
OpenCourseWare (2023)

CHEMISTRY II

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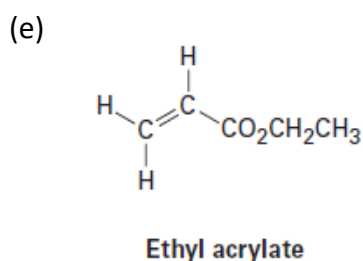
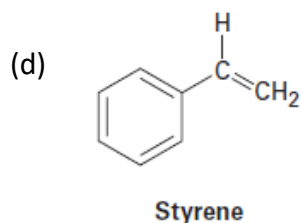
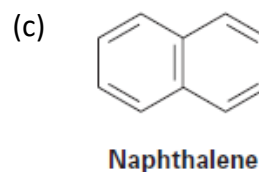
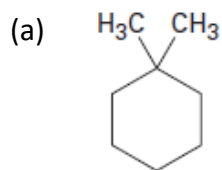
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EXERCISES OF STRUCTURAL DETERMINATION



Exercise 1. How many types of non-equivalent protons are present in each of the following molecules?



Exercise 2. Structural Elucidation from ^1H NMR Spectra. There are several isomeric alcohols and ethers of molecular formula $\text{C}_5\text{H}_{12}\text{O}$. Two of these, A and B, exhibit the following ^1H NMR spectra:

A: $\delta = 1.19$ (s, 9 H), 3.21 (s, 3 H) ppm

B: $\delta = 0.93$ (t, 3 H), 1.20 (t, 3 H), 1.60 (sextet, 2 H), 3.37 (t, 2H), 3.47 (q, 2 H) ppm.

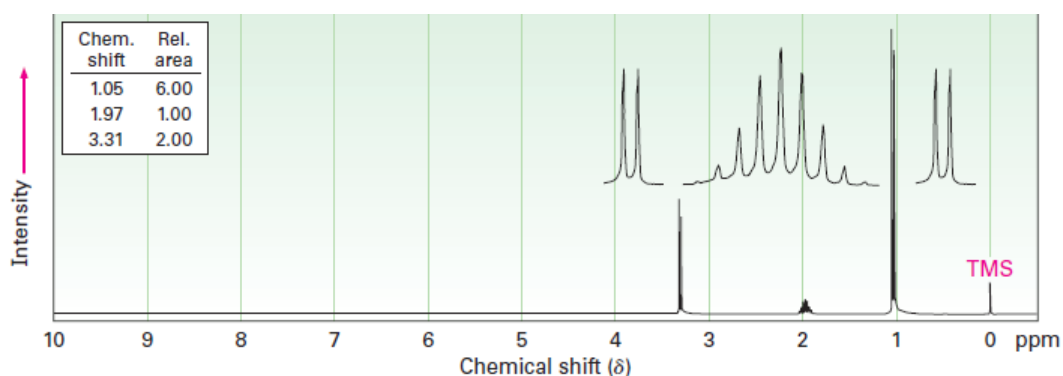
Determine compounds A and B.

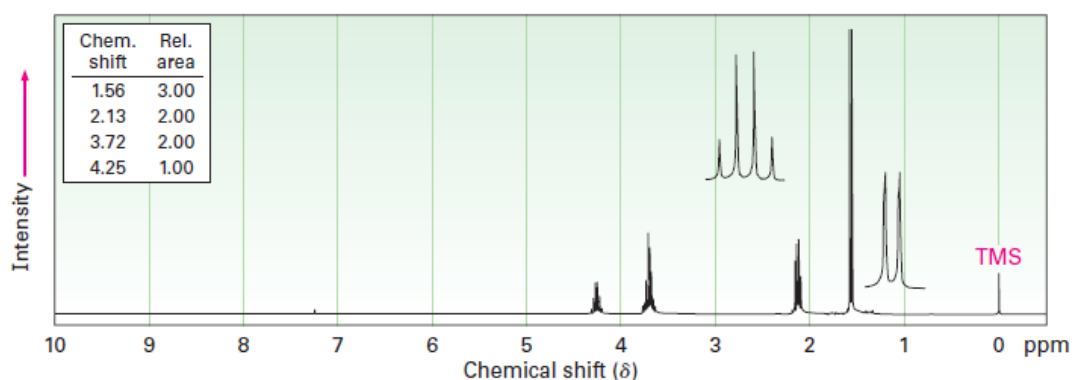
Exercise 3. An isomer of $\text{C}_5\text{H}_{12}\text{O}$ exhibits the following ^1H NMR spectrum: $\delta = 0.92$ (t, 3 H), 1.20 (s, 6 H), 1.49 (q, 2 H), 1.85 (br s, 1 H) ppm. Determine its structure.

