

Molecular Modelling and Simulations: QM Assignment-1
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1. Take five organic reactions of your choice, calculate the reaction energies (in kcal/mol), and include the reactions with structures. [20]
2. Perform conformational analysis of butane and plot the energy (in kcal/mol) as a function of the rotation angle [10]
3. Calculate the energy difference between the chair and boat forms of cyclohexane [10]
4. Calculate the vibrational spectrum of Acetaldehyde, obtain the experimental spectrum and compare the two. [10]
5. Hydrogen bond between two water molecules are stronger than that between two hydrogen sulfide molecules. Prove [10]