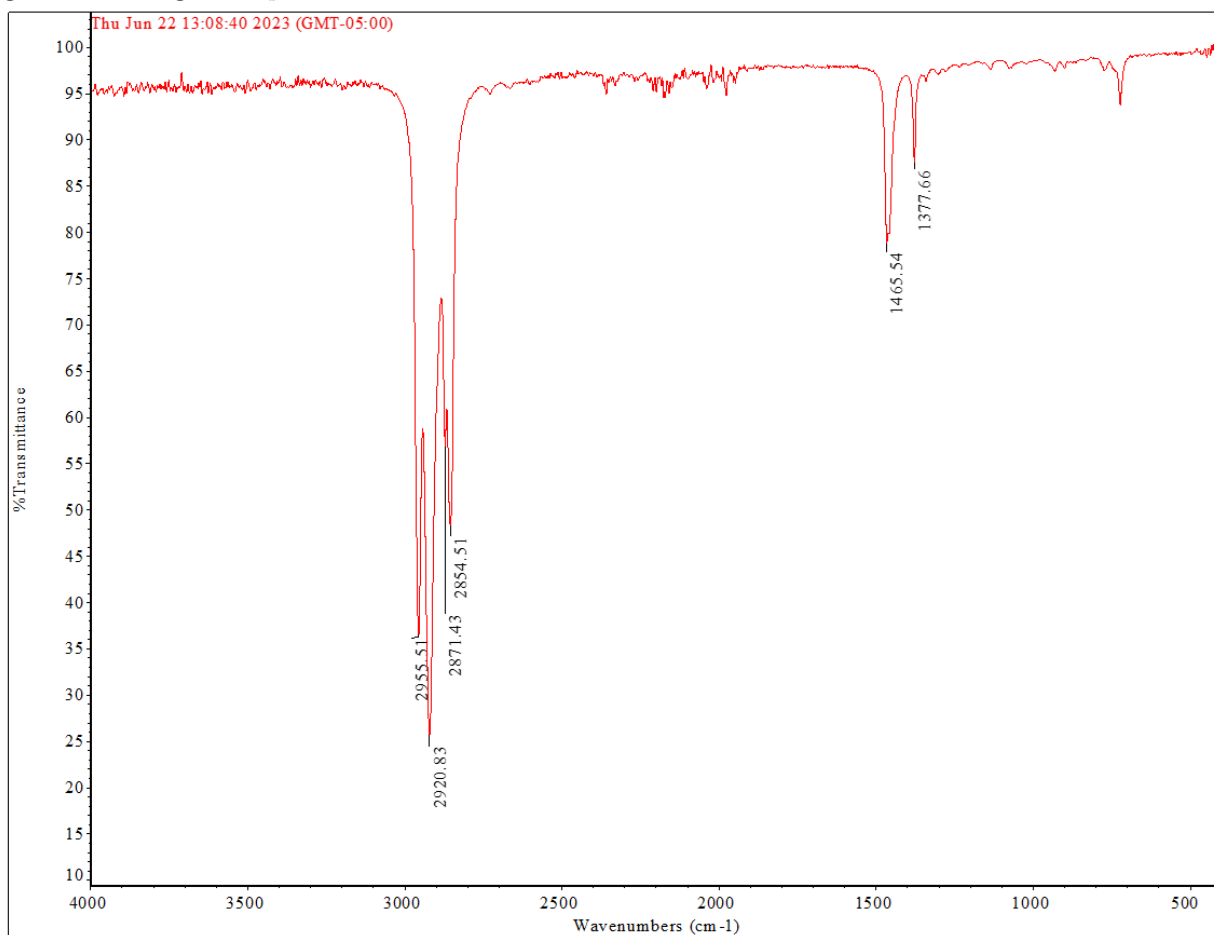


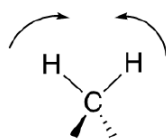
5.4: Exercise Questions

Part 1: Vibrational Modes of Hexane

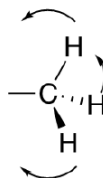
- Using your knowledge of IR spectra please assign the following stretches and bends to the experimental IR spectrum of hexane using an IR stretching chart: sp^3 C – H Stretch, CH_2 bend/scissor, and CH_3 bend.



