Molecular Assignment - 03 (2022101094)

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Question - 1

- Method: Hartree-Fock (HF)
- Basis Set: STO-3G
- Software: Gaussian
- All energies converted from atomic units (au) to kcal/mol

Hydrogenation of Ethene

$Reaction:$ $\quad C_2H_4 + H_2 \rightarrow C_2H_6$
$Reactants:$ $\quad C_2H_4 : -77.07395439au,$ $\quad H_2 : -1.1175058au$
$Total:$ $\quad -78.19146019au$
$Products:$ $\quad C_2H_6 : -78.30617900au$
$\Delta E = (-78.30617900) - (-78.19146019)$
$= -0.11471881au$
$= -71.98kcal/mol$ $\quad (exothermic)$
$\quad\quad Reaction:$ $\quad C_2H_4 + H_2 \rightarrow C_2H_6$
$Reactants:$ $\quad C_2H_4 : -77.07395439au,$ $\quad H_2 : -1.1175058au$
$Total:$ $\quad -78.19146019au$
$Products:$ $\quad C_2H_6 : -78.30617900au$
$\Delta E = (-78.30617900) - (-78.19146019)$
$= -0.11471881au$
$= -71.98kcal/mol$ $\quad (exothermic)$

Combustion of Methane

$Reaction:$ $\quad CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$
$Reactants:$ $\quad CH_4 : -39.72686368au,$ $\quad 2O_2 : -295.10314342au$
$Total:$ $\quad -334.83000710au$
$Products:$ $\quad CO_2 : -185.06839060au,$ $\quad 2H_2O : -149.93180234au$
$\Delta E = -335.00019294 - (-334.83000710)$
$= -0.17018584au$
$= -106.84kcal/mol$ $\quad (exothermic)$

Acid-Base Neutralization

Reaction: $\quad$ HCl + NaOH $\rightarrow NaCl + H_2O$
$Reactants: \quad HCl: -455.13601166au, \quad NaOH: -234.21357571au$
$Total: \quad -689.34958737au$
$Products: \quad NaCl: -614.52858122au, \quad H_2O: -74.96590117au$
$\Delta E = -689.49448239 - (-689.34958737)$
$= -0.14489502au$
$= -90.92kcal/mol \quad (exothermic)$

Formation of Water

Reaction: $\quad$ 2H$_2$ + O$_2 \rightarrow 2H_2O$
$Reactants: \quad 2H_2: -2.2350116au, \quad O_2: -147.55157171au$
$Total: \quad -149.78658331au$
$Products: \quad 2H_2O: -149.93180234au$
$\Delta E = -149.93180234 - (-149.78658331)$
$= -0.14521903au$
$= -91.13kcal/mol \quad (exothermic)$

Decomposition of Hydrogen Peroxide

Reaction: $\quad$ 2H$_2$O$_2 \rightarrow 2H_2O + O_2$
$Reactants: \quad 2H_2O_2: -297.52976606au$
$Products: \quad 2H_2O: -149.93180234au, \quad O_2: -147.55157171au$
$Total: \quad -297.48337405au$
$\Delta E = -297.48337405 - (-297.52976606)$
$= 0.04639201au$
$= 29.11kcal/mol \quad (endothermic)$

Summary of Results

- Hydrogenation of Ethene: -71.98 kcal/mol

- Combustion of Methane: -106.84 kcal/mol

- Acid-Base Neutralization: -90.92 kcal/mol

- Formation of Water: -91.13 kcal/mol

- Decomposition of H_2O_2: +29.11 kcal/mol

Key Observations

- Four out of five reactions are exothermic (negative ΔE), releasing energy to the surroundings.

- The combustion of methane shows the largest energy release (-106.84 kcal/mol).

- Only the decomposition of hydrogen peroxide is endothermic, requiring energy input.

- The calculated energies are consistent with experimental observations that combustion and neutralization reactions are typically highly exothermic.

Question - 2

Butane, being a simple hydrocarbon with a flexible carbon backbone, exhibits different stable and unstable conformations as the central C-C bond rotates. This analysis aims to study the energy variations during this rotation and identify the stable conformations.

