COMPUTING IN SCIENCES-1 Practical Assignment

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CIS-1 Practical Assignment

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Q1

- Perform a 100 ps MD simulation on the tripeptide assigned to you.

* RMSD as a function of time
* End-to-end distance as a function of time
* SASA as a function of time
* Rg as a function of time
* Radial distribution function

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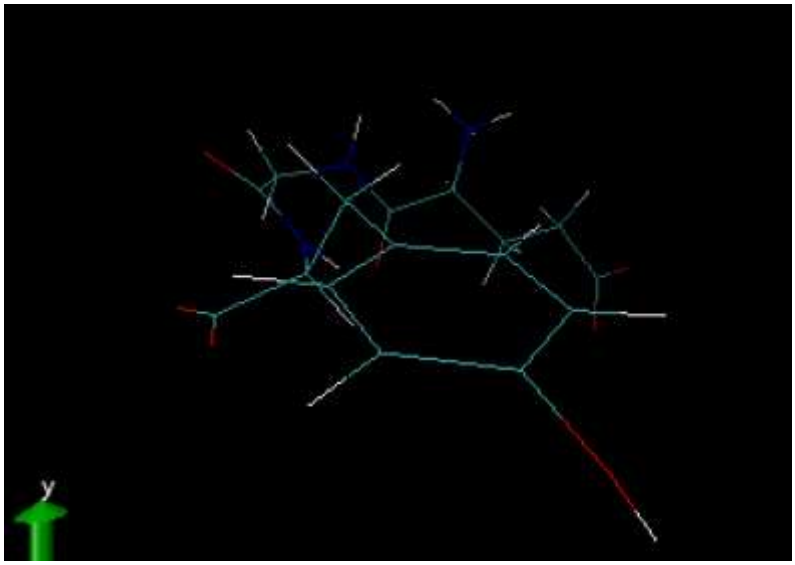
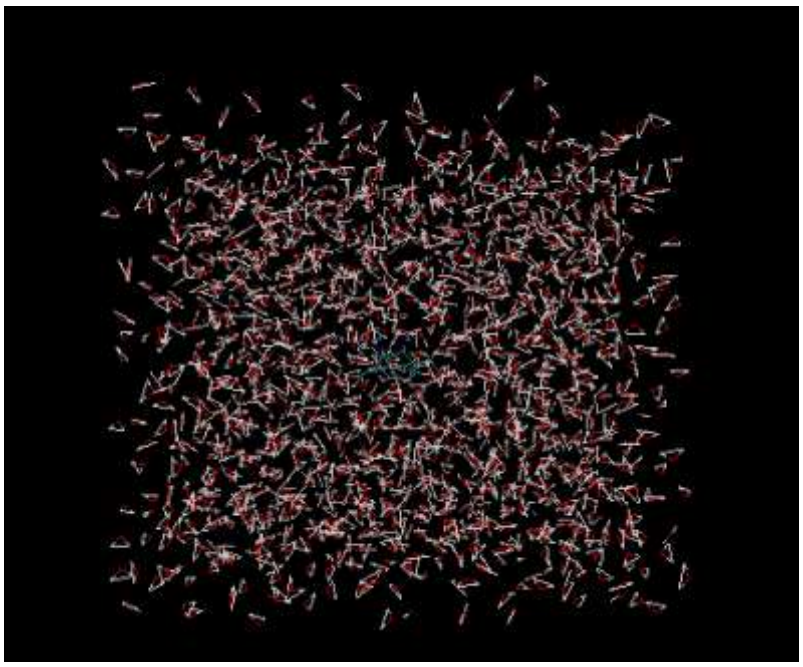


Initial Tripeptide (w/Glutamic acid (Glu), Glycine (Gly) and Tyrosine(Tyr))



