CNS Assignment 3

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1   Introduction

1.1   HF (Hartree Fock method)

This method keyword requests a Hartree-Fock calculation. It also contains the set of approximations to solve the Schrodinger's equation.

1.2   STO-nG

STO-nG basis sets are basis sets, where n basic Gaussian orbitals are combine to form a single Slater-type orbital (STO) An STO-3G basis set has all linear combination of 3 primitive Gaussian functions.
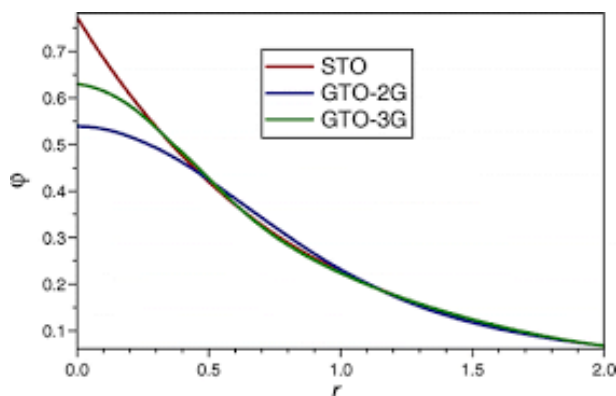
1.3   opt

This keyword requests that a geometry optimization be performed.

1.4   freq

The keyword Freq calls for a second calculation that computes the frequencies and with it the energy of the molecule. For all methods used in Gaussian, the energy will be given in atomic units (au). The atomic unit of energy is called Hartree. Vibrational frequencies are computed by determining the second derivatives of the energy with respect to the Cartesian nuclear coordinates.

1.5   Other specifications used

- opt = (ts,calcfc,noeigentest) :

    - We specify the optimization (Opt) to be a transition state (TS) optimizization.

    - Calcfc Specifies that the force constants be computed at the first point using the current method

- By default, the optimization program checks the curvature (number of negative eigenvalues) of the approximate second derivative matrix at each step of a transition state optimization. If the number is not exactly one negative eigenvalue, the job is aborted. The test can be suppressed with the NoEigenTest option. It appears that Gaussian never finds a transition state unless the NoEigenTest keyword is included.

- opt = modredundant :

  ModRedundant allows us to explicity freeze variables during the optimization and optimizes the geometry in redundant internal coordinates. This keyword is used to perform a scan. Once the geometry is optimized the angle is again increased by the same amount.

- irc = (rcfc,maxpoints=n) geom=check :

  - Transition state geometries may be connected to ground state geometries with an intrinsic reaction coordinate (IRC) calculation. In the process one follows the path downhill from the transition state in either the forward or reverse direction. The direction does not correspond to the user's understanding of forward and reverse for ones particular chemical system.
  - rcfc recalls the force constant from checkpoint file.
  - Maxpoints ensures that the optimizations takes place n number of times in both forward and reverse directions rather than the default 10 times.
  - The Geom keyword specifies the source of the molecule specification input. In this case it points to the check point file wherein the final optimized values are stored.

- %chk :

  Allows us to store the final optimized values of the .COM files as [FILENAME].chk in binary form.

- %nproc :

  Specifies number of processors

- %mem :

  Specifies memory used in the multiple cores

- The .COM files also include the heading of the file and the charge & multiplicity of the molecule being specified in terms of variables in a Z-Matrix using Bond Length, Bond angle and Dihedral angle.

1.6   Configuring the g09.sh file

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Before submitting the **.com** file , we need to create a **.sh** file having the following info:

```
    #!/bin/bash
#SBATCH −A cn4101
#SBATCH −−qos=cn4101
#SBATCH −n 2
```

```
#SBATCH −N 1
#SBATCH −−mem−per−cpu=200
#SBATCH −−time=03:00:00

module load Gaussian/09revC
export GAUSS_SCRDIR=/scratch/$USER.$SLURM_JOBID
/bin/mkdir −p $GAUSS_SCRDIR

g09 [FILE NAME].com

/bin/rm −rf $GAUSS_SCRDIR
```

2 Model of the Diels-Alder reaction between butadiene and ethylene to form cyclohexene and the IRC calculations.

2.1 .COM file

Writing a .COM file which includes the Z-Matrix:

Z-Matrix for the Transition State:

.

```
%nproc=2
%mem=2GB
%chk=diels_alder.chk
#HF STO−3G opt=(ts,noeigentest,calcfc) freq

Diels Adler

0 1
C1
C2 1 1.4
C3 2 1.4 1 109.0
C4 3 1.4 2 109.0 1 0.0
H5 1 1.0 2 120.0 3 180.0
H6 1 1.0 2 120.0 3 0.0
H7 2 1.0 3 120.0 4 180.0
H8 3 1.0 2 120.0 1 180.0
H9 4 1.0 3 120.0 2 180.0
H10 4 1.0 3 120.0 2 0.0
C11 6 1.5 1 90.0 2 90.0
```

```
C12  11  1.3  6  90.0  10  0.0
H13  11  1.0  12  120.0  10  90.0
H14  11  1.0  12  120.0  10  270.0
H15  12  1.0  11  120.0  10  90.0
H16  12  1.0  11  120.0  10  270.0
```

File for Transition State IRC using the optimised Transition state:

.

```
%nproc=2
%mem=2GB
%chk=diels_alder.chk
#hf sto−3g irc=(rcfc, maxpoints=17) geom=check


Diels Alder Reaction


0 1
```

2.2 Observations

Opening the file on Gaussian and reviewing the .LOG file, we observe and tabulate the following data:

