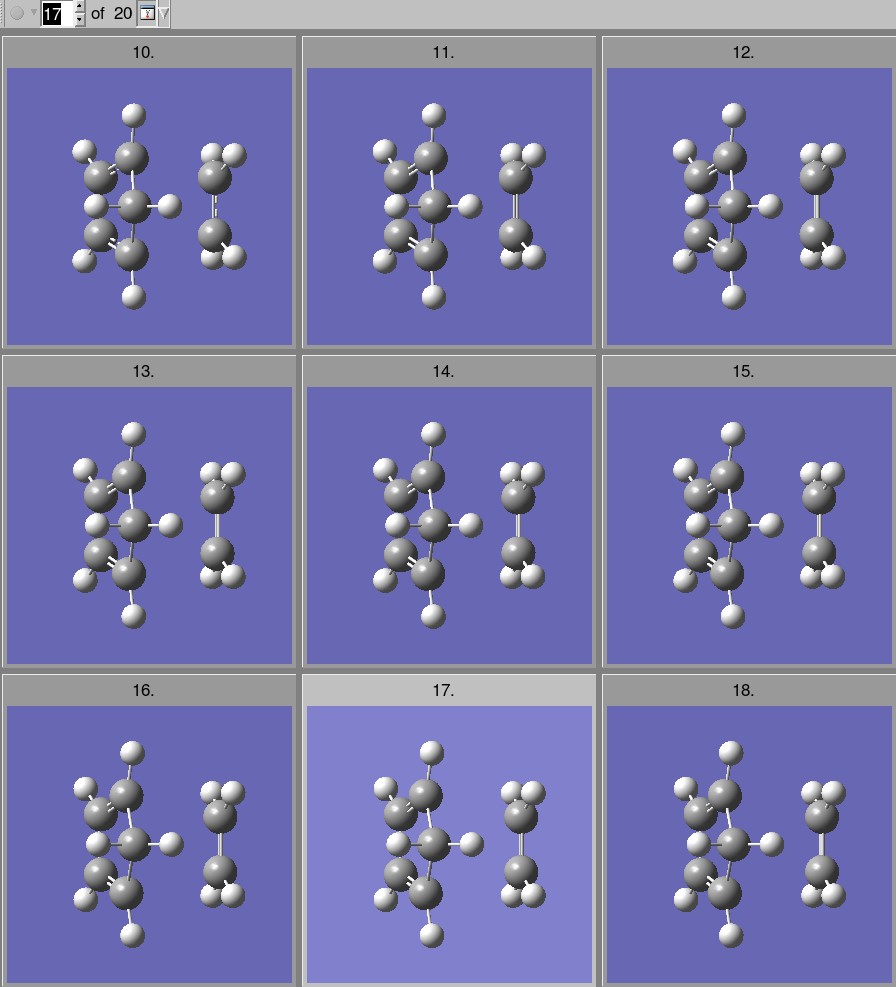


The transition states



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.