Computing in Sciences - I   Assignment - 4

1. π-conjugation is general leads to stabilization of organic compounds. Identify two model systems with same molecular formula with and without π-conjugation to support or refute this.

2. Show that the true transition state involved in an S_N2 reaction (for example, $Cl^- + CH_3I \rightarrow CH_3Cl + I^-$) is more stable than the sum of the energies of the reactants or that of the products. Isn't this incorrect? Explain this phenomenon with any additional calculations you may need to do.

3. Plot the three dimensional potential energy surface corresponding to the two central single bonds of pentane molecule. Identify all unique minimum energy conformers and explain their relative energies.

4. Model the following reaction.
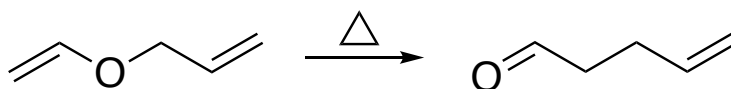
5. Qualitatively compare the rates of the following reactions. Explain the observed trend.

$$n = 1, 2, 3$$
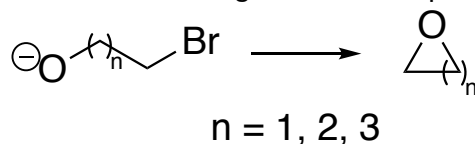
6. One of the key properties for the stability of DNA molecules is base pair interaction. Compare the strength of these interactions in G:C and A:T base pairs.