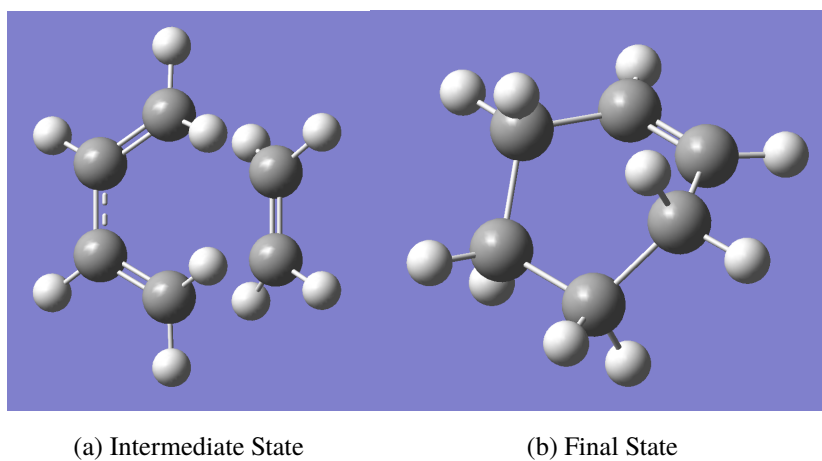(a) Intermediate State   (b) Final State

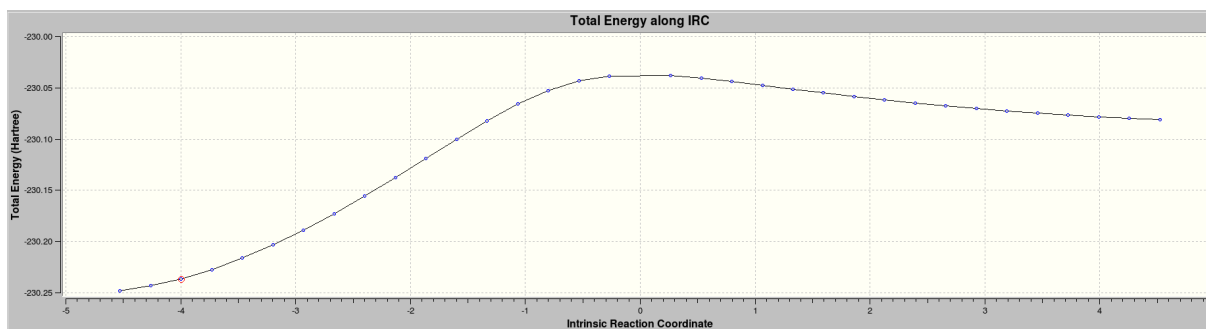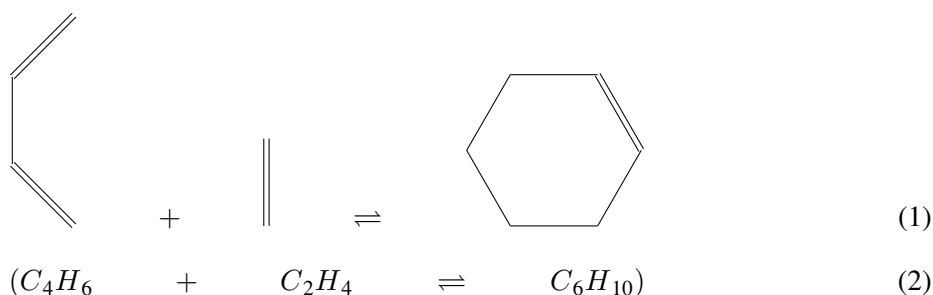Figure 1: Molecule Images of Reaction

Figure 2: IRC Graph

2.3 Inference

The Diels-Alder reaction is a conjugate addition reaction of a conjugated diene to an alkene to produce a cyclohexene. Since the reaction forms a cyclic product, via a cyclic transition state.

Diels Alder reaction is as follows :

$$+ \qquad \rightleftharpoons \qquad \qquad (1)$$

$$(C_4H_6 \quad + \quad C_2H_4 \quad \rightleftharpoons \quad C_6H_{10}) \qquad (2)$$

The transition state formation proceeds as follows:

Scheme 1: The Diels-Alder reaction of 1,3-butadiene and ethylene.
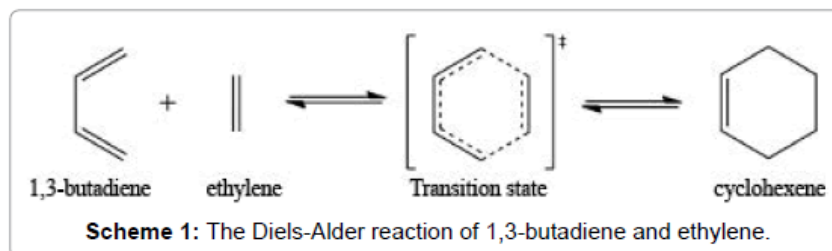
On approaching the transition state, multiple bonds break into different ones, example the the double bond of Ethene converts to a single bond.

The computation results of IRC values in the .LOG files are (the Energy vs Reaction Coordinate table for the reaction):

$$\Delta Energy_{\text{Activation}} = 0.04410 Hartree = 27.673173714 kcal/mol \qquad (3)$$

whereas the Threshhold Energy is :

$$\Delta Energy_{\text{Threshold}} = 0.04410 - 0.21090 Hartree = -104.6686 kcal/mol \qquad (4)$$

These computed values are approximately equal to the expected value and hence the transition state observed is of the required reaction.

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3 Conformational analysis on Ethane, Propane and Butane

3.1 .COM file

Writing a .COM file which includes the Z-Matrix :

Note : To conclude the Z-matrix there is an extra step to be added, X Y Z W (S) [STEPS] [ANGLE]. Here, due to the modredundant keyword the conformational analysis of the molecule takes place as the dihedral angle of plane X-Y-Z and Y-Z-W changes about the central Y-Z bond, where X, Y, Z, W are atoms.

Z-Matrix for Ethane :

.

%nproc=2
%mem=1GB
#HF STO−3G opt=modredundant

Ethane

0 1
C
C 1 1.5
H 1 1.0 2 120.0
H 2 1.0 1 120.0 3 180.0
H 1 1.0 2 120.0 3 120.0
H 1 1.0 2 120.0 3 240.0

H 2 1.0 1 120.0 4 120.0
H 2 1.0 1 120.0 4 240.0

3 1 2 8 S 20 18.0

Z-Matrix for Propane :

.