Final Complex

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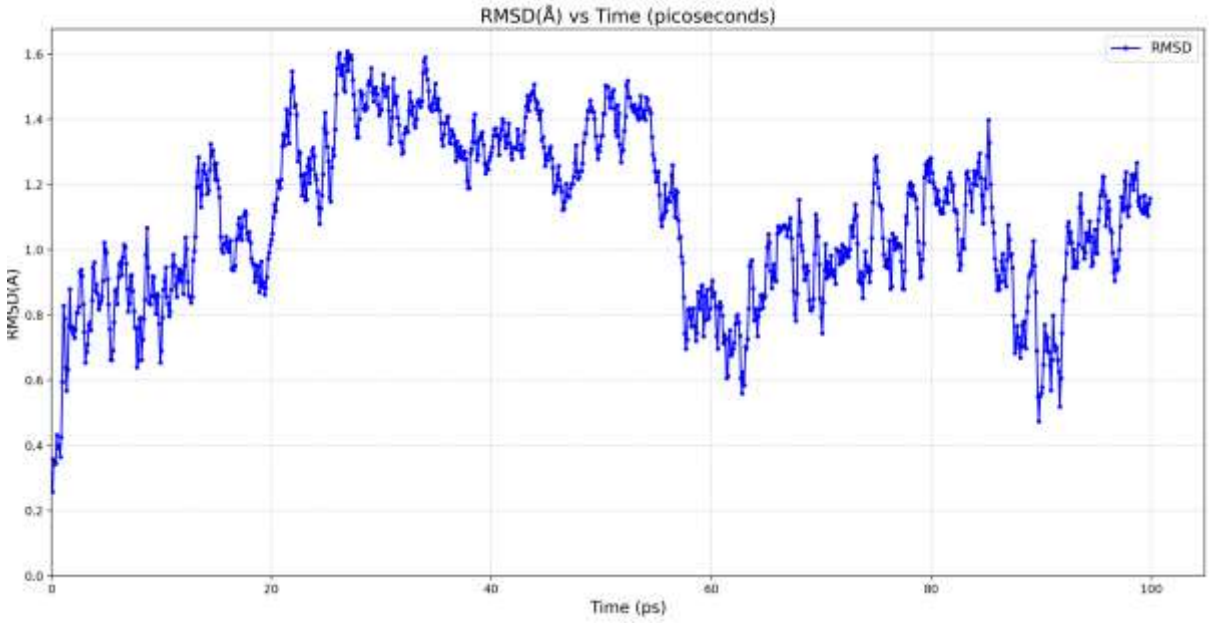
a) RMSD as a function of time



- RMSD (Root Mean Square Deviation) quantifies the difference between the positions of atoms in the tripeptide, at different time points.

- The MSD initially increases, suggesting significant conformational changes, then fluctuates around 1.2 Å after approximately 40 ps, indicating a relatively stable state with minor variations.

- The periodic fluctuations imply dynamic equilibrium, with no large structural deviations after stabilization.

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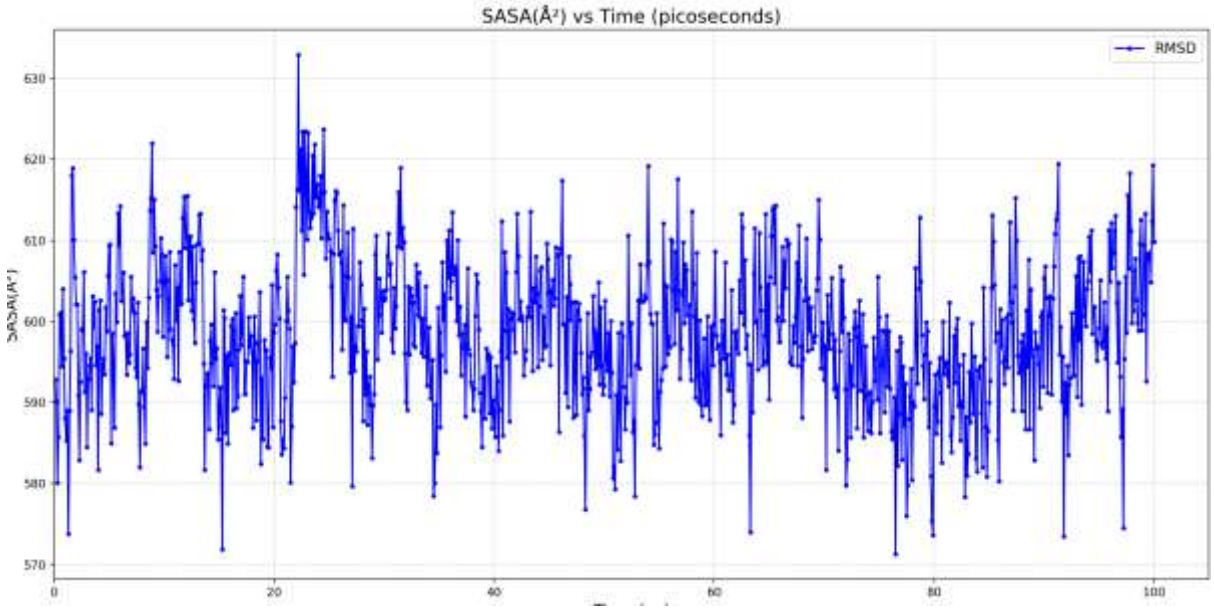
b) SASA as a function of time



