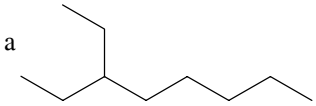
a

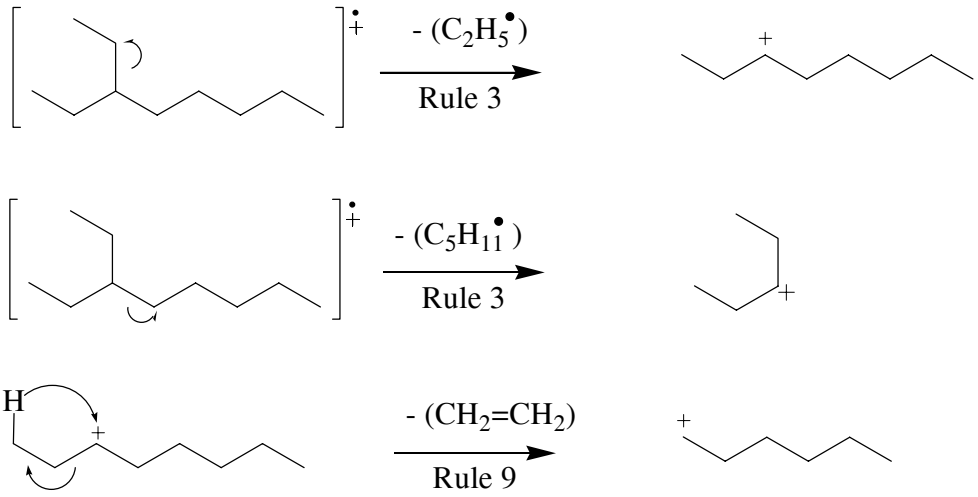


3-ethyloctane
$C_{10}H_{22}$

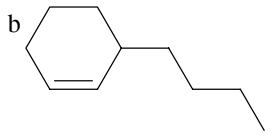
$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 0

| Atom Type | # of Atoms | Mass | Total Mass |
|---|---|---|---|
| Hydrogen | 22 | 1.00783 | 22.17226 |
| Carbon | 10 | 12.00000 | 120.00000 |
| Nitrogen | 0 | 14.0031 | 0.00000 |
| Oxygen | 0 | 15.9949 | 0.00000 |
| Sulfur | 0 | 31.9721 | 0.00000 |
| Bromine | 0 | 78.9183 | 0.00000 |
| | | Exact Mass | 142.17226 |