%nproc=2
%mem=1GB
#HF STO−3G opt=modredundant

Propane

0 1
C
C 1 1.5

```
H  1  1.0  2  109.0
H  1  1.0  2  109.0  3  120.0
C  1  1.5  2  109.0  3  240.0
H  2  1.0  1  109.0  5  180.0
H  2  1.0  1  109.0  3  180.0
H  2  1.0  1  109.0  4  180.0
H  5  1.0  1  109.0  2  120.0
H  5  1.0  1  109.0  2  240.0
H  5  1.0  1  109.0  2  0.0


6  2  1  5  S  20  18.0
```

Z-Matrix for Butane :

  .

```
%nproc=2
%mem=1GB
#HF STO−3G opt=(ts,calcfc,noeigentest) freq

 Butane

0  1
C
C  1  1.5
H  1  1.0  2  120.0
H  1  1.0  2  120.0  3  120.0
C  1  1.0  2  120.0  3  240.0
C  2  1.0  1  120.0  5  180.0
H  2  1.0  1  120.0  3  180.0
H  2  1.0  1  120.0  4  180.0
H  5  1.0  1  120.0  2  120.0
H  5  1.0  1  120.0  2  240.0
H  5  1.0  1  120.0  2  0.0
H  6  1.0  2  120.0  1  120.0
H  6  1.0  2  120.0  1  240.0
H  6  1.0  2  120.0  1  0.0


5  1  2  6  S  20  18.0
```

3.2 Observations

Opening the file on Gaussian and reviewing the .LOG file, we observe and tabulate the following data:
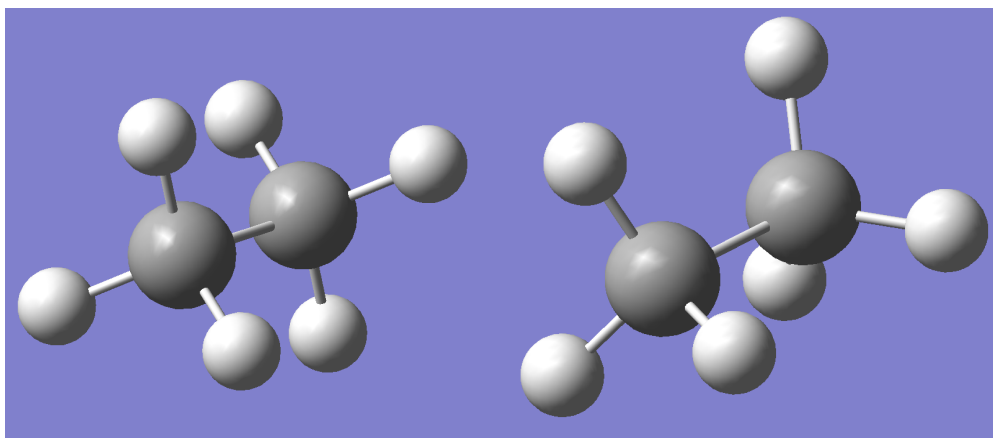

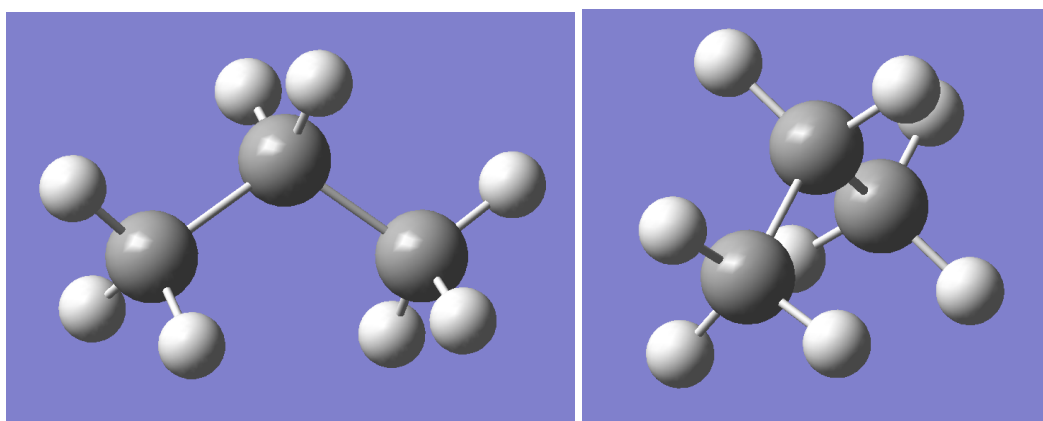Figure 3: Examples of some conformers of Ethane
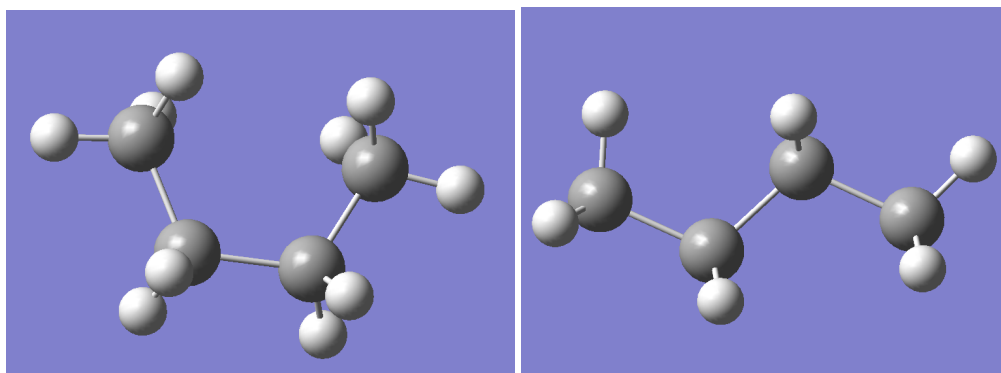

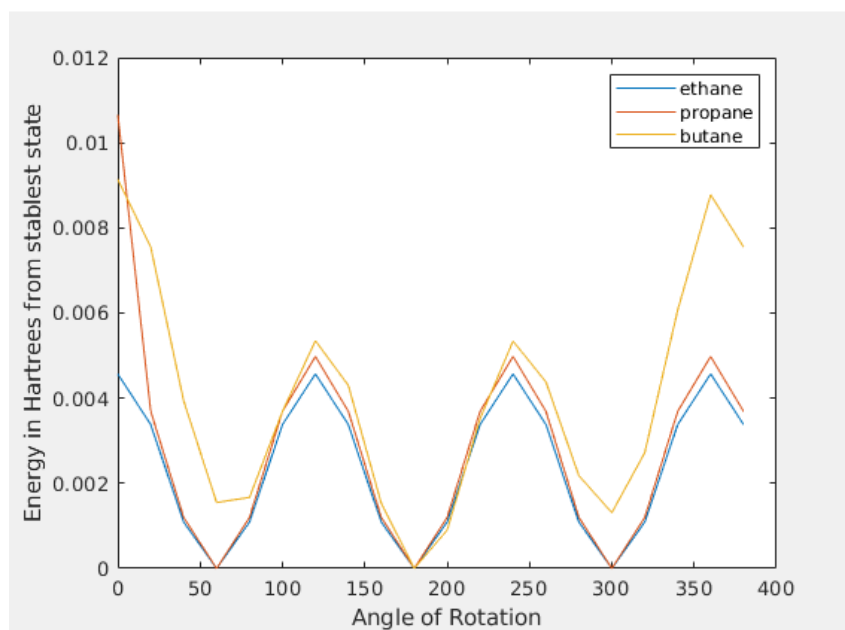Figure 4: Examples of some conformers of Propane

Figure 5: Examples of some conformers of Butane

(a) Relative Energy Graph

3.3 Inference

Conformational Isomerism is a form of stereoisomerism where interconversions of isomers are possible by rotations referring to single bonds.Rotational Energy acts as a barrier in case of single bond rotation. It has to be overcome to interconvert one conformer to another.

The energy barrier must be small for Conformational Isomerism to occur. Since the energy barrier is low (as computed) the rotamers of Ethane, Propane and Butane all interconvert rapidly at room temperature

3.3.1 Conformations of Ethane

The six carbon-hydrogen bonds are shown as solid lines protruding from the two carbons at 120°angles, which is what the actual tetrahedral geometry.

The lowest energy conformation of ethane is called the staggered conformation, in which all of the C-H bonds on the front carbon are positioned at dihedral angles of 60°relative to the C-H bonds on the back carbon. The energy os lowest in this conformer because:

- The distance between the bonds (and the electrons in them) is maximized

- Can form more delocalised molecular orbitals
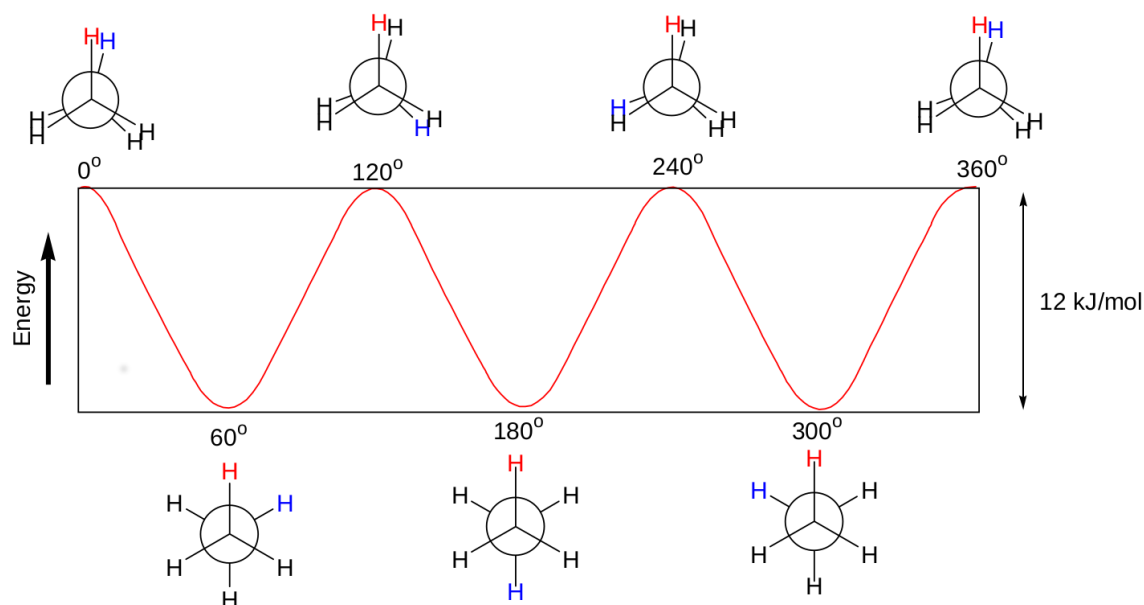
The molecule in the highest energy eclipsed conformation is where the hydrogens on the front carbon are as close as possible to the hydrogens on the back carbon. This is the highest energy conformation because of unfavorable interactions between the electrons in the front and back C-H bonds. Eclipsing interactions are an example of a general phenomenon called steric hindrance, which occurs whenever bulky portions of a molecule repel other molecules or other parts of the same molecule. Because such hindrance causes resistance to rotation, it is also called torsional strain. The energy of the eclipsed conformation is approximately 3 kcal/mol higher than that of the staggered conformation and therefore 3 kcal/mol is needed to overcome this resistance and is called the torsional energy.

Another 60°rotation returns the molecule to a second eclipsed conformation. This process can be continued all around the 360°circle, with three possible eclipsed conformations and three staggered conformations, in addition to an infinite number of variations in between.

3.3.2 Conformations of Propane

The most stable (low energy) conformation is the one in which all of the bonds as far away from each other as possible that is staggered form and the least stable (high energy) conformation is the one in which, for any two adjacent carbon atoms, the six bonds (five C–H and one C–C) are as close as possible that is eclipsed form.
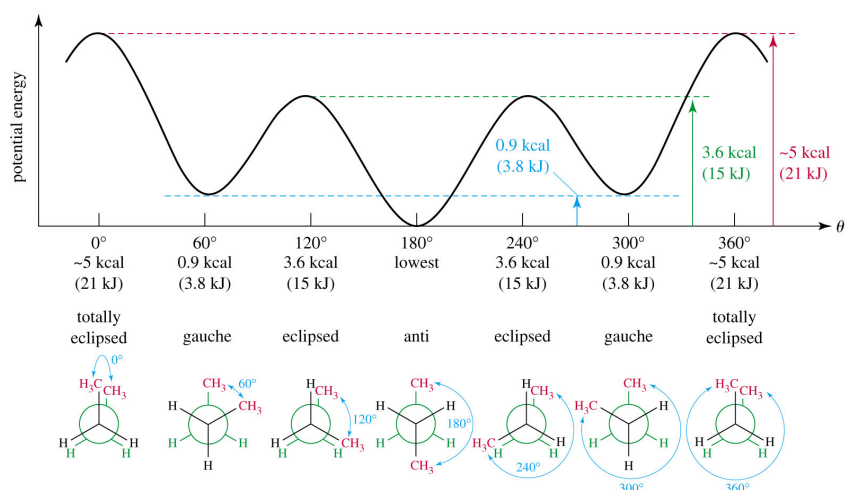
All other conformations lie between these two enrgy values.