- SASA (Solvent Accessible Surface Area) is a measure of the surface area of the tripeptide that is accessible to the water solvent.

- The SASA values oscillate between approximately 570 Å² and 630 Å², indicating a dynamic equilibrium where the molecular conformation changes slightly over time but remains generally stable.

- The periodic fluctuations suggest that the molecule is undergoing minor conformational changes or interactions with the solvent, without significant structural collapse or unfolding.

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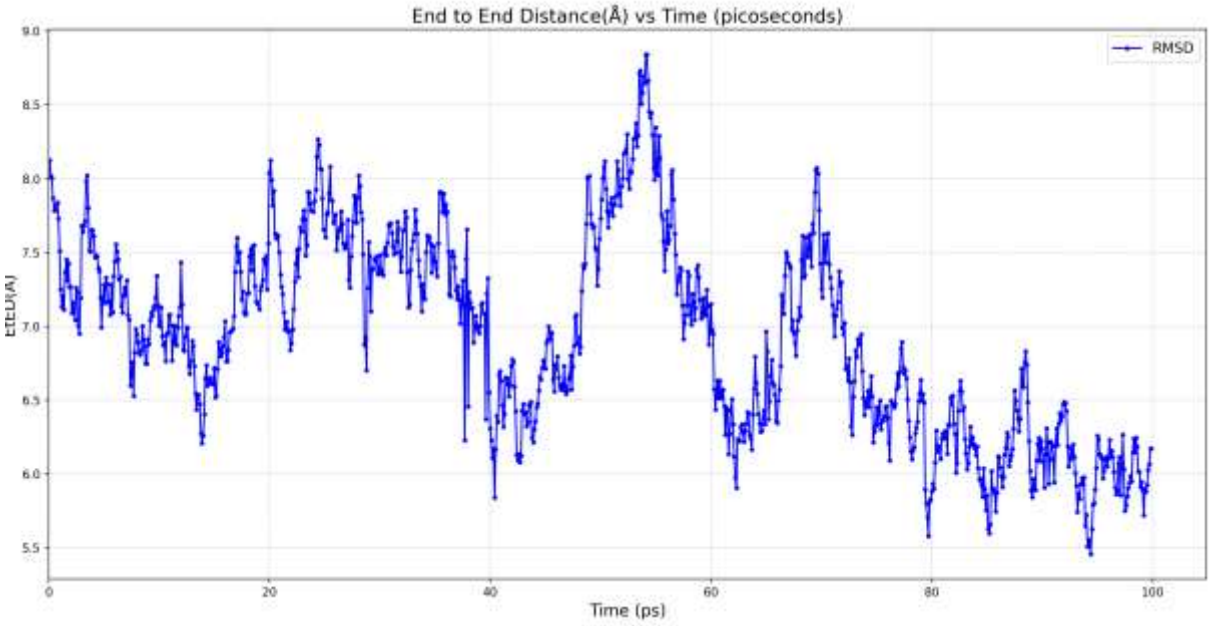
c) End-to-end distance as a function of time



- The end-to-end distance refers to the linear distance between the N-terminal (amine group) of the first amino acid and the C-terminal (carboxyl group) of the third amino acid.