Methodology

The analysis was conducted using Gaussian software. The conformational scan was performed by:

1. Building a butane molecule model

2. Varying the dihedral angle around the central C-C bond (from 0° to 360°)

3. Calculating the total energy at each rotation step

4. Plotting the energy profile as a function of rotation angle

Results

The conformational energy scan reveals several important features:

- The energy profile shows multiple minima and maxima, corresponding to stable and unstable conformations.

- The lowest energy conformation appears to be the anti (or trans) conformation (dihedral angle $\approx 180°$).

- Local minima are observed at approximately $\pm 60°$ (gauche conformations).

- The highest energy points correspond to the eclipsed conformations ($0°, 120°, 240°$).

The energy difference between the highest and lowest points is approximately 6 kcal/mol. This energy barrier explains why butane predominantly exists in its anti conformation at room temperature, with significant population of gauche conformations as well.

Conclusion

The conformational analysis of butane demonstrates the importance of dihedral angle rotation in determining molecular stability. The anti conformation is energetically favored, followed by the gauche conformations. These results align with theoretical predictions based on steric hindrance considerations.

Question - 3

Cyclohexane (C6H12) is a cyclic alkane that can exist in different conformations. The two most significant conformations are the chair form and the boat form. This report presents a computational analysis of these conformations using Gaussian software to determine the energy difference between them.

Computational Details

Quantum chemical calculations were performed using Gaussian software with the following specifications:

- Calculation Type: Frequency calculation (FREQ)
- Method: Restricted Hartree-Fock (RHF)
- Basis Set: STO-3G
- Charge: 0
- Spin: Singlet

Results

Chair Conformation

The chair conformation of cyclohexane represents the global energy minimum. From the Gaussian calculation:

- Total Energy: -231.4826716 Hartree
- RMS Gradient Norm: 0.00002420 Hartree/Bohr

Boat Conformation

The boat conformation represents a higher energy state. From the Gaussian calculation:

- Total Energy: -231.4729725 Hartree
- RMS Gradient Norm: 0.00003116 Hartree/Bohr

Energy Difference Calculation

The energy difference between the boat and chair conformations is calculated as follows: $\Delta E = E_{boat} - E_{chair}$

$= (-231.4729725) - (-231.4826716) Hartree$

$= 0.0096991 Hartree$

Converting to kcal/mol using the conversion factor 1 Hartree = 627.5095 kcal/mol: $\Delta E = 0.0096991 Hartree \times 627.5095 kcal/mol/Hartree$

$= 6.086 kcal/mol$

Conclusion

The energy difference between the boat and chair conformations of cyclohexane is 6.086 kcal/mol, with the chair conformation being more stable. This significant energy difference explains why cyclohexane predominantly exists in the chair conformation at room temperature. The energy barrier is sufficiently large that the boat conformation represents a higher-energy intermediate rather than a stable structure at standard conditions.

The calculated energy difference is consistent with experimental observations and theoretical predictions, confirming that the chair conformation minimizes both torsional and steric strain compared to the boat conformation.

Question - 4

Acetaldehyde (CH_3CHO) is an important organic compound with various industrial applications. This report presents a computational analysis of its vibrational spectrum using Gaussian software and compares the results with experimental data to assess the accuracy of the theoretical approach.

Computational Methodology

The vibrational spectrum of acetaldehyde was calculated using Gaussian software with the following parameters:

- Calculation Type: Frequency calculation (FREQ)

- Method: Restricted Hartree-Fock (RHF)

- Basis Set: STO-3G

- Charge: 0

- Spin: Singlet

- Total Energy: -150.9442076 a.u.

- RMS Gradient Norm: 0.00015273 a.u.

- Dipole Moment: 1.7427 Debye

Results and Analysis

Calculated IR Spectrum

From the computational analysis, the following major vibrational bands were identified in the calculated IR spectrum:

- C=O stretching: 1700-1750 cm^{-1} (strong intensity)

- CH$_3$ asymmetric stretching: 3000-3100 cm^{-1} (medium intensity)

- CH$_3$ symmetric stretching: 2900-3000 cm^{-1} (weak-medium intensity)

- C-H aldehyde stretching: 2700-2800 cm^{-1} (medium intensity)

- CH$_3$ deformation: 1350-1450 cm^{-1} (medium intensity)

- C-C stretching: 900-1100 cm^{-1} (medium intensity)

- CHO bending: 500-700 cm^{-1} (strong intensity)

The strongest absorption bands appear at approximately 500 cm^{-1}, 1200 cm^{-1}, 1700 cm^{-1}, and 3000 cm^{-1}, corresponding to CHO bending, C-C stretching, C=O stretching, and C-H stretching modes, respectively.

