

2018113012

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ASSIGNMENT 1

Steps-

1) Login to your temporary id on abacus

```
ssh -X cn410101@abacus
```

enter password

2) create a vim file with the type ".com"

3) Type the batch submitting prototype

```
%nproc=2
```

```
%mem=1GB
```

```
#HF STO-3G opt freq
```

4) Enter the Z matrix

5) Run the batch file g09.sh

6) Submit batch code'

```
sbatch g09.sh
```

7) Put the code to be run in queue

```
squeue -u $USER
```

8) Open the ".log" created by Abacus using vim editor

9) Press "G" to go to the end of the file. If error occurred in execution of optimisation then rewrite the Z matrix. If no error is displayed, then take data about the molecule from the log file.

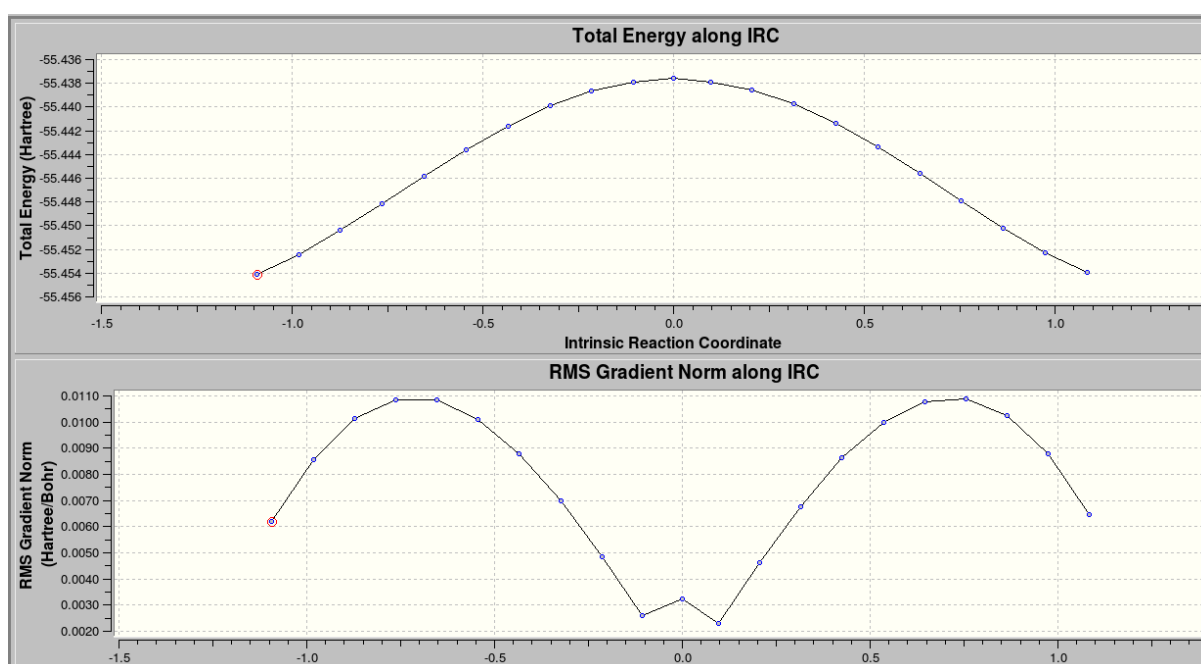
10) Open gview and see the formed molecule.

For Ammonia-

Open IRC graph and check the intermediate stage energy, which can also be called the (activation energy+ initial energy of ammonia). Calculate the activation energy from the graph.

Results-

- 1) Water -74.9648591206 Hartrees or -47041.1693628363 kcal/mol
- 2) Water dimer -149.935321708 Hartrees or -94085.8549549279 kcal/mol
- 3) Ammonia -55.2314424349 Hartrees or -34658.2607932883 kcal/mol
- 4) Hydrogen Sulphide -394.310286735 Hartrees or -247433.49347151 kcal/mol
- 5) Hydrogen Sulphide Dimer -788.0497302 Hartrees or -494508.778437189 kcal/mol



Ammonia Transition State During Inversion

Difference in Energies of Water Dimer and Hydrogen Sulphide Dimer =

638.114408492 Hartrees or 494508.77730642 kcal/mol

Difference in Energies of Water Dimer and Twice of Water Molecule= $(H_2O) - 2*(H_2O)$

-0.0056034668 Hartrees or -3.5162292552804 kcal/mol

Difference in Energies of H₂S Dimer and Twice of H₂S Molecule= $(H_2S) - 2*(H_2S)$

-0.0057084327 Hartrees or -3.209636605 kcal/mol