- The distance fluctuates between approximately 5.5 Å and 9 Å, with an initial increasing trend followed by a gradual decline after 60 ps, suggesting dynamic folding or structural adjustments over time.

- The decreasing trend in the latter half indicates the molecule may be adopting a more compact or stable conformation.

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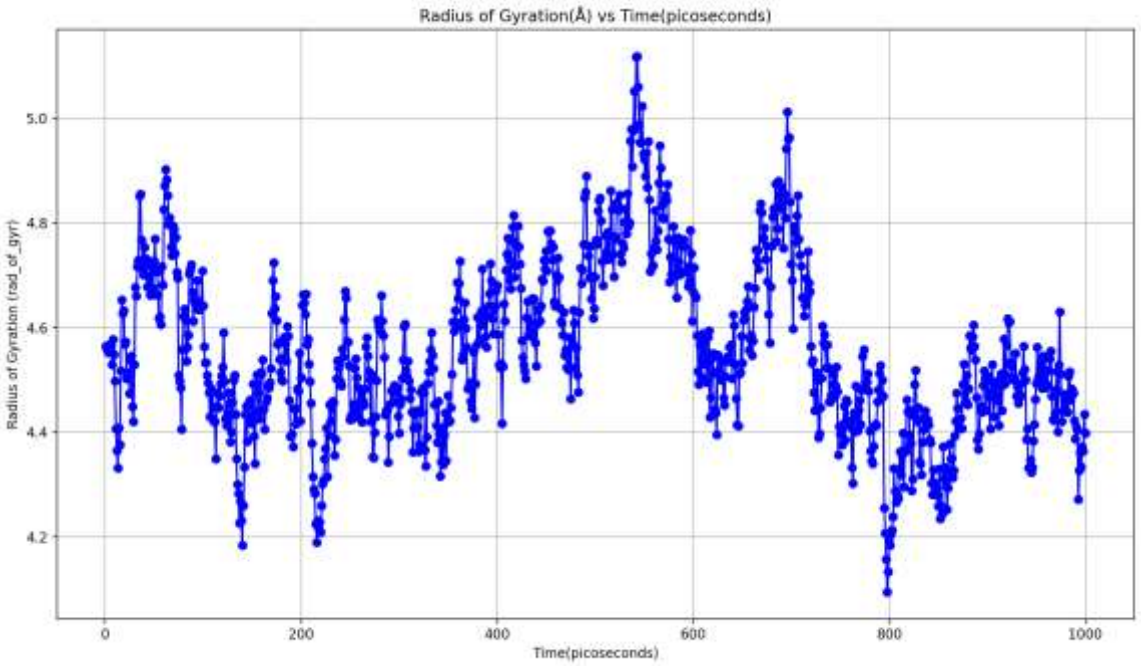
d)Rg(Radius of Gyration) as a function of time



- The radius of gyration (Rg) measures the overall compactness or spatial distribution the tripeptide , relative to its centre of mass.

- The radius of gyration fluctuates between the values of 4 Å and 5.2 Å, suggesting that there is significant conformational flexibility.

- The graph oscillates around 4.6 Å for the duration of the simulation, which could mean that it is the overall most stable conformation of the tripeptide