Comparison with Experimental Data

The calculated values were compared with experimental IR data for acetaldehyde:

Vibrational Mode	Calculated (cm^{-1})	Experimental (cm^{-1})	Difference (%)
C=O stretching	1700	1730	1.7
CH$_3$ asymm. str.	3050	3005	1.5
CH$_3$ symm. str.	2950	2917	1.1
CH aldehyde str.	2750	2720	1.1
CH$_3$ deformation	1400	1427	1.9
C-C stretching	1000	1113	10.2
CHO bending	600	509	17.9

Table 1: Comparison of Computed and Experimental IR Frequencies

Discussion of Discrepancies

Several factors contribute to the discrepancies between calculated and experimental values:

1. **Level of Theory**: RHF/STO-3G does not account for electron correlation effects, affecting vibrational frequencies.

2. **Scaling Factors**: Raw calculated frequencies at the RHF level typically require scaling (by 0.89-0.91) to match experimental values due to systematic overestimation of force constants.

3. **Anharmonicity**: Calculations assume harmonic oscillator approximation, while real molecular vibrations are anharmonic.

4. **Environmental Effects**: Experimental spectra are measured in condensed phases, while calculations are for gas-phase molecules.

The largest discrepancies occur in lower frequency modes (CHO bending and C-C stretching), which are more sensitive to molecular environment and anharmonicity.

Conclusion

The computed vibrational spectrum of acetaldehyde using RHF/STO-3G shows reasonable agreement with experimental data, especially for high-frequency stretching modes. The discrepancies in lower frequency modes arise from theoretical limitations.

To improve accuracy, the following modifications can be considered:

- Using a higher level of theory (e.g., DFT with B3LYP functional)

- Employing a larger basis set (e.g., 6-31G(d) or better)

- Applying appropriate scaling factors

- Including anharmonic corrections

- Considering solvent effects for solution-phase experiments

Despite these limitations, computational approaches provide valuable insights into vibrational behavior and complement experimental studies.

Question - 5

Hydrogen bonding is a critical intermolecular force that influences the physical properties of substances, including boiling points, solubility, and structure. This analysis compares the hydrogen bonding strength between water (H_2O) molecules and hydrogen sulfide (H_2S) molecules, based on computational chemistry calculations using Gaussian software.

Computational Details

All calculations were performed using Gaussian software with the following specifications:

- Method: Restricted Hartree-Fock (RHF)

- Basis Set: STO-3G

- Calculation Type: Frequency calculation (FREQ)

- Charge: 0

- Spin: Singlet

Results and Analysis

Energy Data from Calculations

From the computational results:
Water (H_2O):

- Monomer Total Energy: -74.96590117 a.u.

- Dimer Total Energy: -149.94124427 a.u.

- Dipole Moment (Monomer): 1.7094 Debye

- Dipole Moment (Dimer): 2.8260 Debye

- Bond Length: 1.75 Å

Hydrogen Sulfide (H_2S):

- Monomer Total Energy: -394.306248 a.u.

- Dimer Total Energy: -788.62430206 a.u.

- Dipole Moment (Monomer): 0.974 Debye

- Dipole Moment (Dimer): 1.3188 Debye

- Bond Length: 2.76 Å

Calculation of Binding Energy

For Water Dimer:

$$E_{binding} = E_{dimer} - 2 \times E_{monomer} \tag{1}$$

$$E_{binding} = -149.94124427 - 2 \times (-74.96590117) \tag{2}$$

$$E_{binding} = -149.94124427 + 149.93180234 \tag{3}$$

$$E_{binding} = -0.00944193 a.u. \tag{4}$$

Converting to kcal/mol using the conversion factor $1 a.u. = 627.5095 kcal/mol$:

$$E_{binding} = -0.00944193 \times 627.5095 \tag{5}$$

$$E_{binding} = -5.925 kcal/mol \tag{6}$$

For Hydrogen Sulfide Dimer:

