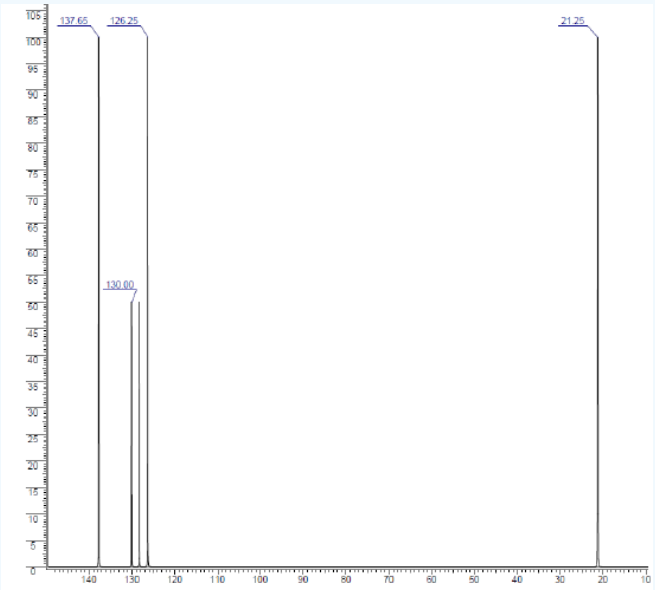
6.7: Structure Determination Problems with C-13 NMR and 1-H NMR

Learning Objectives

- Solve unknown problems using ^{13}C and ^{1}H NMR spectra and molecular formula.

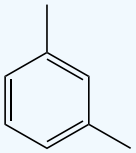
Exercise 6.7.1

Which isomer of ortho, meta, or para xylene do you have based on the ^{13}C NMR spectrum?



Answer

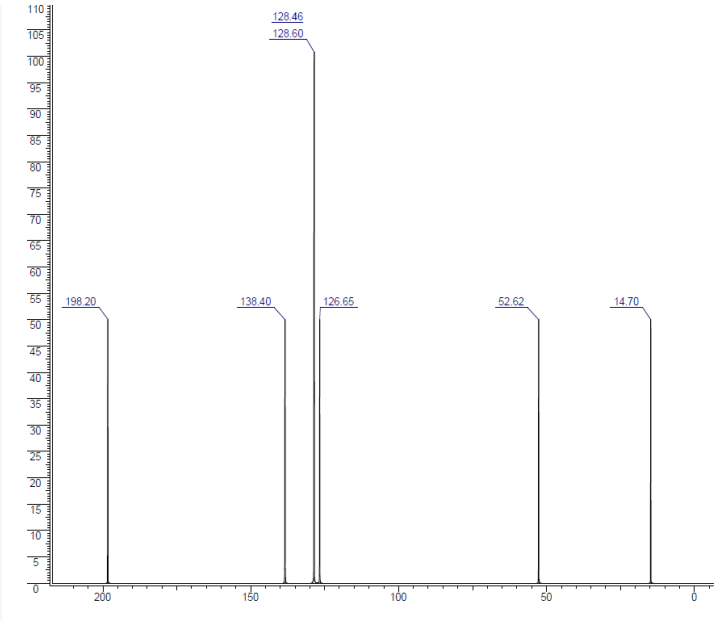
There are 5 different carbons in the spectrum with four different aromatic carbons. *p*-Xylene would have 2 types of aromatic carbons and *o*-xylene would have 3 types. *m*-Xylene is the only one with 4 different types of aromatic carbons, which fits this spectrum. The methyl groups would all be similary, so not a point of difference.



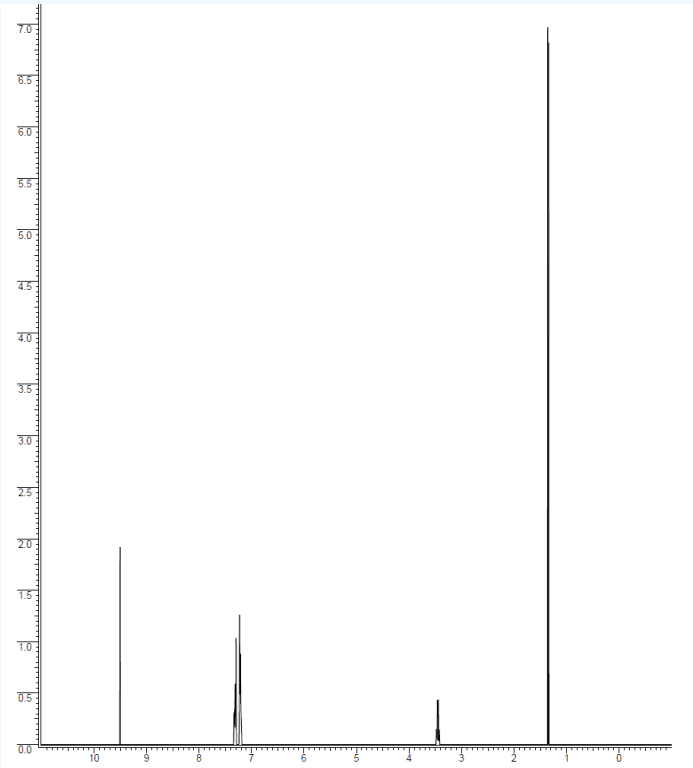
Exercise 6.7.2

Propose a structure using the spectral data below for $C_9H_{10}O$.

