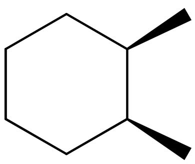
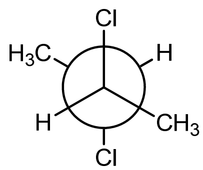
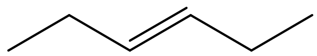
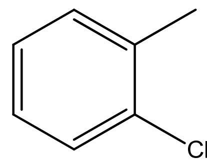
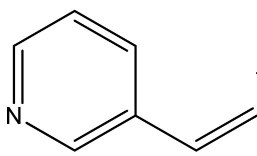
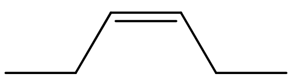
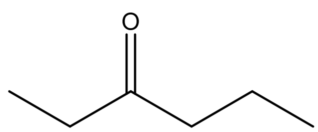
Homework #6: NMR theory, equivalent nuclei, and ^{13}C NMR

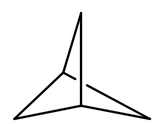
1. What two nuclei are most commonly investigated by NMR in organic chemistry?
2. What does NMR stand for? How are each of these words descriptive of an important aspect of this spectroscopy?
3. What happens to nuclei when placed in an external magnetic field? Why does this allow for investigation of the nuclei by electromagnetic radiation?
4. What is meant by shielding? What is deshielding? How does deshielding affect the frequency of light absorbed by nuclei?
5. Why are NMR spectra reported in units of ppm rather than Hertz?
6. What is the 0 ppm standard for proton NMR? Why is this substance used?
7. Label all sets of equivalent protons in these molecules.

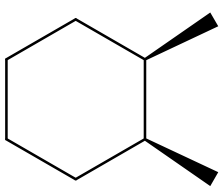
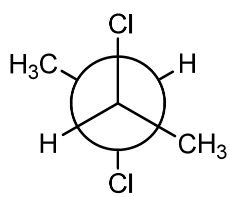



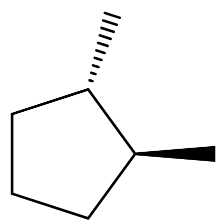
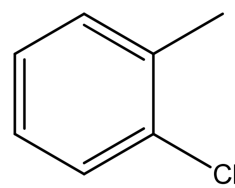


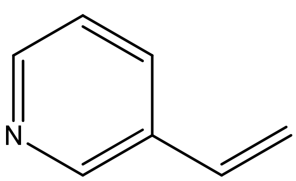



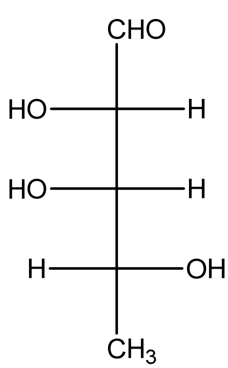


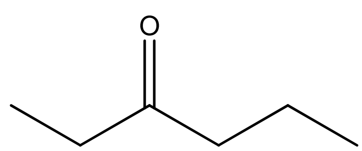
8. Label all sets of equivalent carbons in these molecules. How many ^{13}C NMR signals would you expect to see for each compound?

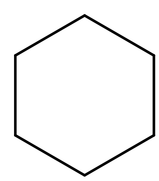
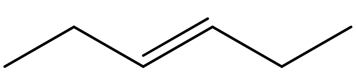
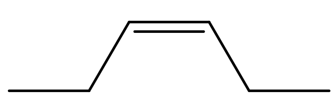
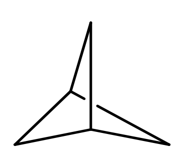



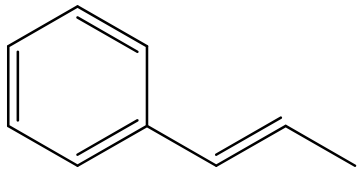


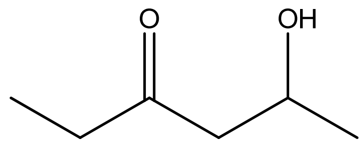


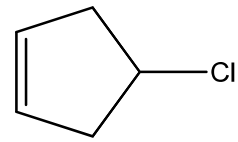


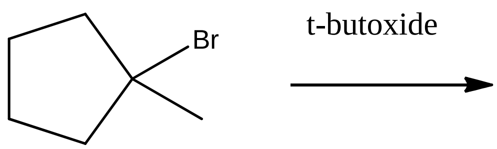
9. Give estimated ^{13}C NMR chemical shift ranges for the carbons in these molecules. Draw a predicted ^{13}C NMR spectrum for each compound.

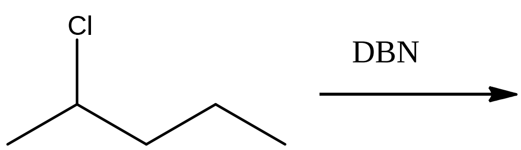




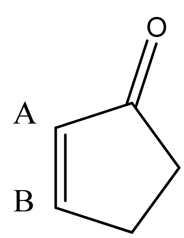


10. The following elimination reactions were carried out, and the major and minor products were isolated from each other. Would ^{13}C NMR data alone be able to differentiate the identity of the major and minor products?