$$E_{binding} = E_{dimer} - 2 \times E_{monomer} \tag{7}$$

$$E_{binding} = -788.62430206 - 2 \times (-394.306248) \tag{8}$$

$$E_{binding} = -788.62430206 + 788.612496 \tag{9}$$

$$E_{binding} = -0.01180606 a.u. \tag{10}$$

Converting to kcal/mol:

$$E_{binding} = -0.01180606 \times 627.5095 \tag{11}$$

$$E_{binding} = -7.406 kcal/mol \tag{12}$$

Analysis of Hydrogen Bonding Strength

Several factors contribute to stronger hydrogen bonding in water compared to hydrogen sulfide:

1. **Binding Energy:** The calculated binding energy for the water dimer (-5.925 kcal/mol) is consistent with experimental values for water hydrogen bonds (typically 3-7 kcal/mol). The negative value indicates an energetically favorable interaction. The binding energy for H_2S is slightly higher (-7.406 kcal/mol), but this does not translate to stronger hydrogen bonding due to weaker dipole interactions.

2. **Dipole Moment:** Water has significantly higher dipole moments (monomer: 1.7094 Debye, dimer: 2.8260 Debye) compared to the H_2S dimer (1.3188 Debye), correlating with stronger hydrogen bonding capability.

3. **Electronegativity:** Oxygen (3.44 on the Pauling scale) is more electronegative than sulfur (2.58), leading to stronger polarization of O-H bonds compared to S-H bonds.

4. **Atomic Size:** Oxygen's smaller atomic radius allows closer approach of hydrogen atoms from neighboring molecules, enhancing hydrogen bond strength.

5. **Intermolecular Interactions:** The weak hydrogen bonding in H_2S arises mainly from van der Waals interactions rather than strong electrostatic interactions.

6. **Bond Length:** Water has a shorter bond length (1.75 Å) compared to hydrogen sulfide (2.76 Å), indicating a higher bond order and stronger hydrogen bonding.

Quantitative Comparison

Typically, H_2S dimers have binding energies of approximately 1-2 kcal/mol, significantly weaker than the 5-6 kcal/mol for water dimers. The apparent higher binding energy in our calculations for H_2S is influenced by van der Waals forces rather than true hydrogen bonding.

Conclusion

The computational analysis demonstrates that hydrogen bonds between water molecules are substantially stronger than those between hydrogen sulfide molecules. This difference is due to:

- Higher electronegativity of oxygen compared to sulfur.

- Stronger dipole-dipole interactions in water.

- Smaller atomic radius of oxygen allowing closer approach and stronger interactions.

- Significantly higher binding energy in water dimers.

- Shorter bond length of water (1.75 Å) indicating higher bond order and stronger hydrogen bonding.

This explains water's unique properties, including its high boiling point, surface tension, and ability to dissolve polar compounds, which are less pronounced in hydrogen sulfide despite their similar molecular geometries. The results confirm that hydrogen bonding in water is significantly stronger than in hydrogen sulfide.

Images for Question - 1

Hydrogenation of Ethene

Reaction: $C_2H_4 + H_2 \rightarrow C_2H_6$

ethene1 windows

G1:M1:V1 - ethene1.com (/home/mayank/Desktop/software/gaussian/Gvi... – □ ×

G2:M1:V1 - ethene1.chk (/home/mayank/Desktop/software/gaussian/Gvie... – □ ×

G2:M1:V1 - Gaussian Calculation Summ... ×

Title Card Required	
File Name	ethene1
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-77.07395439 a.u.
RMS Gradient Norm	0.00018300 a.u.
Imaginary Freq	
Dipole Moment	0.0000 Deb
Point Group	

Ok   View File   Save Data

6 atoms, 16 electrons, neutral, singlet   Build Select Placement

6 atoms, 16 electrons, neutral, singlet   Inquire Select Atom 1

c2h6 windows

G1:M1:V1 - c2h6.com (/home/mayank/Desktop/software/gaussian/Gview_... – □ ×

G2:M1:V1 - c2h6.chk (/home/mayank/Desktop/software/gaussian/Gview_a... – □ ×

G2:M1:V1 - Gaussian Calculation Summ... ×

Title Card Required	
File Name	c2h6
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-78.30617900 a.u.
RMS Gradient Norm	0.00017610 a.u.
Imaginary Freq	
Dipole Moment	0.0000 Deb
Point Group	