The staggered conformation is the most stable because the bonds are furthest away from each other and the electron repulsions are least. This energy difference between the two conformations is called torsional strain. In the conformational energy diagram, we are looking down the C1-C2 bond, and the CH_3 is coming off the back carbon.

The energy difference between the maxima and minima is the total repulsion of three bond pairs, two C-H, C-H repulsions and a C-H, C-CH_3 repulsion.

We know from the conformational analysis of ethane that one C-H, C-H repulsion contributes some amount of torsional enrgy, so a C-H, C-CH_3 repulsion contributes more to the torsional strain.

3.3.3   Conformations of Butane

The four major conformers of butane in increasing order of energy are:

- Anit/Staggered (180°)

- Partially Eclipsed (120°)

- Gauche (60°)

- Fully Eclipsed (0°)

Butane Conformations
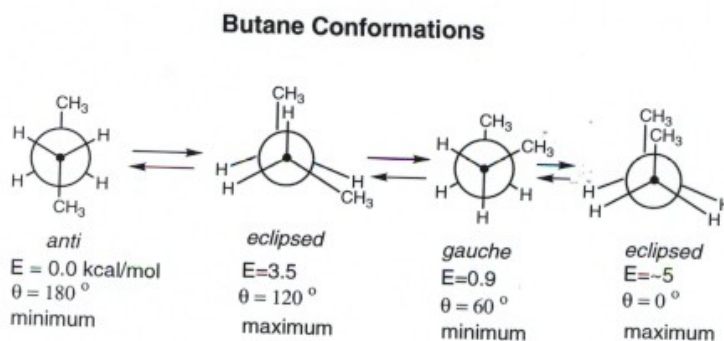
As in the case of ethane, the staggered conformers are more stable than the eclipsed conformers. However due to a factor called stearics there is destabilization in the initial conformation at 0 degrees, in favour of the Z-shaped one with the methyl groups 180 degrees apart from each other due to over-crowding. When they get farther apart, crowding subsides and the energy in the molecule goes down. In case of Butane, there exists stearic strain in addition to the torsional strain that existed in ethane and hence torsion and sterics both contribute to strain energy. Therefore Butane has the highest peak in the graph.

4   Infrared (vibrational) spectrum of formaldehyde

4.1   .COM file

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```
%nproc=2
%mem=1GB
#HF STO−3G opt freq

 Formaldehyde

0  1
C
H  1  1.0
H  1  1.0  2  120.0
O  1  1.2  2  120.0  3  180.0

.
```
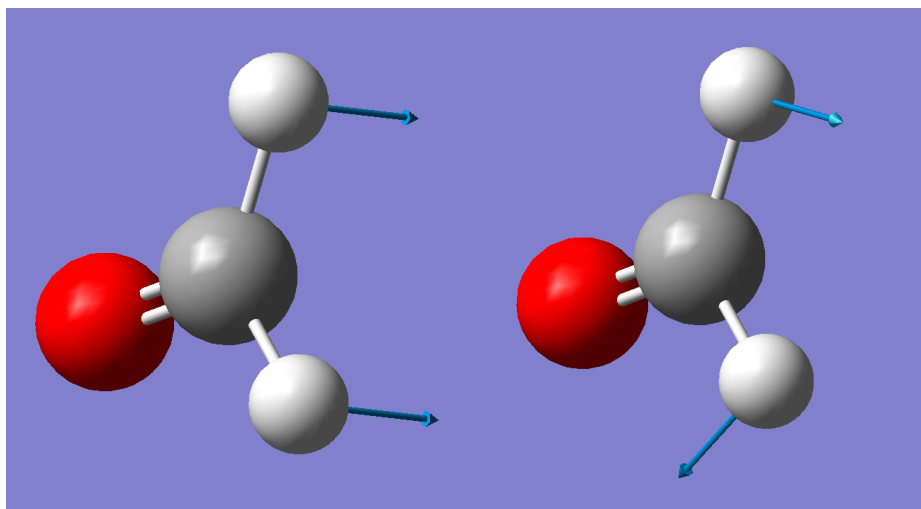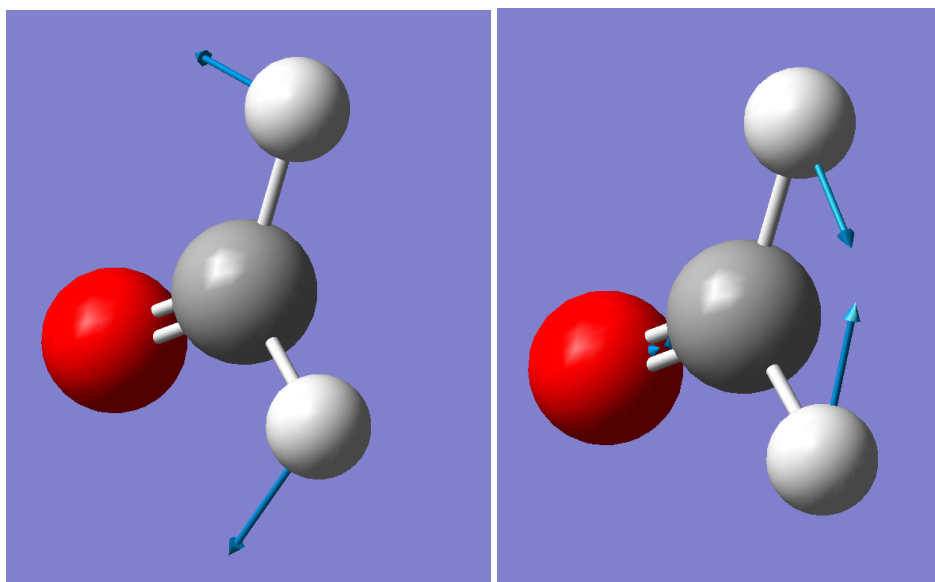

4.2 Observation

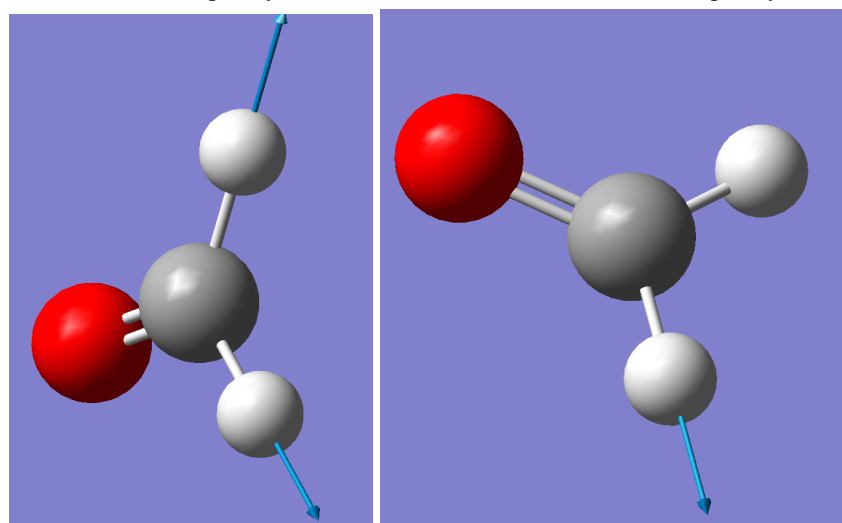There are 6 different vibration modes for Formaldehyde.

(a) wag - frequency mode 1

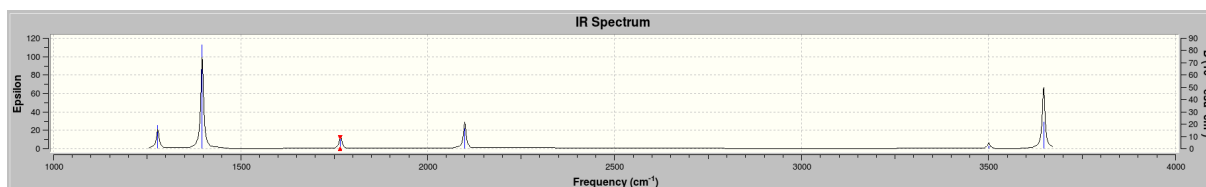(b) rock - frequency mode 2

(c) scissor - frequency mode 3

(d) C=O stretch - frequency mode 4

(e) sym stretch - frequency mode 5

(f) asym stretch - frequency mode 6

4.3 Inference

Mode #	Freq	Infrared	Raman Activity	Depolar-P	Depolar-U
1	1278.30	6.1636	0.0075	0.7500	0.8571
2	1397.15	29.5591	3.0418	0.7500	0.8571
3	1767.10	4.1673	16.3924	0.7071	0.8284
4	2099.35	8.4443	6.7100	0.0756	0.1406
5	3500.16	1.8361	38.6485	0.1865	0.3144
6	3647.13	19.8495	24.5197	0.7500	0.8571

The values computed are not in correspondence with the values given in the problem statement.However the labelling is correct as energy orders concur with those given.
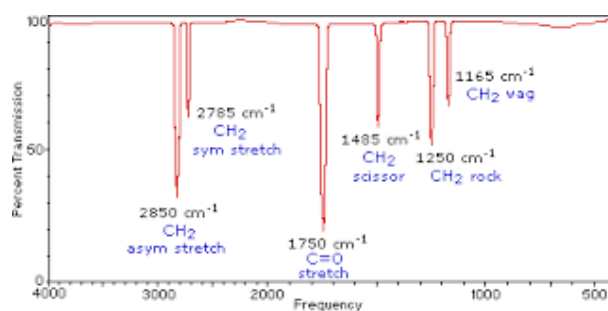
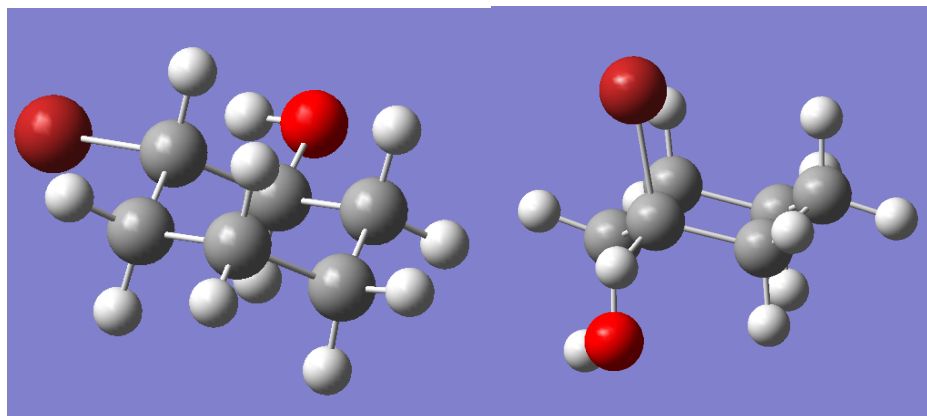# 5 Studying the Energy differences between the two given conformational states

5.1 .COM file

Writing a .COM file which includes the Z-Matrix for all the 8 cases. (Refer to Appendix)
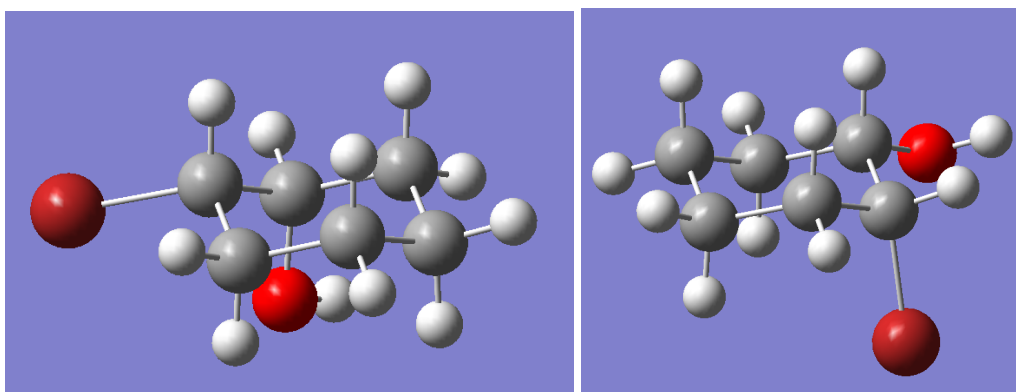
5.2 Observations

(a) 4(a)-1   (b) 4(a)-2

Figure 8: -OH and -Br at eq-eq/ax-ax

(a) 4(b)-1   (b) 4(b)-2

Figure 9: -OH and -Br at eq-ax/ax-eq
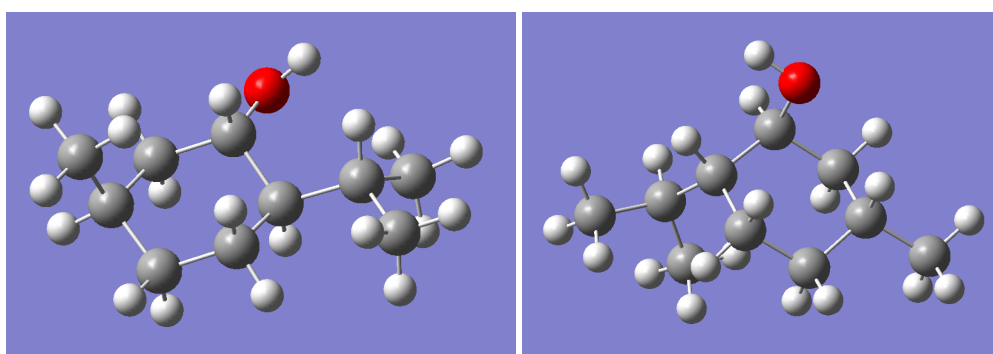