Exercise 4. Predict the splitting pattern for each kind of hydrogen in isopropyl propanoate, $\text{CH}_3\text{CH}_2\text{CO}_2\text{CH}(\text{CH}_3)_2$.

Exercise 5. Propose structures for the two compounds whose ^1H NMR spectra are shown:

(a) $\text{C}_4\text{H}_9\text{Br}$



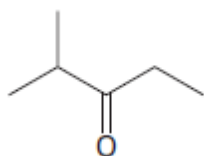
(b) $C_4H_8Cl_2$ 

Exercise 6. Predict the number of carbon resonance lines you would expect in the ^{13}C NMR spectra of the following compounds:

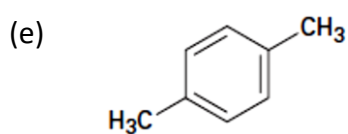
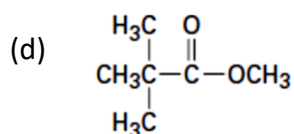
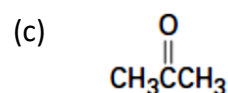
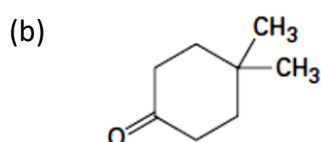
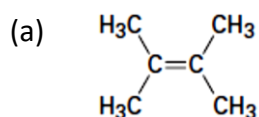
(a) 1-Methylcyclohexene

(b) 2-Methyl-2-butene

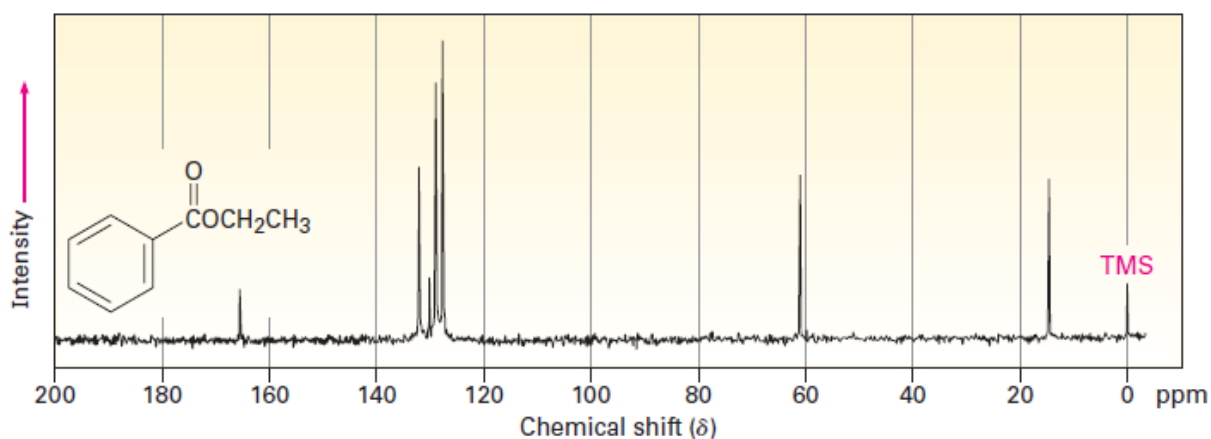
(c)



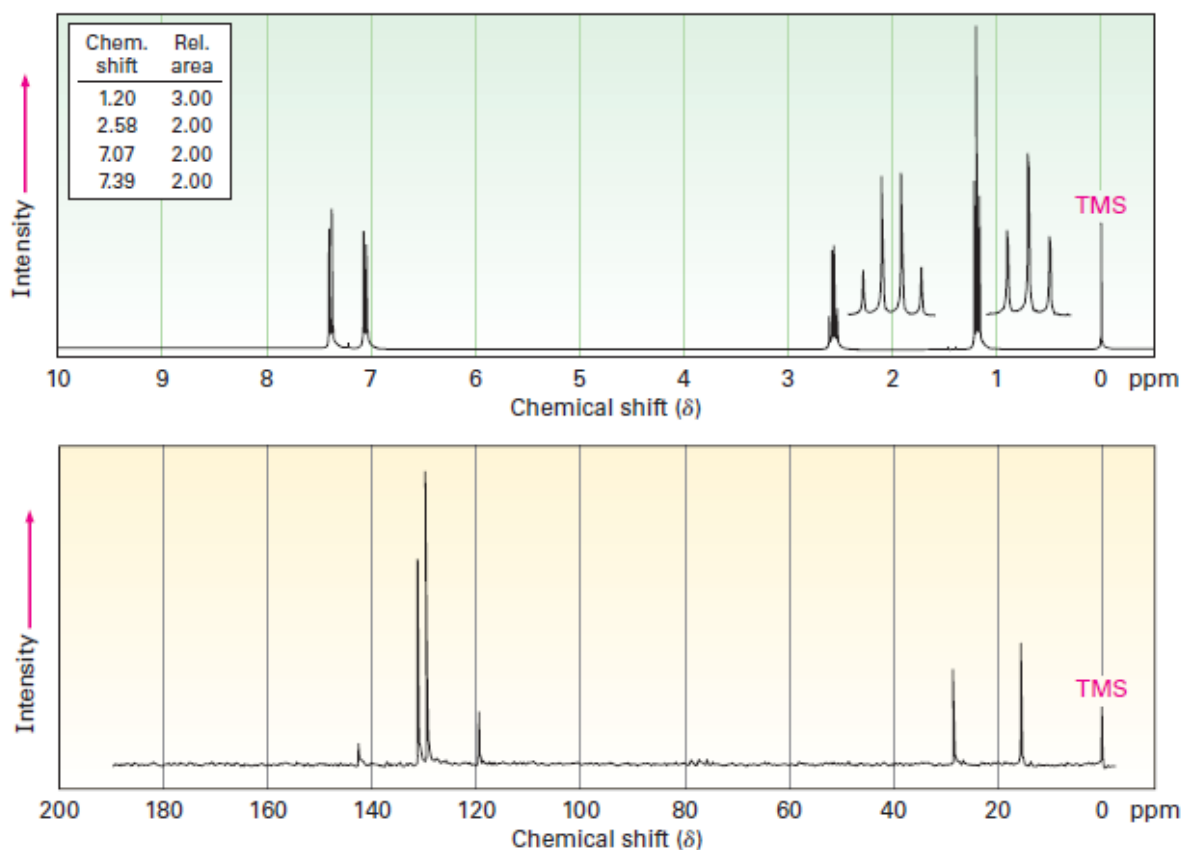
Exercise 7. How many signals would you expect each of the following molecules to have in its 1H and ^{13}C spectra?



Exercise 8. Assign as many of the resonances as you can to specific carbon atoms in the ^{13}C NMR spectrum of ethyl benzoate.



Exercise 9. The ^1H and ^{13}C NMR spectra of compound A, $\text{C}_8\text{H}_9\text{Br}$, are shown. Propose a structure for A and assign peaks in the spectra to your structure.



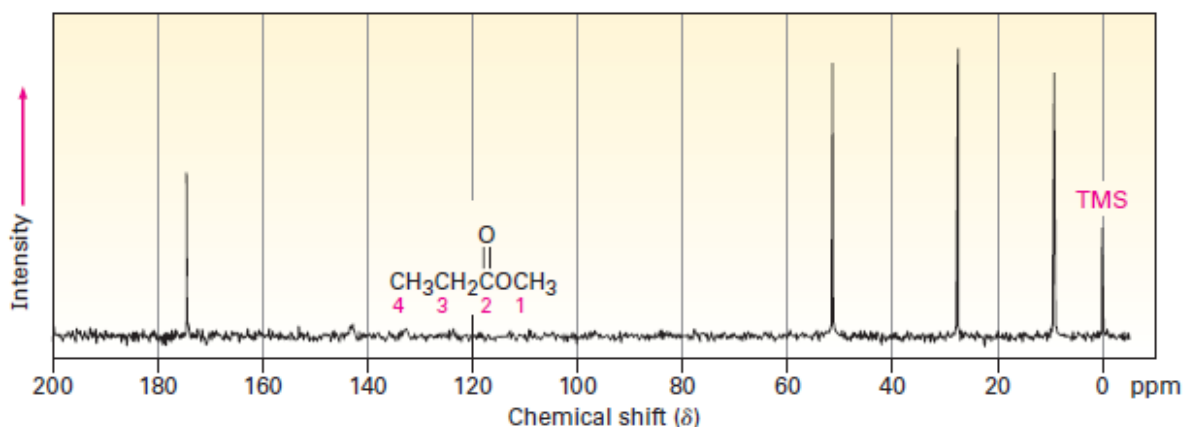
Exercise 10. Assume that you have a compound with formula $\text{C}_3\text{H}_6\text{O}$.

- How many double bonds and/or rings does your compound contain?
- Propose as many structures as you can that fit the molecular formula.
- If your compound shows an infrared absorption peak at 1715 cm^{-1} , what functional group does it have?
- If your compound shows a single ^1H NMR absorption peak at $2.1\ \delta$, what is its structure?

Exercise 11. How could you use infrared spectroscopy to distinguish between the following pairs of isomers?

- (a) $\text{HC}\equiv\text{CCH}_2\text{NH}_2$ and $\text{CH}_3\text{CH}_2\text{C}\equiv\text{N}$
 (b) CH_3COCH_3 and $\text{CH}_3\text{CH}_2\text{CHO}$

Exercise 12. Assign the resonances in the ^{13}C NMR spectrum of methyl propanoate, $\text{CH}_3\text{CH}_2\text{CO}_2\text{CH}_3$.



Exercise 13. Two compounds of molecular formula $\text{C}_2\text{H}_6\text{O}$ show large intensity IR peaks at 2870 and 1150 cm^{-1} for the first isomer, and at 3400, 2950, and 1090 cm^{-1} for the second. What are their structures?

Exercise 14. How would you use infrared spectroscopy to distinguish between the following pairs of constitutional isomers?

- (a) but-2-yne and but-1-yne; (b) pent-3-en-2-one and pent-4-en-2-one; (c) methoxyethene and propanal.

Exercise 15. Assume that you are carrying out the dehydration of 1-methylcyclohexanol to yields 1-methylcyclohexene. How could you use infrared spectroscopy to determine when the reaction is complete?

Exercise 16. The figure shows the IR spectrum of a compound with the formula $\text{C}_8\text{H}_8\text{O}$. What functional groups does the compound contain?

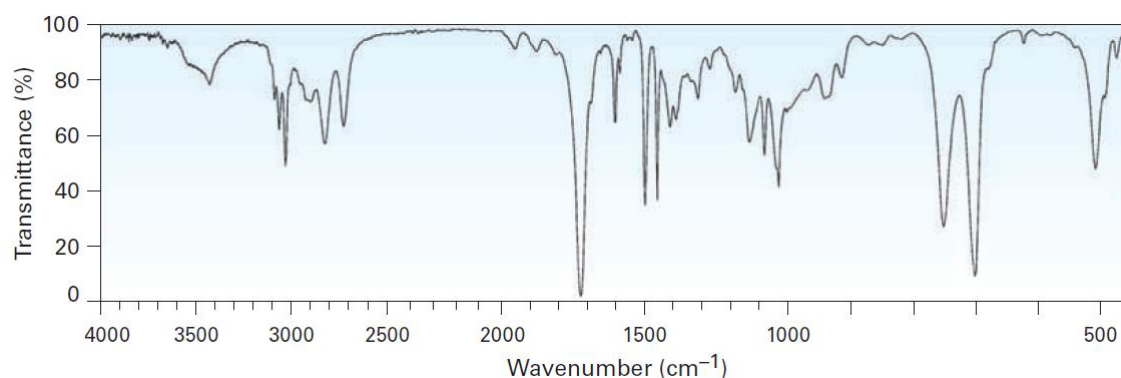


IMAGE CREDITS

- Images of exercises 5, 7-9, 12, and 16: Organic Chemistry. A tenth Edition. John McMurry, Cornell University (Emeritus), CC BY-SA 4.0, <https://openstax.org/details/books/organic-chemistry>.
- Images of exercises 1 and 6 were made by authors.