TIKI Report :

Introduction:

The goal of this project is to use DFT (Density Functional Theory) to model various multi-configurational transition states. We calculate the activation energy of dhb and its branch molecules using DFT and compare with our previous study (put reference), which was done using MCSCF (Multi-configurational self-consistent field). We want to compare if we can do a faster calculation with DFT compared to MCSCF, which is slow and expect to get comparable results. We studied various molecules, including 3-aza-3-ium; 3,4-diaza-3-ium; 3,4-diaza-34-diium; dhb (dihydrobenzvalence).

Previous Study:

The table (reference) below shows the activation energy of difference transition states from our previous study using MCSCF/cc-pVDZ. We used DFT/cc-pVTZ in our new study.

Computational Details:

There are different computational steps involved in this research. We prepared an input file with co-ordinates of molecules, molecule name\*\*\*, model name. Then we prepared an job submission script, which takes input file and submit jobs to supercomputer and produces an output file with optimized results. Then we analyze the output file for any potential errors (ex: not converged, no negative eigenvalue, termination error etc). If any error is found, then we have to repeat again the process starting from the beginning. If no errors found, then we use the output to produce two different types of results: use MacMolPlt (reference) to draw molecule shapes and frequency calculation to get the activation energy.

Challenges faced:

We used several new technologies in this research including linux, bash script, super computer job submission, Gaussian 09, many job submission tools, MacMolplt. Each input file usually runs 5 to 48+ hours to get the optimized output. There are several errors we encountered in this process including termination error, unrestricted error, convergent error, restricted error, mixing error, error on dis-molecule. We followed each steps carefully to minimize the error and processing time.

Results:

The output file contains two types of table, with coordinates (X, Y, Z) of molecules in Angstroms. The standard orientation table is used for frequency calculation and zero-point energy is found. The input orientation table is used in MacMolPlt to draw the shapes of molecules.

Show the results table here

Activation Energies (kcal/mol) for 3-aza-3-ium

|  |  |  |
| --- | --- | --- |
| TS | Ea (DFT) | Ea (MCSCF) |
| TSconA |  |  |
| TSconB |  |  |
| TSdisA\_mix |  |  |
| TSdisB\_mix |  |  |
| TSezA |  |  |
| TSezA\_mix |  |  |

Activation Energies (kcal/mol) for 34-diaza-3-ium

|  |  |  |
| --- | --- | --- |
| TS | DFT | MCSCF |
| TSconA | 53.7 | 57.4 |
| TSconB | 57.1 | 56.9 |
| TSconC | 52.5 | 54.2 |
| TSconD | 50 | 55.5 |
| TSdisA | X | 56.6 |
| TSdisB | X | 60.8 |
| TSdisC | X | 61.4 |
| TSdisD\_mix | 61.0 | 57.3 |
| TSezA | X | 2.8 |
| TSezB | 91.3 | 1.2 |
| TSezC | 54.8 | 3.1 |
| TSezD | 94.5 | 2.2 |

Activation Energies (kcal/mol) for 34-diaza-34-diium

|  |  |  |
| --- | --- | --- |
| TS | DFT | MCSCF |
| TSconA | X | 69.2 |
| TSconB | X |  |
| TSdisA | X | 67.0 |
| TSdisB | X |  |
| TSezA | X | 2.1 |
| TSezB | x |  |

Activation Energies (kcal/mol) (dhb)

|  |  |  |
| --- | --- | --- |
| TS | DFT | MCSCF |
| TSconA | 41.8 | 43 |
| TSdisA | 51.4 | 55 |
| TSezA | 9.1 | 3 |

Molecule Structures:

Pictures of Reactant 🡪 Transition 🡪 Product

Summary :

We studied four different types of molecules: 3-aza-3-ium; 3,4-diaza-3-ium; 3,4-diaza-34-diium; dhb (dihydrobenvalene). Most of the results are found to be consistent with previous study. TSezB,C,D for 3,4-diaza-3-ium are higher than previous study, which we would like to investigate in future studies. In conclusion, our new method DFT is found to be much faster than the previous method MCSCF.