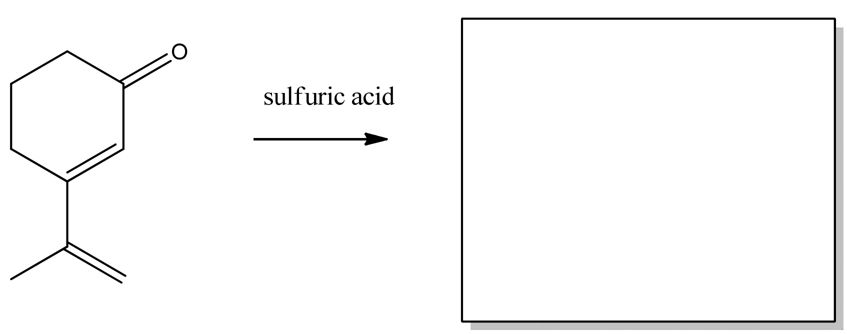




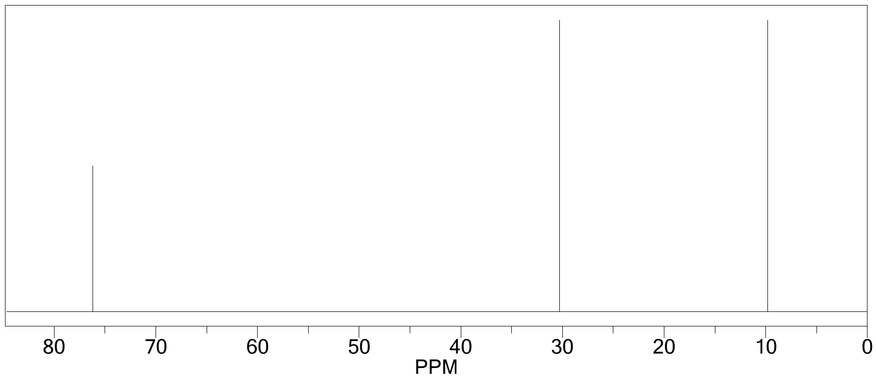
11. The following compound has ^{13}C NMR signals at 29, 34, 134, 164, and 210 ppm. Which signals correspond to carbons A and B? Give a physical explanation for your prediction.



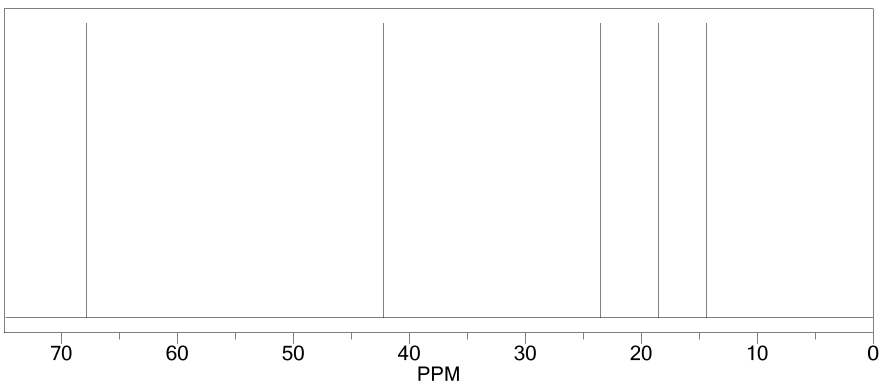
12. You performed this rearrangement of carvone reaction in lab. Use your IR and C-13 NMR to predict the product of the reaction. Explain how your C-13 data is consistent with the product you proposed. How is the C-13 data you collected inconsistent with the structure of the starting material?



13. Propose structures for **$C_5H_{12}O$** compounds consistent with these C-13 NMR.



A.



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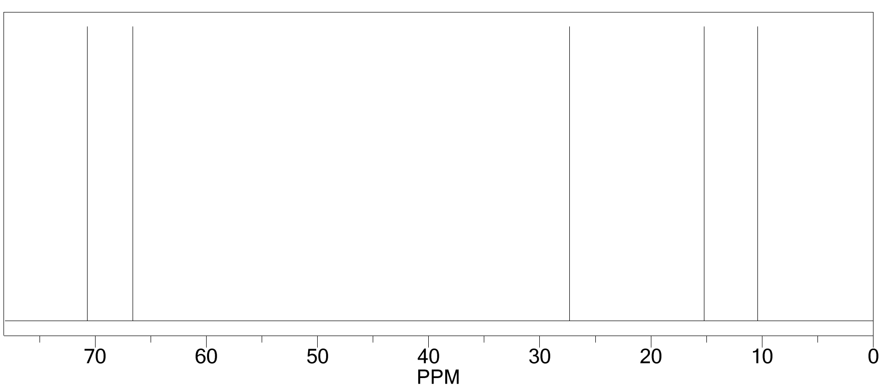
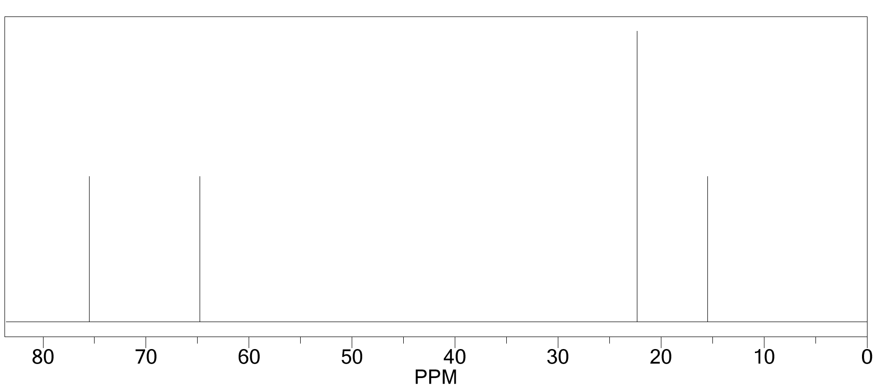


C.



D.