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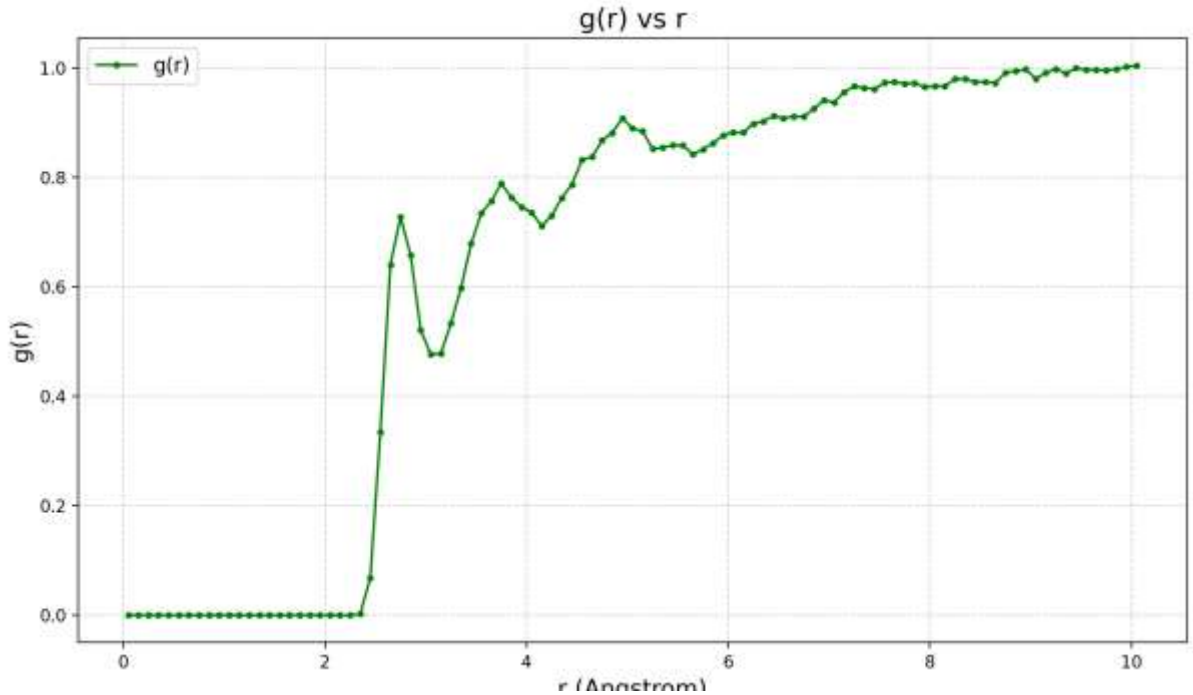
e) Radial distribution function



- The radial distribution function g(r) of the tripeptide describes how the density of atoms or molecules is distributed the centre of mass of the tripeptide, as a function of distance.

- The initial distance upto 2 Å has a g(r) of 0, meaning that the probability of a finding particles at that distance,

- The peak at around 2.5 Å indicates that is probably the first coordination shell, with high particle density. The graph then slowly rises to 1, which indicates that the system becomes disordered, beyond around 4.5 Å.

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Q2

Calculate the transition barrier and reaction energy corresponding to the Diels-Alder reaction between butadiene and ethylene; Depict the three-dimensional structures of reactants, transition state and product.

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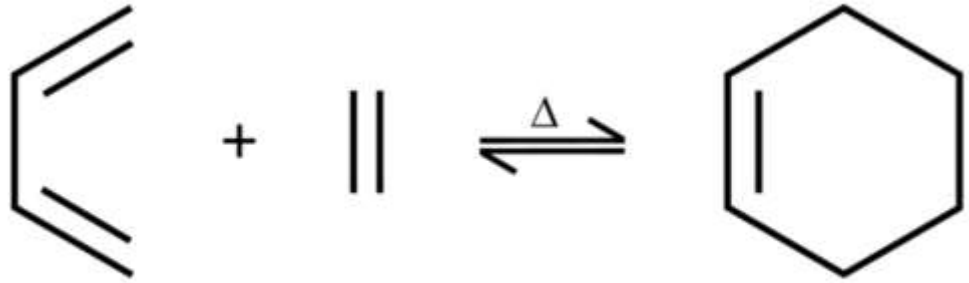
Dier's Alder Reaction-