(a) 4(c)-1   (b) 4(c)-2

Figure 10: -OH, -C_3H_7 and -CH_3 at eq-ax
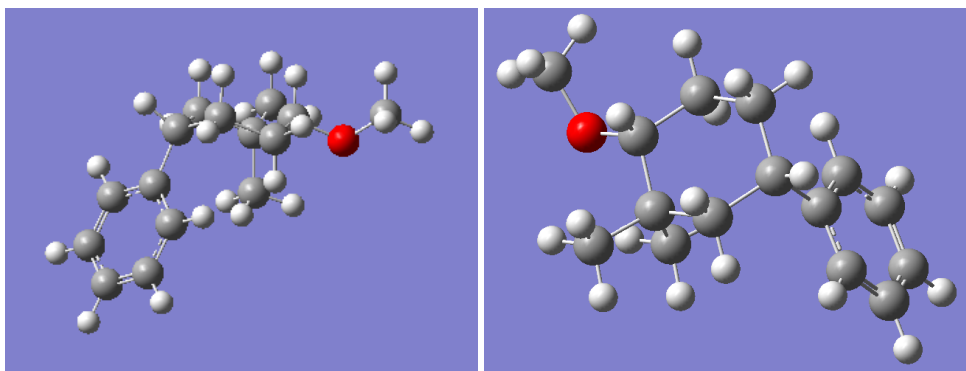
(a) 4(d)-1   (b) 4(d)-2

Figure 11: $-OCH_3$, $-CH_3$, $-CH_3$ and $-C_6H_6$ at eq-ax

5.3 Inference

The data values for Enrergies are as observed:
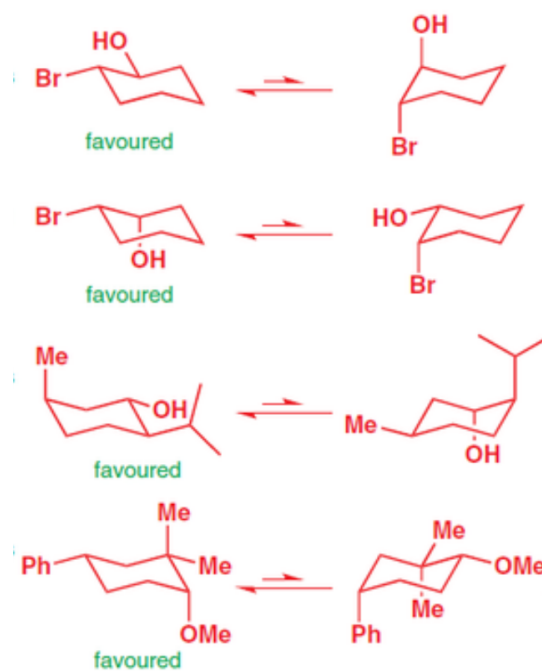
(a)   Energy of (1) = -2849.40420135 Hartree   Energy of (2) = -2849.40139652 Hartree

(b)   Energy of (1) = -2849.40141433 Hartree   Energy of (2) = -2849.40060558 Hartree

(c)   Energy of (1) = -459.62149398 Hartree   Energy of (2) = -459.62052479 Hartree

(d)   Energy of (1) =-647.799420967 Hartree   Energy of (2) = -647.79183703 Hartree

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It can be observed that the molecules with lower energy are the all conformer (1) molecules when compared to conformer (2) molecules and hence are more favored. Thus, verifying the given problem statement.

6 Appendix

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Z-matrix for 4(a)-1

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−a1

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
Br7 1 1.94 2 109.0 3 180.0
H8 1 1.0 2 109.0 3 60.0
O9 2 1.5 3 109.0 4 180.0
H10 2 1.0 3 109.0 4 −60.0
H11 3 1.0 4 109.0 5 180.0
H12 3 1.0 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
H19 9 0.98 2 104.0 4 180.0

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Z-matrix for 4(a)-2

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−a2 Cyclohexane