b

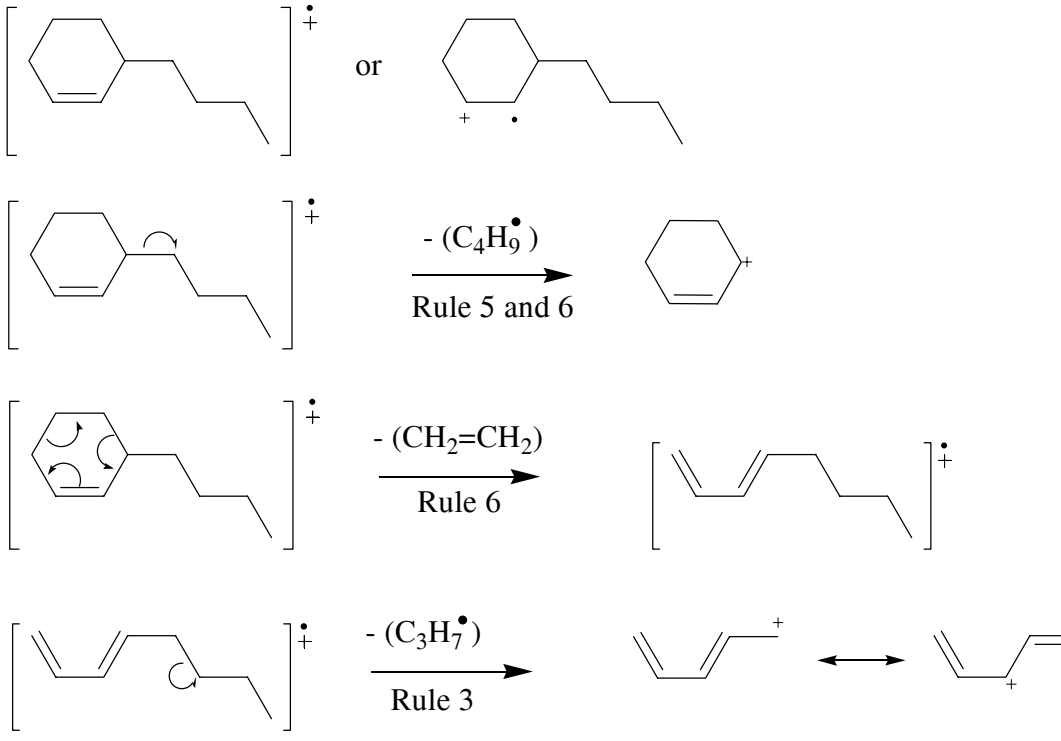


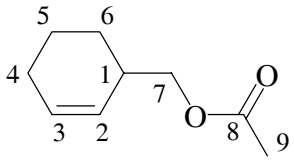
3-butylcyclohex-1-ene
$C_{10}H_{18}$

$C_nH_mX_xN_yO_z$ IHD

Index = (n) - (m/2) - (x/2) + (y/2) + 1 = 2

| Atom Type | # of Atoms | Mass | Total Mass |
|---|---|---|---|
| Hydrogen | 18 | 1.00783 | 18.14094 |
| Carbon | 10 | 12.00000 | 120.00000 |
| Nitrogen | 0 | 14.0031 | 0.00000 |
| Oxygen | 0 | 15.9949 | 0.00000 |
| Sulfur | 0 | 31.9721 | 0.00000 |
| Bromine | 0 | 78.9183 | 0.00000 |
| | | Exact Mass | 138.14094 |






(b) (cyclohex-2-enyl)methyl acetate

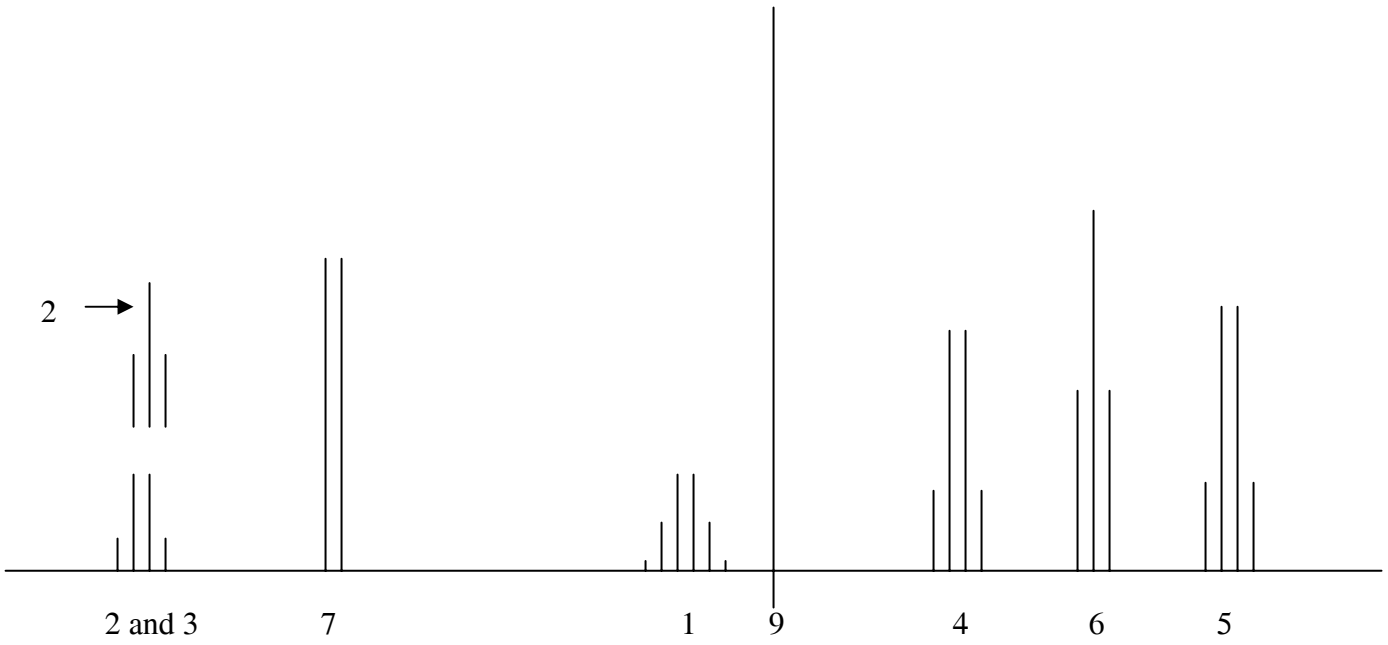
3.1 (b) 1,2,3,4,5,6,7 are one spin system, and 9 is the second. 4,4' ; 5,5' ; 6,6'and 7,7' are diastereotopic.

3.2 (b)

| Spin | Appr. δ | Table or Calculation | Coupled with | Multiplet (n+1) | Integration |
|---|---|---|---|---|---|
| 1 | δ 2.80 | Appendix A, Chart A.2 | 6,2,7 | Sextet* | 1 |
| 2 | δ 5.59 | Appendix D, Chart D2 | 3,1 | Triplet* | 1 |
| 3 | δ 5.59 | Appendix D, Chart D2 | | Quartet* | 1 |
| 4 | δ 1.96 | Appendix D, Chart D2 | | Quartet** | 2 |
| 5 | δ 1.65 | Appendix D, Chart D2 | 4,6 | Quartet** | 2 |
| 6 | δ 1.80 | Appendix A, Chart A.2 | 1,5 | Triplet** | 2 |
| 7 | δ 4.05 | Appendix A, Chart A.2 | 1 | Doublet** | 2 |
| 9 | δ 2.10 | Appendix A, Chart A.1 | none | Singlet | 3 |

* Coupling constants may not be the same, but make the assumption that they are.
**These are diastereotopic, and are coupled to diastereotopic protons, they would not be first order. We will assume they are first order for the drawn spectrum.

3.3 (b)



Spin System $ab_2c_3$

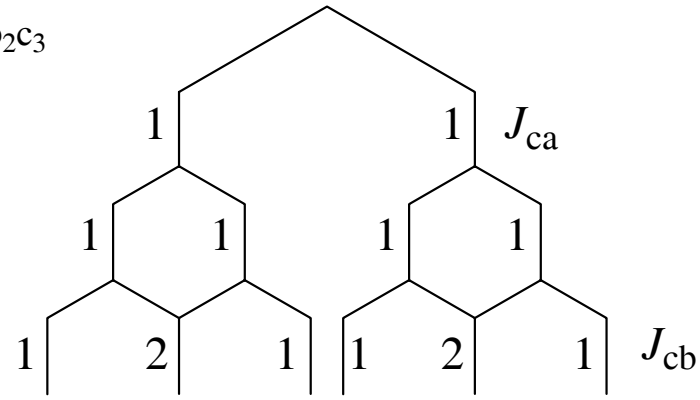
Coupling

a-b 6 Hz

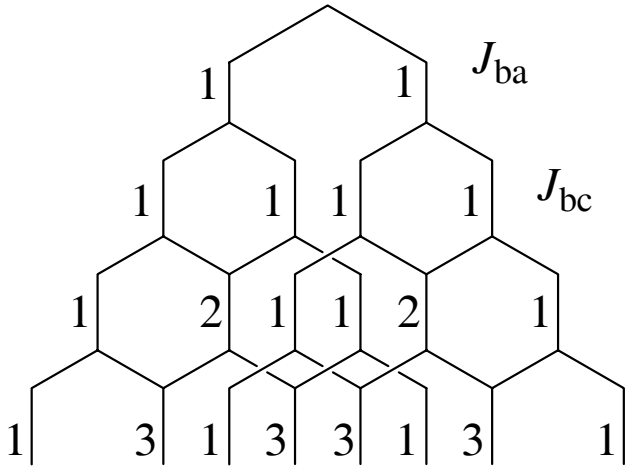
b-c 4Hz

a-c 9 Hz

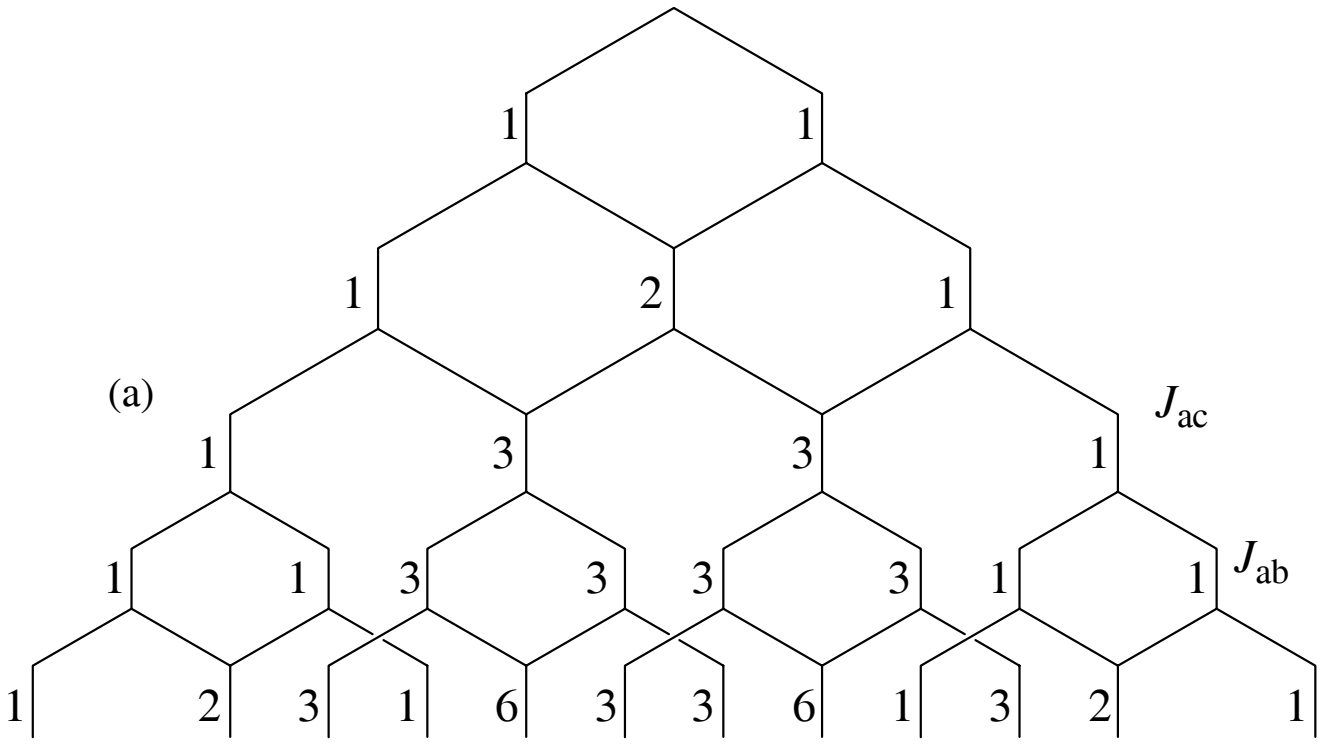
(c)



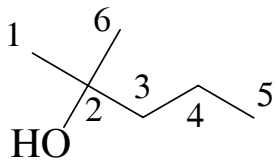

(b)




(a)

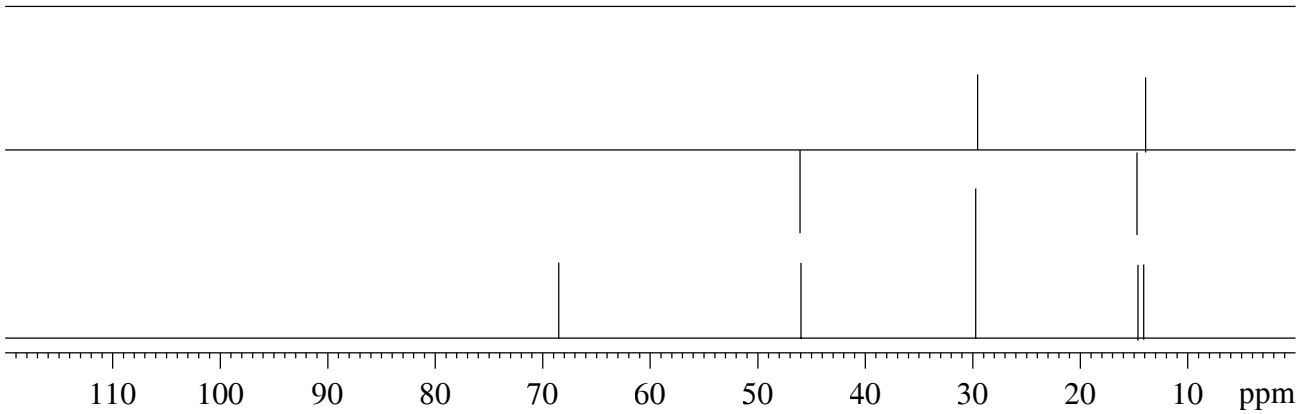


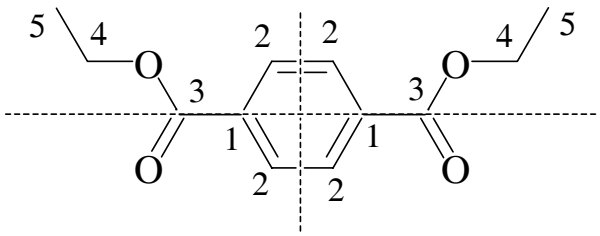
Answers for Student Exercise 4.2-3 (i)




(i) 2-methylpentan-2-ol

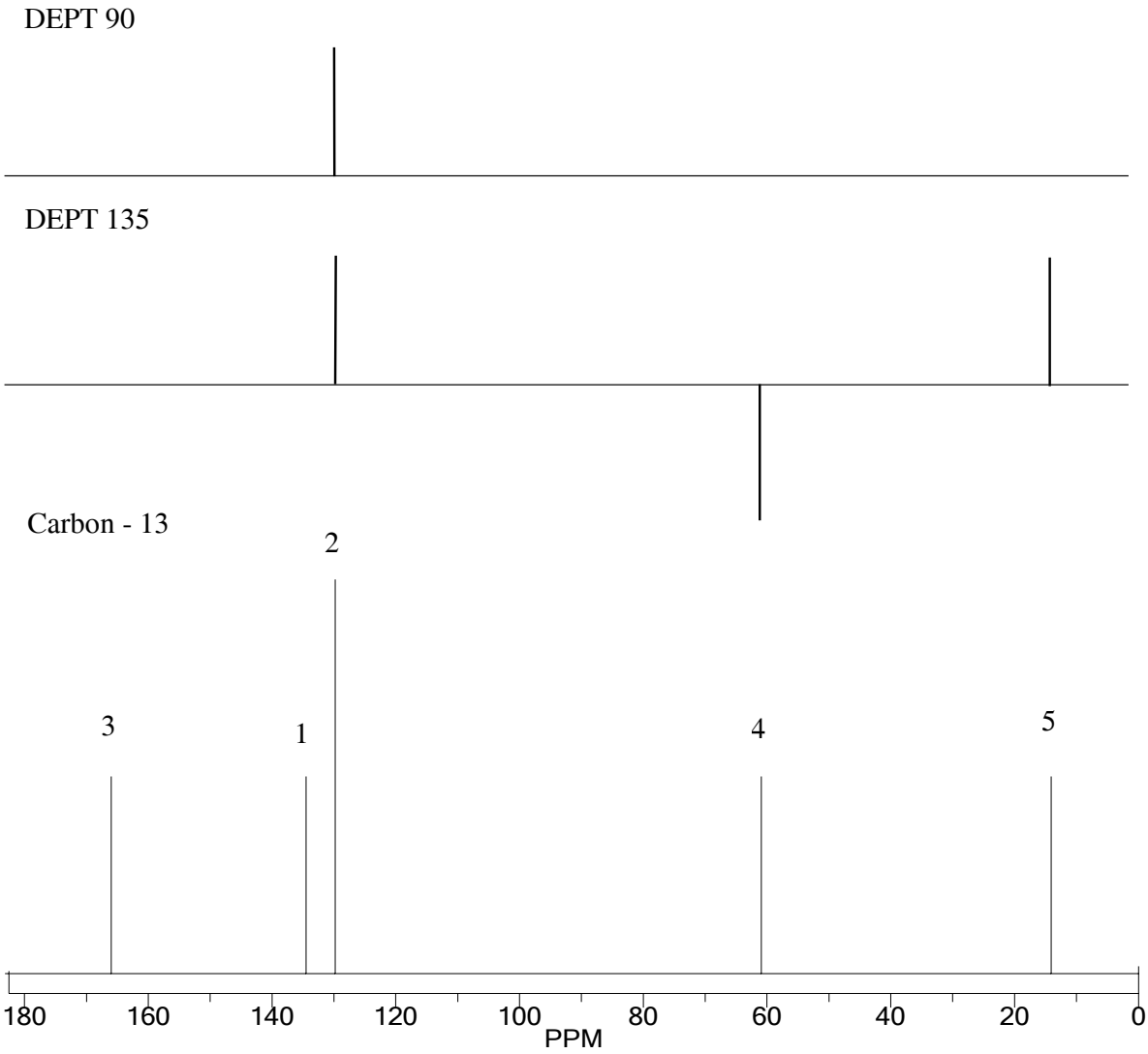
| Atom | Base | α | β | γ | δ | ε | Other | Calc Shift | Comments |
|---|---|---|---|---|---|---|---|---|---|
| C1 | methane | 2 | 6,3,OH | 4 | 5 | | 1°(4°) | | The base and shifts |
| | -2.5 | 9.1 | 2(9.4)+10 | -2.5 | 0.3 | | -3.4 | | are from Table 4.4 |
| | -2.5 | 9.1 | 28.8 | -2.5 | 0.3 | | -3.4 | 29.8 | Increments from table 4.6 |
| C2 | methane | 1,6,3,OH | 4 | 5 | | | 4°(2(1°)+2°) | | See Table 4.14 for |
| | -2.5 | 3(9.1)+48 | 9.4 | -2.5 | | | (2)(-1.5)+-8.4 | | comparison |
| | -2.5 | 75.3 | 9.4 | -2.5 | | | -11.4 | 68.3 | |
| C3 | methane | 2,4 | 1,6,OH,5 | | | | 2°(4°) | | |
| | -2.5 | 9.1(2) | 3(9.4)+10 | | | | -7.2 | | |
| | -2.5 | 18.2 | 38.2 | | | | -7.2 | 46.7 | |
| C4 | methane | 3,5 | 2 | 1,6,OH | | | | | |
| | -2.5 | 2(9.1) | 9.4 | 2(-2.5)+(-5) | | | | | |
| | -2.5 | 18.2 | 9.4 | -10 | | | | 15.1 | |
| C5 | methane | 4 | 3 | 2 | 1,6 | | | | |
| | -2.5 | 9.1 | 9.4 | -2.5 | (2).3 | | | | |
| | -2.5 | 9.1 | 9.4 | -2.5 | 0.6 | | | 14.1 | |
| C6 | methane | 2 | 6,3,OH | 4 | 5 | | 1°(4°) | | |
| | -2.5 | 9.1 | 2(9.4)+10 | -2.5 | 0.3 | | -3.4 | | |
| | -2.5 | 9.1 | 28.8 | -2.5 | 0.3 | | -3.4 | 29.8 | |



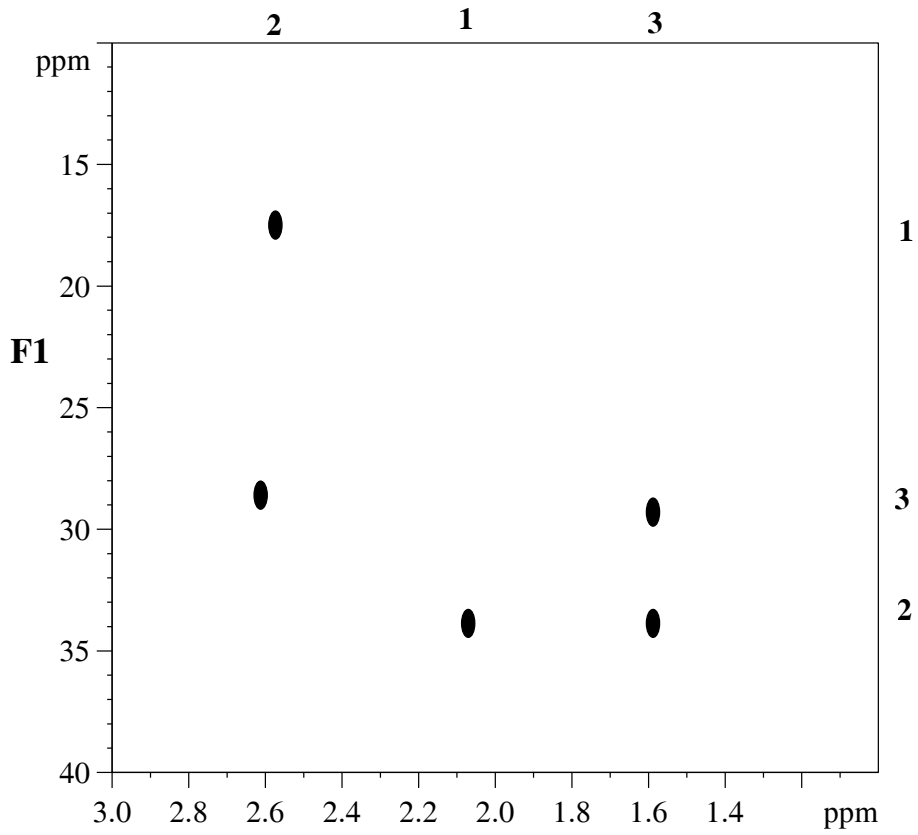



*para*-diethyl phthalate

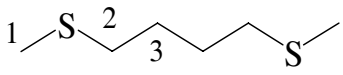
There are two mirror images. There are 5 nonequivalent carbons, and there are 3 distinct proton signals, 2,4,5 with a integration ratio of 4:4:6, or 1:1:3.