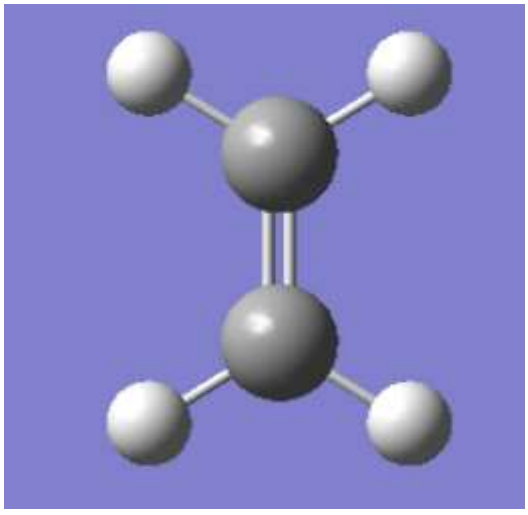


Butadiene Ethylene Cyclohexene

- The Diels–Alder reaction is a chemical reaction that occurs between a conjugated diene and a substituted alkene (dienophile) to form a substituted cyclohexene derivative.
- It has served as a powerful and widely applied tool for the introduction of chemical complexity in the synthesis of natural products and new materials.
- It is believed to occur via a single, cyclic transition state, with no intermediates generated during the course of the reaction.

Depiction of Structures-

a) Ethylene (Reactant)



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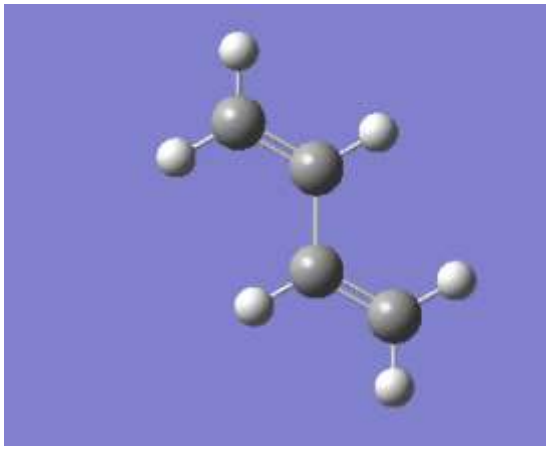
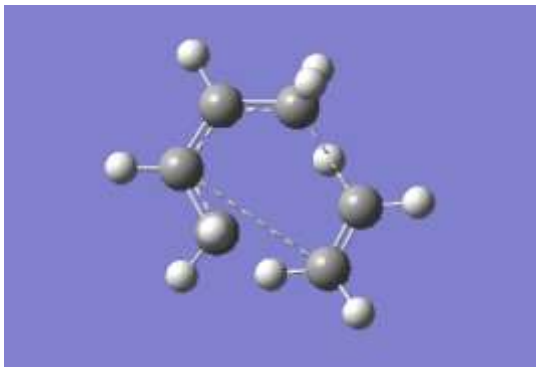
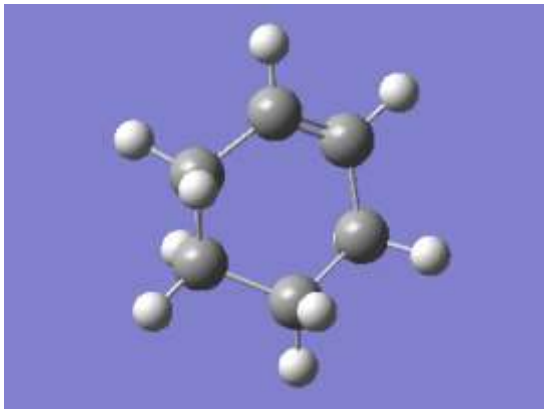
b) Butadiene (Reactant)



c)Transition State



d)Cyclohexene (Product)



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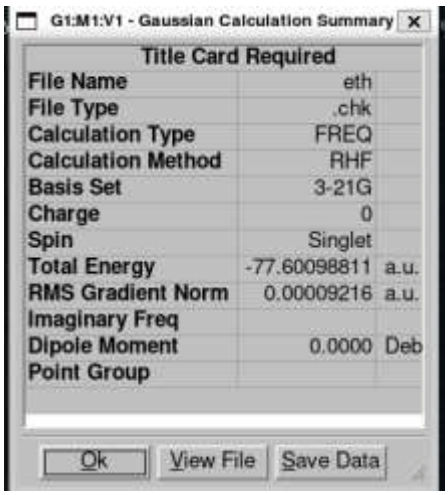
Procedure-