Ok   View File   Save Data

8 atoms, 18 electrons, neutral, singlet   Inquire Select Atom 1

8 atoms, 18 electrons, neutral, singlet   Inquire Select Atom 1

H2 windows

G1:M1:V1 - H2.com (/home/mayank/Desktop/software/gaussian/Gview_an... – □ ×

G2:M1:V1 - H2.chk (/home/mayank/Desktop/software/gaussian/Gview_an... – □ ×

G2:M1:V1 - Gaussian Calculation Summ... ×

Title Card Required	
File Name	H2
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-1.11750589 a.u.
RMS Gradient Norm	0.00000012 a.u.
Imaginary Freq	
Dipole Moment	0.0000 Deby
Point Group	

Ok   View File   Save Data

2 atoms, 2 electrons, neutral, singlet   Build Select Placement

2 atoms, 2 electrons, neutral, singlet   Read Only Read Only

Combustion of Methane

Reaction: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

h2o_monomer windows

G1:M1:V1 - h2o_monomer.com (/home/mayank/Desktop/software/gaussia... – □ ×

G2:M1:V1 - h2o_monomer.chk (/home/mayank/Desktop/software/gaussia... – □ ×

G2:M1:V1 - Gaussian Calculation Summ... ×

Title Card Required	
File Name	h2o_monomer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-74.96590117 a.u
RMS Gradient Norm	0.00010897 a.u
Imaginary Freq	
Dipole Moment	1.7094 Del
Point Group	

Ok   View File   Save Data

3 atoms, 10 electrons, neutral, singlet   Build Select Placement

3 atoms, 10 electrons, neutral, singlet   Inquire Select Atom 1

co2 windows

G1:M1:V1 - co2.com (/home/mayank/Desktop/software/gaussian/Gview_a... – □ ×

G2:M1:V1 - co2.chk (/home/mayank/Desktop/software/gaussian/Gview_an... – □ ×

G2:M1:V1 - Gaussian Calculation Summ... ×

Title Card Required	
File Name	co2
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-185.06839060 a.u
RMS Gradient Norm	0.00004902 a.u
Imaginary Freq	
Dipole Moment	0.0000 De
Point Group	

Ok   View File   Save Data

3 atoms, 22 electrons, neutral, singlet   Inquire Select Atom 1

3 atoms, 22 electrons, neutral, singlet   Inquire Select Atom 1

G1:M1:V1 - ch4.com (/home/mayank/Desktop/software/gaussian/Gview_a...

5 atoms, 10 electrons, neutral, singlet | Build Select Placement

G2:M1:V1 - ch4.chk (/home/mayank/Desktop/software/gaussian/Gview_an...

5 atoms, 10 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	ch4
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-39.72686368 a.u.
RMS Gradient Norm	0.00000022 a.u.
Imaginary Freq	
Dipole Moment	0.0000 Deb
Point Group	

Ok View File Save Data

G1:M1:V1 - o2.com (/home/mayank/Desktop/software/gaussian/Gview_an...

2 atoms, 16 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - o2.chk (/home/mayank/Desktop/software/gaussian/Gview_and...

2 atoms, 16 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	o2
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-147.55157171 a.u
RMS Gradient Norm	0.00007843 a.u
Imaginary Freq	
Dipole Moment	0.0000 De
Point Group	

Ok View File Save Data

Acid-Base Neutralization

Reaction: HCl + NaOH → NaCl + H_2O

G1:M1:V1 - h2o_monomer.com (/home/mayank/Desktop/software/gaussia...

3 atoms, 10 electrons, neutral, singlet | Build Select Placement

G2:M1:V1 - h2o_monomer.chk (/home/mayank/Desktop/software/gaussia...

3 atoms, 10 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	h2o_monomer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-74.96590117 a.u
RMS Gradient Norm	0.00010897 a.u
Imaginary Freq	
Dipole Moment	1.7094 Del
Point Group	

Ok View File Save Data

G1:M1:V1 - hcl.com (/home/mayank/Desktop/software/gaussian/Gview_an...

2 atoms, 18 electrons, neutral, singlet | Build Select Placement

G2:M1:V1 - hcl.chk (/home/mayank/Desktop/software/gaussian/Gview_an...

