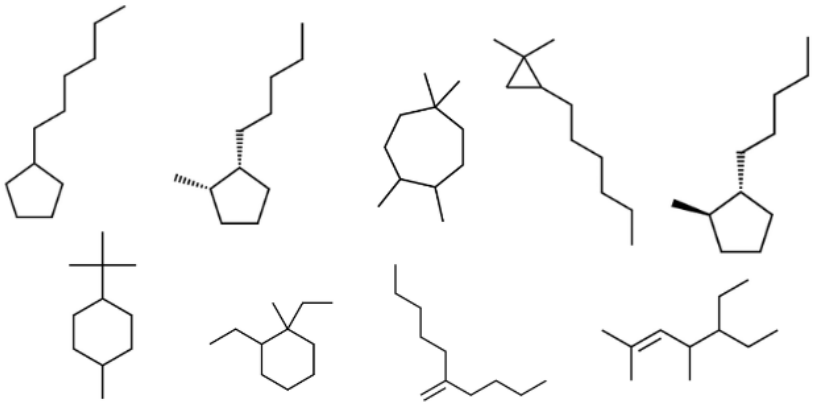
Gaussian Assignment

Computing in Sciences - 1

June 30, 2022

Problem 1. Calculate and plot the relative energies for the following C11H22 isomers



Problem 2. Perform conformational analysis for the following dihedral angles of n-hexane(see figure 1). Choose appropriate step sizes and identify various points of interest(staggered, eclipsed etc).

- Dihedral angle formed by the carbons 1,2,3,4
- Dihedral angle formed by the carbons 3,4,5,6
- 2D scan of the above two dihedral angles

Figure 1: n-hexane

Problem 3. Calculate the vibrational spectrum of ethanol. Perform normal mode analysis and assign major peaks in the experimental spectrum(see figure

2) through comparisons (i.e label peaks on the obtained spectra and map it to the experimental one, also explain what kind of vibrations each labelled peak corresponds to with suitable images).

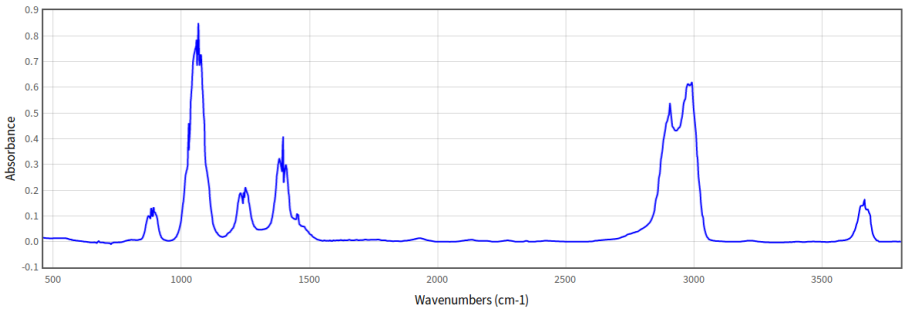


Figure 2: IR spectrum of ethanol

Problem 4. Model the following reactions(Reactants, products, transition state and reaction pathway) and summarize the results (i.e show images of the reactants, products and transition states along with their energy summaries, also show the IRC plot of the reaction and mention if the reaction is endo or exo thermic)

- Tautomerism of Acetone
- Diels-Alder reaction between ethylene and butadiene
- Nucleophilic Substitution Reaction between Methyl Chloride and Bromide ion
- Intramolecular hydrogen transfer between the two oxygens of malonaldehyde
- The Huisgen Reaction of Acetylene with Hydrazoic Acid

Problem 5. Read the attached study on "The intrinsic reaction coordinate". Perform IRC scans for the reactions (HCN and CH3+H rxns only) described in the paper and draw comparisons.

SUBMISSION FORMAT: A single PDF clearly and precisely answering the questions. Use kcal/mol to report energies (unless specified). Present the numbers after rounding them off to appropriate number of digits for each unit of energy.