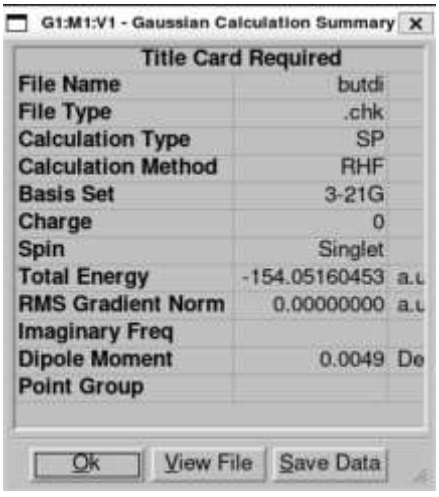
1. Create structures of ethylene, butadiene and cyclohexene.
2. Optimize structures to a minimum, and obtain energies of the optimized structures
3. Create an approximate transition state.
4. Optimize to a TS(Berny), by ignoring symmetry, calculating force constants and using the no-eigen parameter, and obtain the energy of the transition state.
5. Use the obtained energies to calculate the transition barrier and the reaction energy

Result-

- The obtained energies are-

a) Ethylene- -77.60098811 au (Reactant)
b) Butadiene- -154.05160453 au (Reactant)
c) Cyclohexene- -231.71058819 au
d) Transition State- -231.60320857 au (Product)





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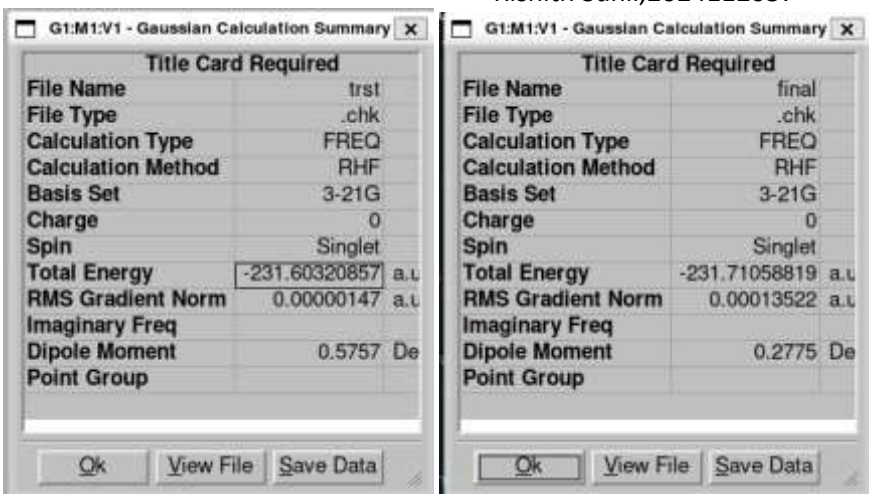

- Transition Barrier (Activation Energy)-
  Energy of Transition State - (Energy of Reactants)
  =-231.0632-(-154.0516+-77.6009)
  =0.049 au
  =30.747 kcal/mol (1 au energy= 627.51 kcal/mol)
- Reaction Energy-
  Energy of Product - (Energy of Reactants)
  =-231.7105-(-154.0516+-77.6009)
  =0.059 au
  =37.023 kcal/mol (1 au energy= 627.51 kcal/mol)

Notes-

- The values calculated are in the margin of error compared to the actual values.
  https://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/enrgtop.htm#:~:text=Despite%20the%20favorable%20overall%20energy,exergonic%20%2D19.4%20kcal%2Fmole. (Reaction Energy-40kcal/mol)
  https://www.ch.ic.ac.uk/rzepa/motm/porphyrins/introDA.html
  (Transition Barrier-27.5kcal/mol)
- This can be due to approximations in the method, as well as environmental and solvent factors.