CNS Assignment 1

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1 Optimizing the structure of a water dimer and hydrogen sulphide dimer single point energies of both

1.1 Configuring the g09.sh file

- 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
```

1.2 Procedure - .COM file

Writing a .COM file which includes the Z-Matrix for the H_2O dimer and H_2S dimer.

Z-Matrix for H_2O dimer:

.

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

Water Dimer Optimization

0 1
```

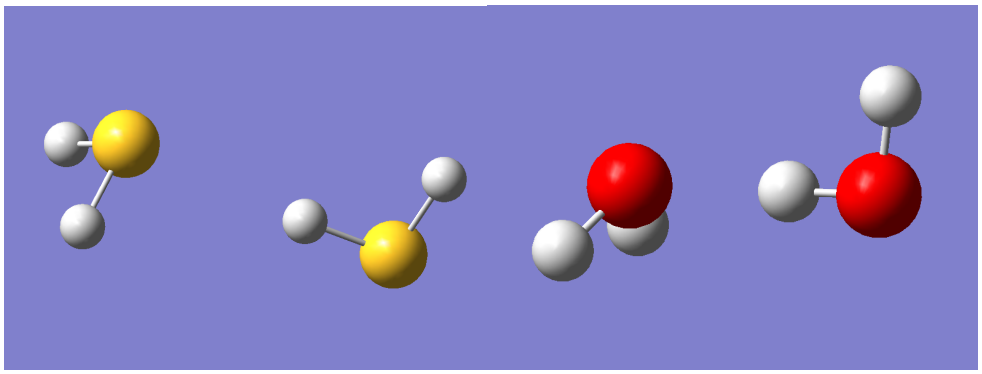
```
H
O 1 1.0
H 2 1.0 1 104.0
O 3 2.0 2 175.0 1 0.0
H 4 1.0 3 133.0 1 90.0
H 4 1.0 3 -133.0 1 90.0
```

Z-Matrix for H_2S dimer:

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

H2S optimization

0 1
H
S 1 1.0
H 2 1.0 1 92.0
S 3 2.0 2 175.0 1 0.0
H 4 1.0 3 92.0 2 120.0
H 4 1.0 3 92.0 2 -120.0
```

1.3 Observations

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



(a) H_2S Dimer (b) H_2O Dimer

Figure 1: Molecule Images

H2S optimization		
File Name	H2S	
File Type	.log	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	STO-3G	
Charge	0	
Spin	Singlet	
E(RHF)	-788.62430206	a.u.
RMS Gradient Norm	0.00000179	a.u.
Imaginary Freq	0	
Dipole Moment	1.3185	Debye
Point Group	CS	
Job cpu time: 0 days 0 hours 0 minutes 3.2 seconds.		

Figure 2: H_2S Summary

Water Dimer Optimization		
File Name	water-dimer	
File Type	.log	
Calculation Type	FREQ	
Calculation Method	RHF	
Basis Set	STO-3G	
Charge	0	
Spin	Singlet	
E(RHF)	-149.94124433	a.u.
RMS Gradient Norm	0.00004459	a.u.
Imaginary Freq	0	
Dipole Moment	2.8241	Debye
Point Group	CS	

Figure 3: H_2O Summary

1.4 Inference

As infered from the log file, the energy of the dimers lowers :

$$2H_2O \rightarrow (H_2O)_2 \tag{1}$$

$$2H_2S \rightarrow (H_2S)_2 \tag{2}$$

- H_2S molecule E(RHF) = -394.311630017

- H_2O molecule E(RHF) = -74.9659011302

- H_2S dimer E(RHF) = -788.624302056
- H_2O dimer E(RHF) = -149.941244334
- Lowering of Energy in H_2O dimer

$$E_{H_2O} = -149.941244334 - 2(-74.9659011302) = -244.3798278 Hatrees \quad (3)$$

- Lowering of Energy in H_2S dimer

$$E_{H_2S} = -788.624302056 - 2(-394.311630017) = -0.00104202199 Hatrees \quad (4)$$

Lowering of energy in the case of H_2O dimer and H_2S dimer is observed. It is more in case of H_2O dimer due to formation of Hydrogen bonds.

2 Determining the activation energy of NH3 inversion through a planar transition state

2.1 Configuring the g09.sh file

- 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
```

2.2 Procedure - .COM file

Writing a .COM file which includes the Z-Matrix for the H_2O dimer and H_2S dimer.