- By clicking on and viewing the vibrational frequencies, how many distinct vibrational modes does hexane have that involve the stretching of an sp^3 C – H bond? (Hint: where do these types of stretches occur on the IR spectrum)
- Do the C – H stretching modes typically involve one C – H bond or multiple C – H bonds?
- In addition to stretching, C – H bonds can bend as well. As shown below, $-CH_2-$ and CH_3 groups will bend when excited by IR light. Please indicate the wavenumber of IR light that you have calculated that causes CH_2 and CH_3 bending as shown below. How do the calculated frequencies compare to the experimental frequencies in question 5.2.1?



CH_2 Bend



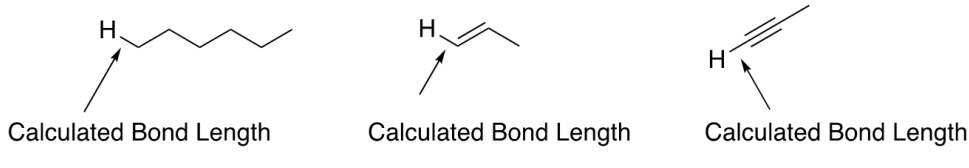
CH_3 Bend

- At around 720 cm^{-1} long chain alkanes tend to have a characteristic vibrational mode. In your computation, this absorption occurs at 718 cm^{-1} . Please describe the molecular motion in this vibrational mode. Why do you think that this mode is used by scientists to determine the presence of a long chain alkane?

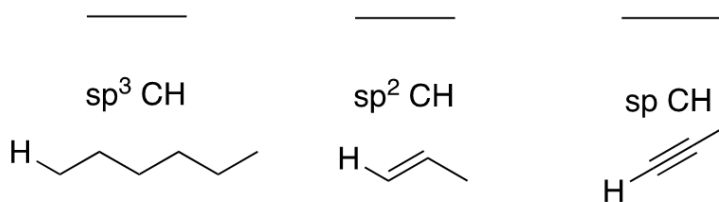
Part 2: Impact of Hybridization of the C-H Stretching Frequency

When examining the IR spectrum of hydrocarbons, you will see that the C – H stretching frequencies are strongly dependent upon the hybridization of the carbon. This is because the hybridization of the carbon influences the length and strength of the C – H bond. Let's examine this phenomenon using computation.

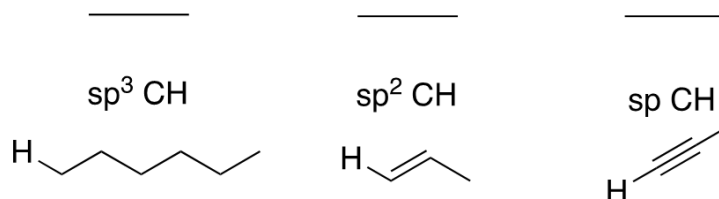
6. Open the output file of hexane (that you calculated), propene (provided), and propyne (provided) and measure indicated bond lengths.



7. Please briefly describe the relationship between carbon hybridization and bond length. Propose an explanation that describes why certain hybridizations have shorter bond lengths (Hint: remember that different hybridizations are made of differing proportions of *s* and *p* orbitals. *S* orbitals, on average, hold electrons closer to the nucleus than *p* orbitals.)
8. In the case of the three C – H bonds measured above, we can correlate homolytic bond strength with bond length. Specifically, the shorter the bond length, the stronger the corresponding bond. Please rank the three bonds in order of increasing strength (1 weakest, 3 strongest).



9. Given the relationship between bond strength (*f*) and vibrational frequency in wavenumber $\tilde{\nu}$ please rank the order of stretching frequencies involving the C – H bonds indicated above. Briefly explain the order that you chose. (1 lowest wavenumber, 3 highest wavenumber).



10. Examine the IR stretching modes of hexane, propene, and propyne. Were your predictions about the order of the stretching frequencies correct?

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