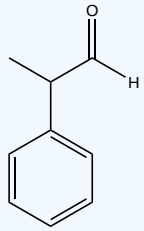
^{13}C broadband decoupled spectrum:



^{1}H NMR spectrum: Integration: 1 (doublet; J = 1 Hz):5 (multiplet):1 (quartet of doublets;J = 7 Hz and 1 Hz):3 (doublet; J = 7 Hz)



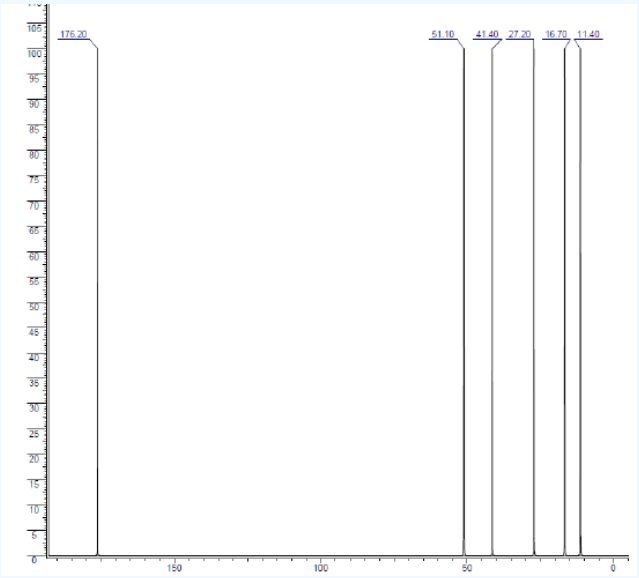
Answer



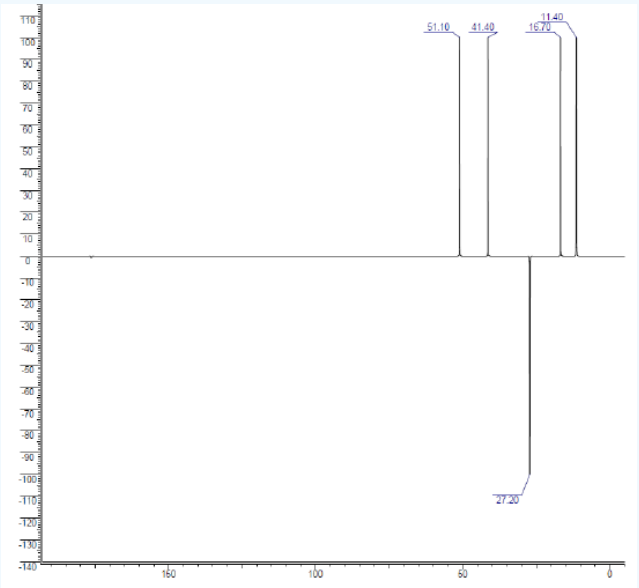
Exercise 6.7.3

Propose a structure using the spectral data below for $C_6H_{12}O_2$.

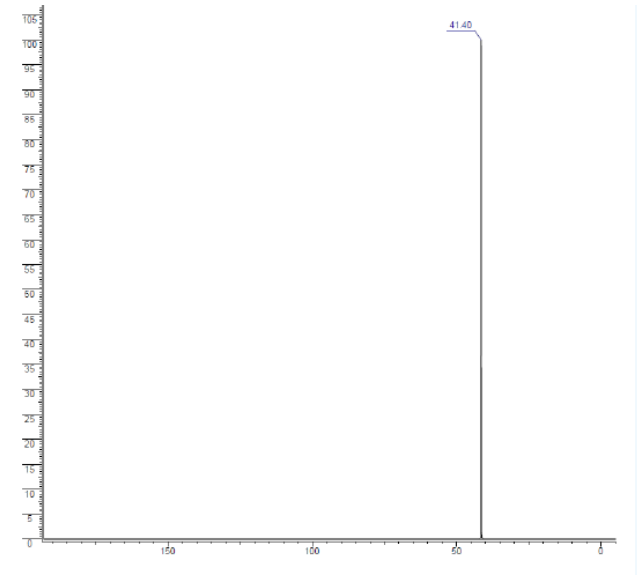
^{13}C broadband decoupled spectrum:



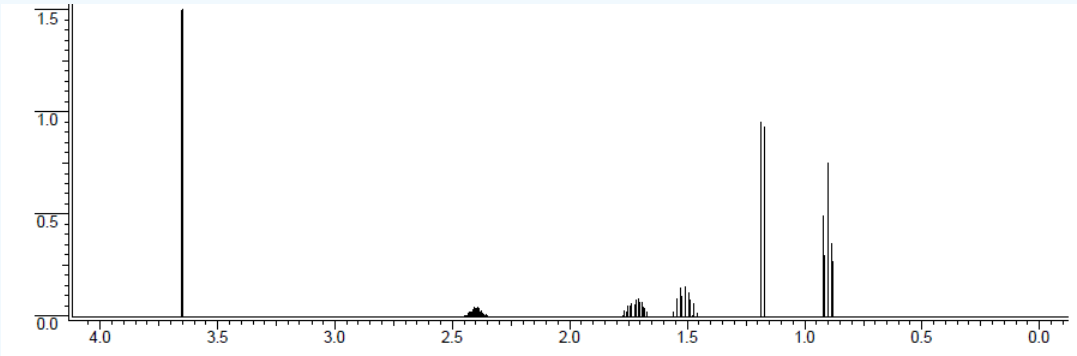
DEPT-135:



DEPT-90:



^{1}H NMR spectrum: Integration: 3 (singlet):1 (sextet; J = 8 Hz):1 (multiplet;J = 25 Hz and 8 Hz):1(multiplet; J = 25 Hz and 8 Hz):3 (doublet; J = 8 Hz):3 (triplet; J = 8 Hz)



Answer

Structure: