5.11: Proton NMR problems

Objectives

- Solve unknown problems using ^{1}H NMR spectra and molecular formula.

Note

Helpful resources for solving these types of problems:

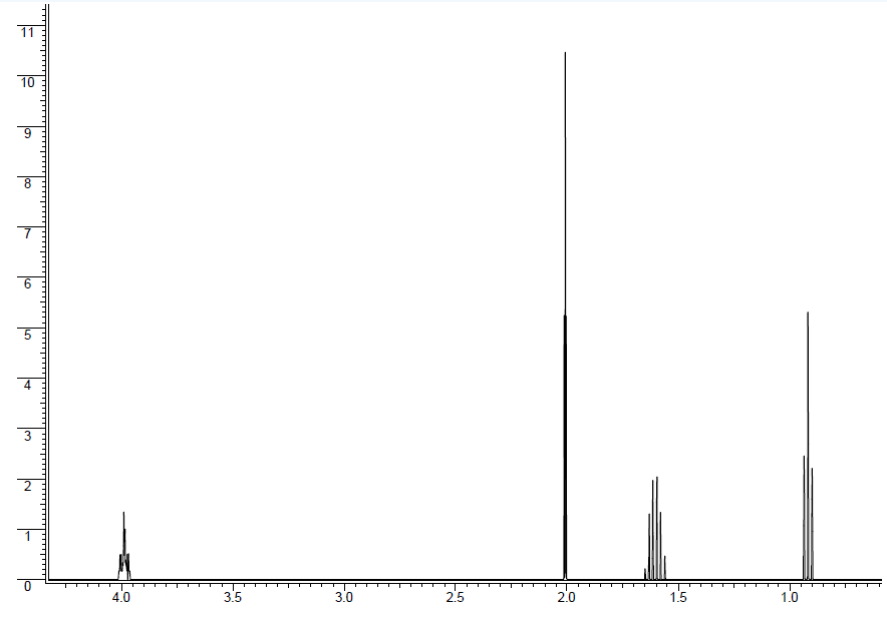
1. Degree of Unsaturation Equation
2. Chemical Shift Data Table
3. Coupling Constant Data Table
4. IR Data Table

You may also want to read through some worked problems on how to solve unknown structure determination problems (Section 5.10).

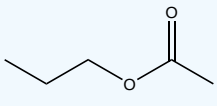
Exercise 5.11.1

Determine the structure for the unknown molecule with the molecular formula of $C_5H_{10}O_2$.

^{1}H NMR: The ratio of protons is 2:3:2:3. J = 7 Hz for all coupling.



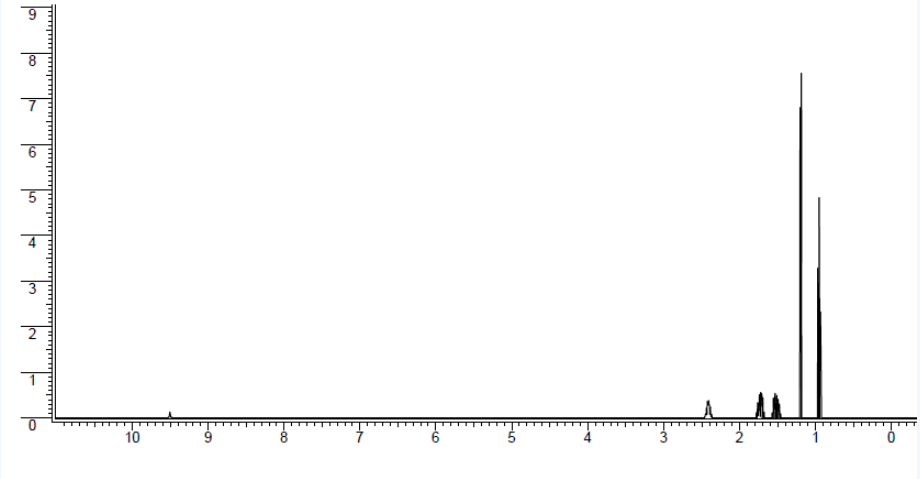
Answer



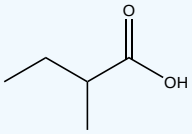
Exercise 5.11.2

Determine the structure for the unknown molecule with the molecular formula of $C_5H_{10}O_2$.

^{1}H NMR: The ratio of protons is 1:1:1:1:3:3. The peak at 9.5 ppm is a singlet. The peak at 2.41 ppm is sextet (J = 7 Hz). The peak at 1.72 ppm is a multiplet (J = 7Hz, 25 Hz). The peak at 1.53 ppm is a multiplet (J = 7 Hz, 25 Hz). The peak at 1.20ppm is a doublet (J = 7 Hz). The peak at 0.95 ppm is a triplet (J = 7 Hz).



Answer

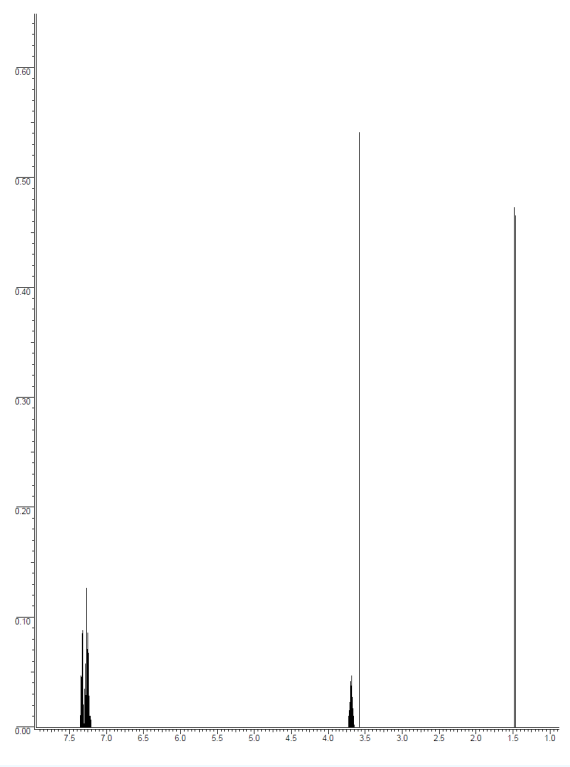


Note: The -CH_2- protons are diastereotopic, so they show up differently in ^{1}H NMR spectra.

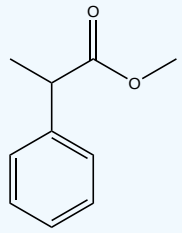
Exercise 5.11.3

Determine the structure for the unknown molecule with the molecular formula of $C_{10}H12O_2$.

^{1}H NMR: The ratio of protons is 5:1:3:3. The peak at 7.5 ppm is a multiplet. The peak at 3.70 ppm is quartet (J = 7 Hz). The peak at 3.58 ppm is a singlet. The peak at 1.48 ppm is a doublet (J = 7 Hz).



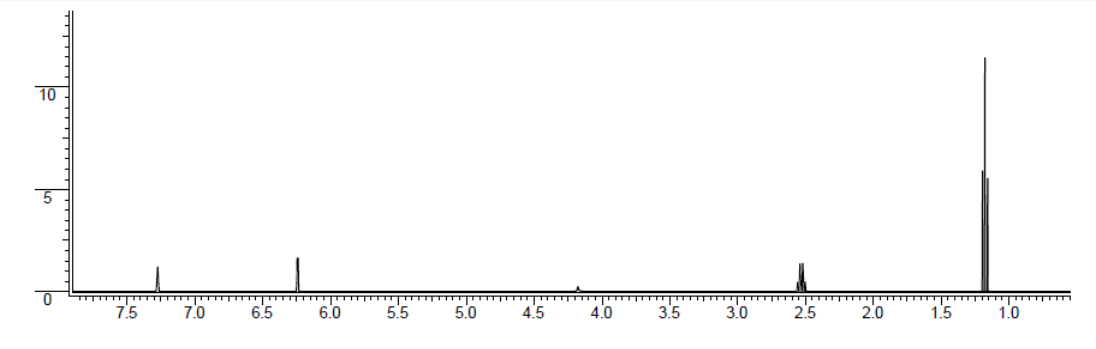
Answer



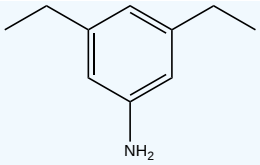
Exercise 5.11.4

Determine the structure for the unknown molecule with the molecular formula of $C_{10}H_{15}N$.

^1H NMR: The ratio of protons is 1:2:2:4:6. The peak at 7.3 ppm is a triplet (J = 2Hz) and the peak at 6.24 ppm is a doublet (J = 2 Hz).



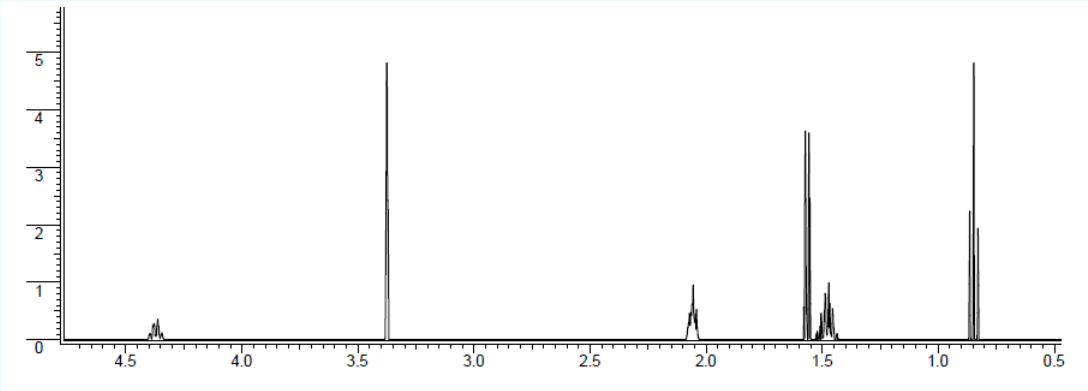
Answer



Exercise 5.11.5

Determine the structure for the unknown molecule with the molecular formula of $C_7H_{14}O$.

^{1}H NMR: The ratio of protons is 1:3:2:3:2:3. The peak at 4.36 ppm is a triplet of quartets (J = 17 Hz and 7Hz). The peak at 3.37 ppm is a singlet. The peak at 2.04 ppm is a doublet of triplets (J = 17 Hz and 7Hz). The peak at 1.56 ppm is a doublet (J = 7 Hz). The peak at 1.48 ppm is a sextet (J = 7 Hz). The peak at 0.85 ppm is a triplet (J = 7 Hz).



Answer