Z-Matrix for H_2O dimer:

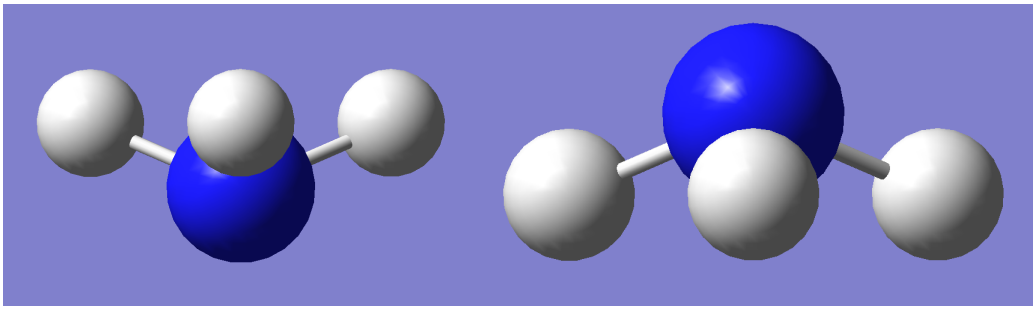
.

```
%nproc=2
%mem=1GB
#irc=calcfc  hf/sto-3g

Ammonia-Planar

0 1
N
H 1 1.0
H 1 1.0 2 120.0
H 1 1.0 2 120.0 3 179.9
```

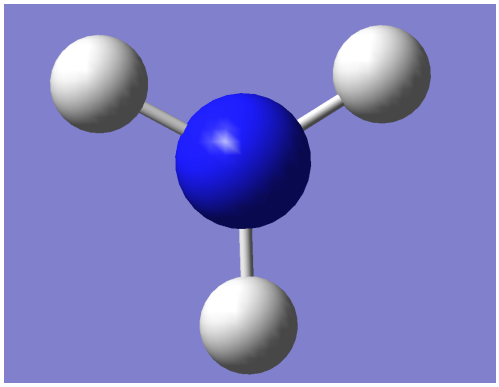
.

2.3 Observations

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



(a) NH_3-1 (b) NH_3-2



(c) NH_3-Planar

Inversion.png

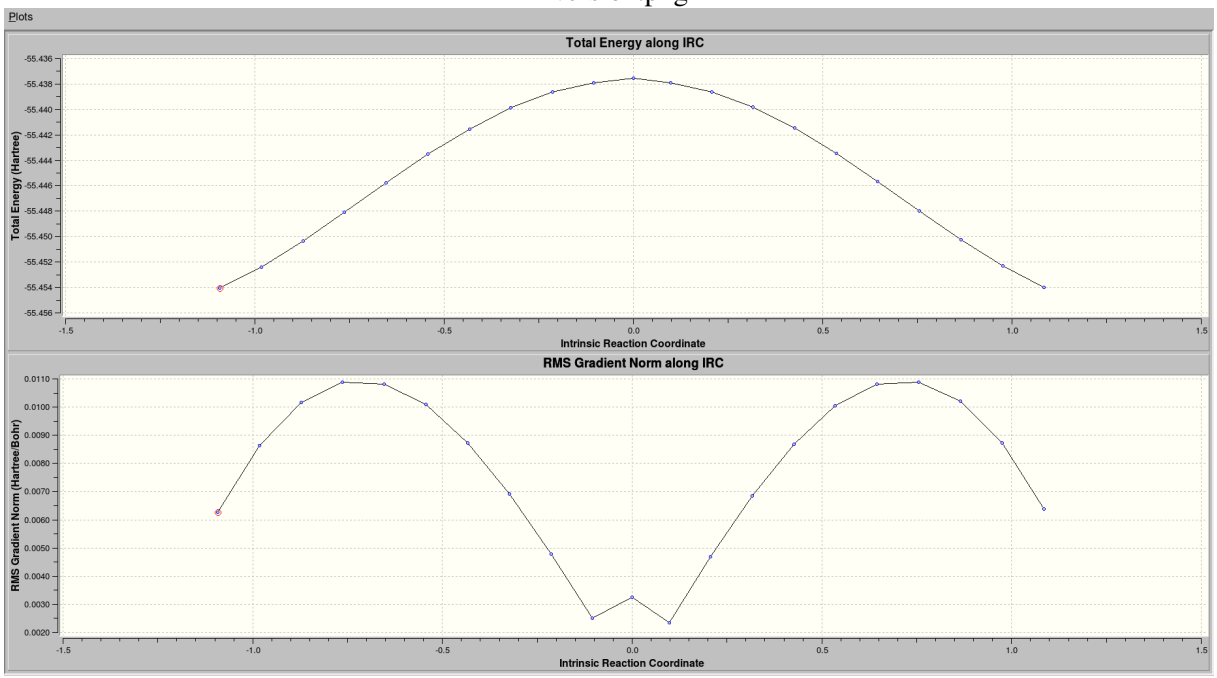


Figure 5: NH_3 IRC Graph

2.4 Inference

From the graph obtained we can infer that the enrgy diffenece betwwen the initial state and transition state of the NH_3 molecule is the Activation Energy.

$$\Delta Energy = E_{\text{transition}} - E_{\text{initial}} = (-55.437) - (-55.454) = 0.017 Hatrees \tag{5}$$

Umbrella inversion of Nitrogen is a process in compounds with a nitrogen atom that has a pyramidal geometry, such as ammonia (NH3), whereby the molecule "turns inside out". It is a rapid oscillation of the nitrogen atom from one side of the plane formed by the substituents to the other side, passing through a planar transition state.

The ammonia interconversion is rapid at room temperature. One of the factors contribute to the rapidity of the inversion is a low energy barrier as observed.