```
0 1
C1
C2  1  1.5
C3  2  1.5  1  109.0
C4  3  1.5  2  109.0  1  60.0
C5  4  1.5  3  109.0  2  −60.0
C6  5  1.5  4  109.0  3  60.0
H7  1  1.0  2  109.0  3  180.0
Br8  1  1.94  2  109.0  3  60.0
H9  2  1.0  3  109.0  4  180.0
O10  2  1.5  3  109.0  4  −60.0
H11  3  1.0  4  109.0  5  180.0
H12  3  1.0  4  109.0  5  60.0
H13  4  1.0  5  109.0  6  180.0
H14  4  1.0  5  109.0  6  −60.0
H15  5  1.0  6  109.0  1  180.0
H16  5  1.0  6  109.0  1  60.0
H17  6  1.0  1  109.0  2  180.0
H18  6  1.0  1  109.0  2  −60.0
H19  10  0.98  2  104.0  4  −60.0
```

.

———.

———.

Z-matrix for 4(b)-1

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−b1 Cyclohexane

```
0  1
C1
C2  1  1.5
C3  2  1.5  1  109.0
C4  3  1.5  2  109.0  1  60.0
C5  4  1.5  3  109.0  2  −60.0
C6  5  1.5  4  109.0  3  60.0
Br7  1  1.94  2  109.0  3  180.0
H8  1  1.0  2  109.0  3  60.0
H9  2  1.0  3  109.0  4  180.0
O10  2  1.5  3  109.0  4  −60.0
```

H11 3 1.0 4 109.0 5 180.0
H12 3 1.0 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
H19 10 0.98 2 104.0 4 −60.

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.

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Z-matrix for 4(b)-2

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−b2 Cyclohexane

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
H7 1 1.0 2 109.0 3 180.0
Br8 1 1.94 2 109.0 3 60.0
O9 2 1.5 3 109.0 4 180.0
H10 2 1.0 3 109.0 4 −60.0
H11 3 1.0 4 109.0 5 180.0
H12 3 1.0 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
H19 9 0.98 2 104.0 4 180.0

.

Z-matrix for 4(c)-1

```
%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−c1 Cyclohexane

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
C7 1 1.5 2 109.0 3 180.0
H8 1 1.0 2 109.0 3 60.0
O9 2 1.5 3 109.0 4 180.0
H10 2 1.0 3 109.0 4 −60.0
H11 3 1.0 4 109.0 5 180.0
C12 3 1.5 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
C19 7 1.5 1 120.0 2 120.0
C20 7 1.5 1 120.0 2 240.0
H21 7 1.0 1 120.0 2 0.0
H22 19 1.0 7 120.0 1 0.0
H23 19 1.0 7 120.0 1 120.0
H24 19 1.0 7 120.0 1 240.0
H25 20 1.0 7 120.0 1 0.0
H26 20 1.0 7 120.0 1 120.0
H27 20 1.0 7 120.0 1 240.0
H28 12 1.0 1 120.0 2 120.0
H29 12 1.0 1 120.0 2 240.0
H30 12 1.0 1 120.0 2 0.0
H31 9 0.98 2 104.0 4 180.0
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Z-matrix for 4(c)-2

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−c2 Cyclohexane

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
H7 1 1.0 2 109.0 3 180.0
H8 1 1.0 2 109.0 3 60.0
H9 2 1.0 3 109.0 4 180.0
C10 2 1.5 3 109.0 4 −60.0
H11 3 1.0 4 109.0 5 180.0
O12 3 1.5 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
C15 5 1.5 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
C19 10 1.5 1 120.0 2 120.0
C20 10 1.5 1 120.0 2 240.0
H21 10 1.0 1 120.0 2 0.0
H22 19 1.0 7 120.0 1 0.0
H23 19 1.0 7 120.0 1 120.0
H24 19 1.0 7 120.0 1 240.0
H25 20 1.0 7 120.0 1 0.0
H26 20 1.0 7 120.0 1 120.0
H27 20 1.0 7 120.0 1 240.0
H28 15 1.0 1 120.0 2 120.0
H29 15 1.0 1 120.0 2 240.0
H30 15 1.0 1 120.0 2 0.0

H31 12 0.98 2 104.0 4 180.0

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Z-matrix for 4(d)-1

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−d Cyclohexane

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
H7 1 1.0 2 109.0 3 180.0
O8 1 1.5 2 109.0 3 60.0
C9 2 1.5 3 109.0 4 180.0
C10 2 1.5 3 109.0 4 −60.0
H11 3 1.0 4 109.0 5 180.0
H12 3 1.0 4 109.0 5 60.0
C13 4 1.5 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
H16 5 1.0 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
C19 8 1.5 1 180.0 3 60.0
H20 19 1.0 8 120.0 1 240.0
H21 19 1.0 8 120.0 1 120.0
H22 19 1.0 8 120.0 1 0.0
H23 9 1.0 1 120.0 2 120.0
H24 9 1.0 1 120.0 2 240.0
H25 9 1.0 1 120.0 2 0.0
H26 10 1.0 1 120.0 2 120.0
H27 10 1.0 1 120.0 2 240.0
H28 10 1.0 1 120.0 2 0.0
X29 13 1.4 4 180.0 14 0.0

X30 13 1.4 4 90.0 14 0.0
C31 29 1.4 13 60.0 30 90.0
C32 29 1.4 13 120.0 30 90.0
C33 29 1.4 13 180.0 30 90.0
C34 29 1.4 13 240.0 30 90.0
C35 29 1.4 13 300.0 30 90.0
H36 31 1.0 29 180.0 30 60.0
H37 32 1.0 29 180.0 30 120.0
H38 33 1.0 29 180.0 30 180.0
H39 34 1.0 29 180.0 30 240.0
H40 35 1.0 29 180.0 30 300.0

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Z-matrix for 4(d)-2

%nproc=2
%mem=1GB
#HF STO−3G opt freq

4−d Cyclohexane

0 1
C1
C2 1 1.5
C3 2 1.5 1 109.0
C4 3 1.5 2 109.0 1 60.0
C5 4 1.5 3 109.0 2 −60.0
C6 5 1.5 4 109.0 3 60.0
H7 1 1.0 2 109.0 3 180.0
H8 1 1.0 2 109.0 3 60.0
O9 2 1.5 3 109.0 4 180.0
H10 2 1.0 3 109.0 4 −60.0
C11 3 1.5 4 109.0 5 180.0
C12 3 1.5 4 109.0 5 60.0
H13 4 1.0 5 109.0 6 180.0
H14 4 1.0 5 109.0 6 −60.0
H15 5 1.0 6 109.0 1 180.0
C16 5 1.5 6 109.0 1 60.0
H17 6 1.0 1 109.0 2 180.0
H18 6 1.0 1 109.0 2 −60.0
C19 9 1.5 2 180.0 4 180.0

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H20  19  1.0  8  120.0  1  120.0
H21  19  1.0  8  120.0  1  240.0
H22  19  1.0  8  120.0  1  0.0
H23  11  1.0  3  120.0  5  120.0
H24  11  1.0  3  120.0  5  240.0
H25  11  1.0  3  120.0  5  0.0
H26  12  1.0  3  120.0  5  120.0
H27  12  1.0  3  120.0  5  240.0
H28  12  1.0  3  120.0  5  0.0
X29  16  1.4  5  180.0  15  0.0
X30  16  1.4  5  90.0  15  0.0
C31  29  1.4  16  60.0  30  90.0
C32  29  1.4  16  120.0  30  90.0
C33  29  1.4  16  180.0  30  90.0
C34  29  1.4  16  240.0  30  90.0
C35  29  1.4  16  300.0  30  90.0
H36  31  1.0  29  180.0  30  60.0
H37  32  1.0  29  180.0  30  120.0
H38  33  1.0  29  180.0  30  180.0
H39  34  1.0  29  180.0  30  240.0
H40  35  1.0  29  180.0  30  300.0
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