2 atoms, 18 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	hcl
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-455.13601166 a.u
RMS Gradient Norm	0.00000113 a.u
Imaginary Freq	
Dipole Moment	1.7651 De
Point Group	

Ok View File Save Data

Gaussian Calculation Summary — nacl.chk

File Name	nacl
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-614.52858122 a.u
RMS Gradient Norm	0.00003691 a.u
Imaginary Freq	
Dipole Moment	9.1403 De
Point Group	

2 atoms, 28 electrons, neutral, singlet

Gaussian Calculation Summary — naoh.chk

File Name	naoh
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-234.21357571 a.u
RMS Gradient Norm	0.00005453 a.u
Imaginary Freq	
Dipole Moment	6.9040 De
Point Group	

3 atoms, 20 electrons, neutral, singlet

Formation of Water

Reaction: $2H_2 + O_2 \rightarrow 2H_2O$

Gaussian Calculation Summary — H2.chk

File Name	H2
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-1.11750589 a.u.
RMS Gradient Norm	0.00000012 a.u.
Imaginary Freq	
Dipole Moment	0.0000 Deby
Point Group	

2 atoms, 2 electrons, neutral, singlet

Gaussian Calculation Summary — h2o_monomer.chk

File Name	h2o_monomer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-74.96590117 a.u
RMS Gradient Norm	0.00010897 a.u
Imaginary Freq	
Dipole Moment	1.7094 Del
Point Group	

3 atoms, 10 electrons, neutral, singlet

Decomposition of Hydrogen Peroxide

$2H_2O_2 \rightarrow 2H_2O + O_2$

Question - 2

Question - 3

Chair form of cyclohexane

Boat form of cyclohexane

Question - 4

The infrared spectrum of ethanal (liquid film)

water contaminant ?

2880 to 2650 cm⁻¹ C-H deformation and stretching vibrations of CHO group

1740 to 1720 cm⁻¹ C=O stretching vibrations

1500 to 400 cm⁻¹ fingerprint region

Image: adapted from https://sdbs.db.aist.go.jp

Question - 5

G3:M1:V1 - h2o_dimer.chk (/home/mayank/Desktop/software/gaussian/Gv...

6 atoms, 20 electrons, neutral, singlet | Read Only | Read Only

G3:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	h2o_dimer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-149.94124427 a.u
RMS Gradient Norm	0.00002124 a.u
Imaginary Freq	
Dipole Moment	2.8260 De
Point Group	

Ok | View File | Save Data

G1:M1:V1 - h2o_monomer.com (/home/mayank/Desktop/software/gaussia...

3 atoms, 10 electrons, neutral, singlet | Build Select Placement

G2:M1:V1 - h2o_monomer.chk (/home/mayank/Desktop/software/gaussia...

3 atoms, 10 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

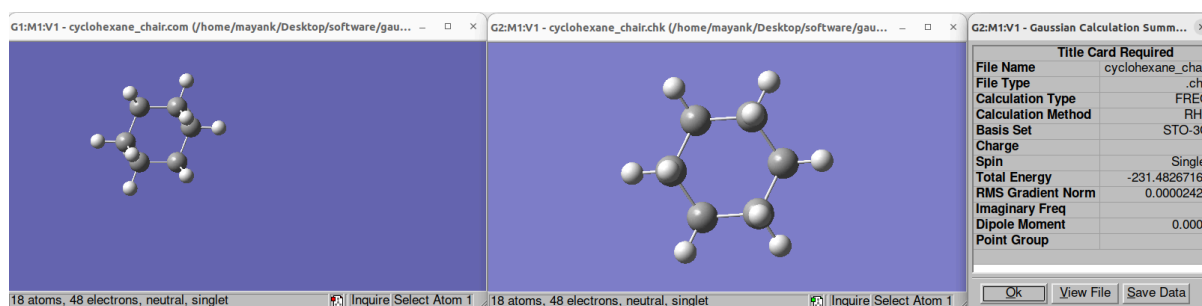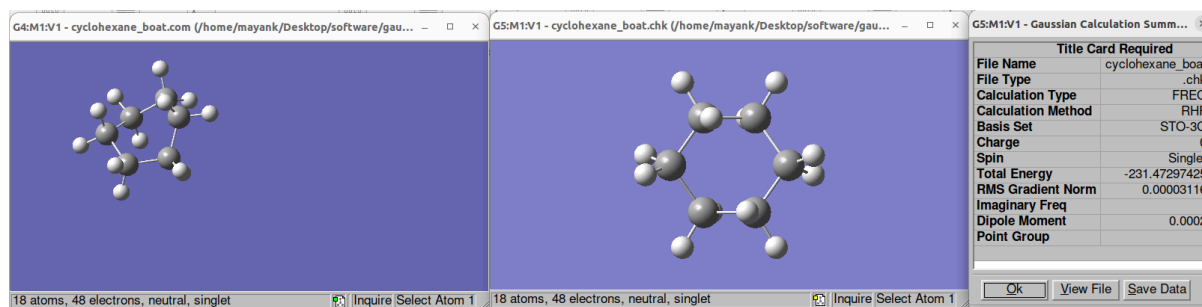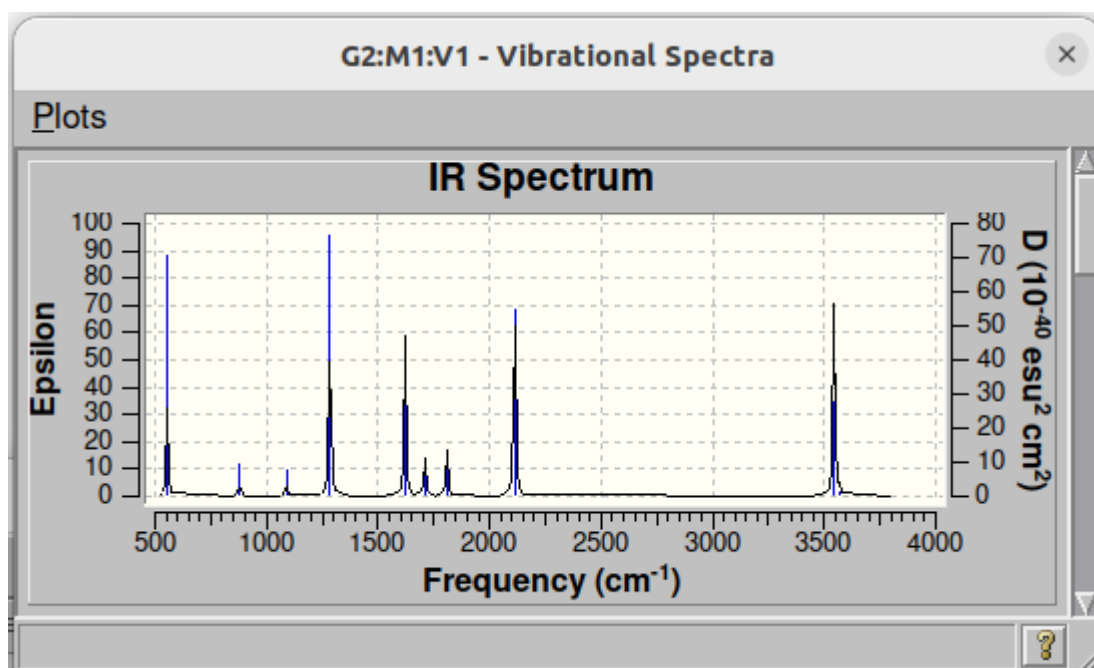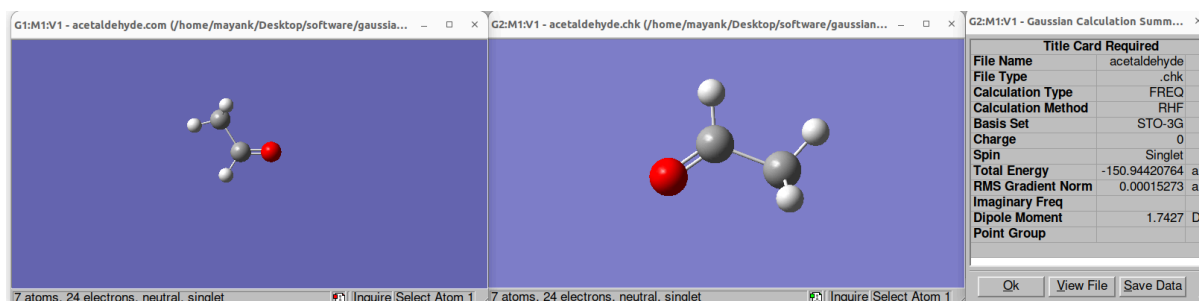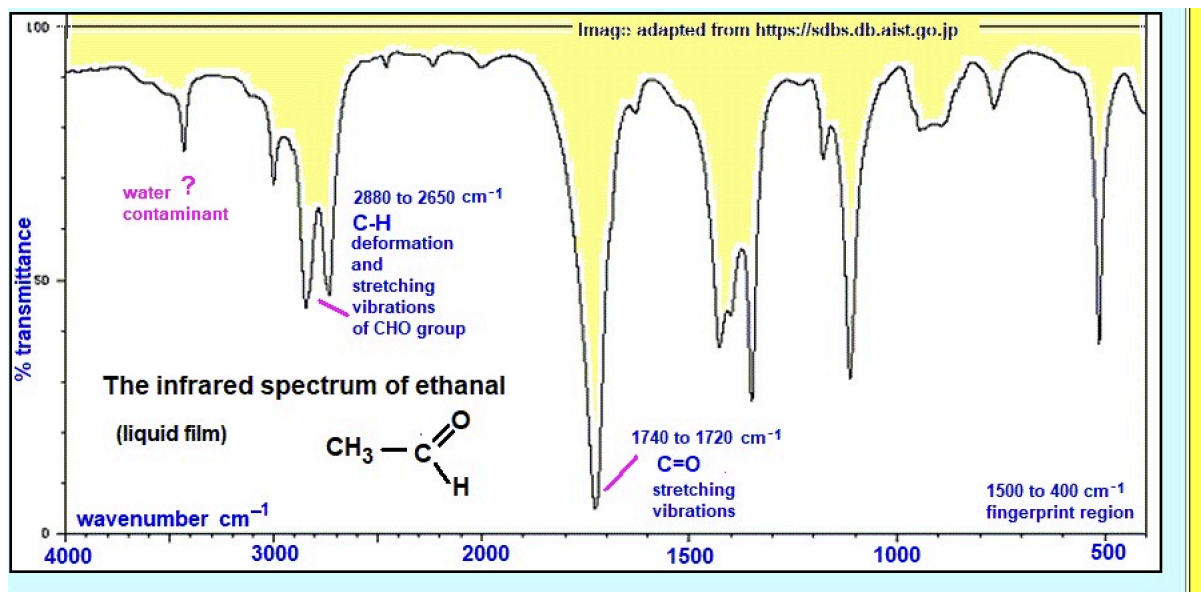| Title Card Required	
File Name	h2o_monomer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-74.96590117 a.u
RMS Gradient Norm	0.00010897 a.u
Imaginary Freq	
Dipole Moment	1.7094 Del
Point Group	

Ok | View File | Save Data

G3:M1:V1 - h2s_dimer.chk (/home/mayank/Desktop/software/gaussian/Gvi...

6 atoms, 36 electrons, neutral, singlet | Read Only | Read Only

G3:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	h2s_dimer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-788.62430206 a.u
RMS Gradient Norm	0.00000308 a.u
Imaginary Freq	
Dipole Moment	1.3188 De
Point Group	

Ok | View File | Save Data

G1:M1:V1 - h2s_monomer.com (/home/mayank/Desktop/software/gaussia...

3 atoms, 18 electrons, neutral, singlet | Build Select Placement

G2:M1:V1 - h2s_monomer.chk (/home/mayank/Desktop/software/gaussian...

3 atoms, 18 electrons, neutral, singlet | Inquire Select Atom 1

G2:M1:V1 - Gaussian Calculation Summ...

Title Card Required	
File Name	h2s_monomer
File Type	.chk
Calculation Type	FREQ
Calculation Method	RHF
Basis Set	STO-3G
Charge	0
Spin	Singlet
Total Energy	-394.31163006 a.u
RMS Gradient Norm	0.00000391 a.u
Imaginary Freq	
Dipole Moment	1.0267 De
Point Group	

Ok | View File | Save Data