**HMBC**

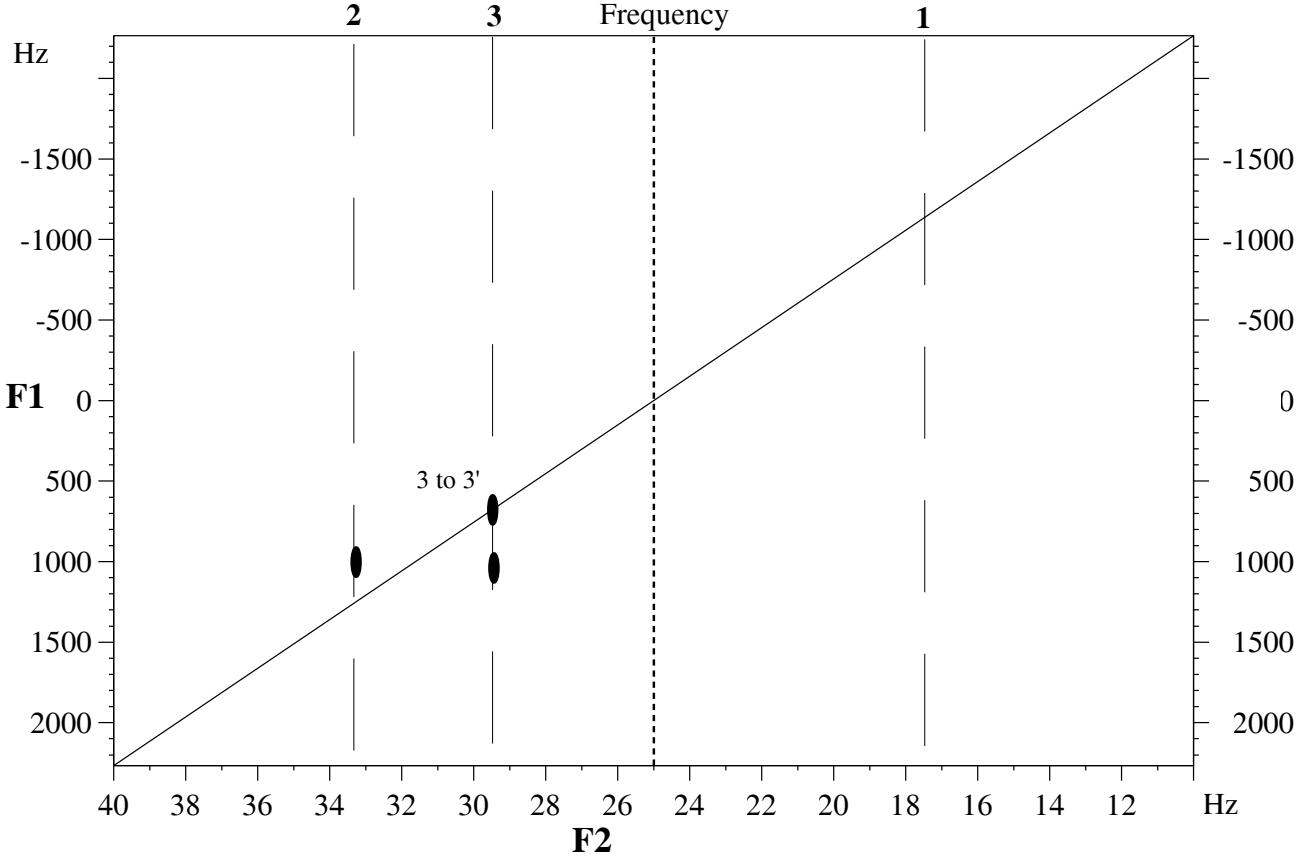



**(j)**

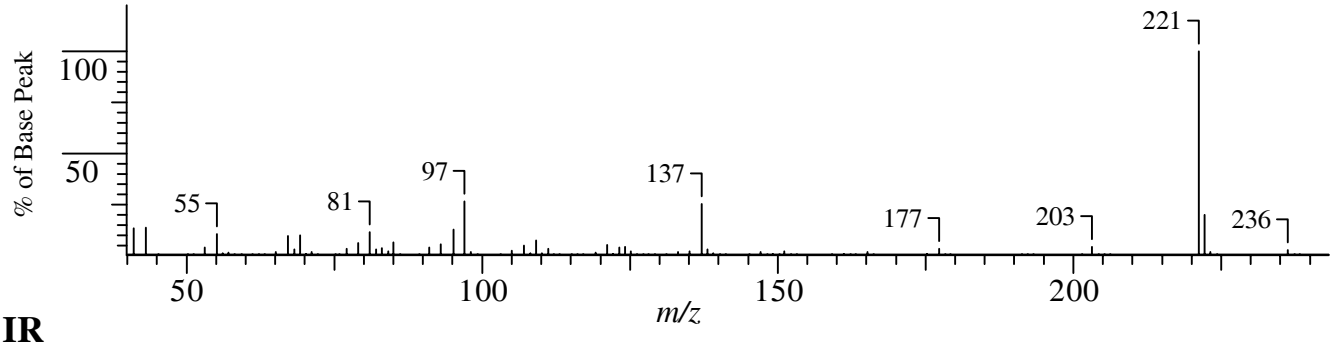



| Group # | δH | δC |
|---|---|---|
| 1 | 2.10 | 17.5 |
| 2 | 2.60 | 33.5 |
| 3 | 1.60 | 29.6 |

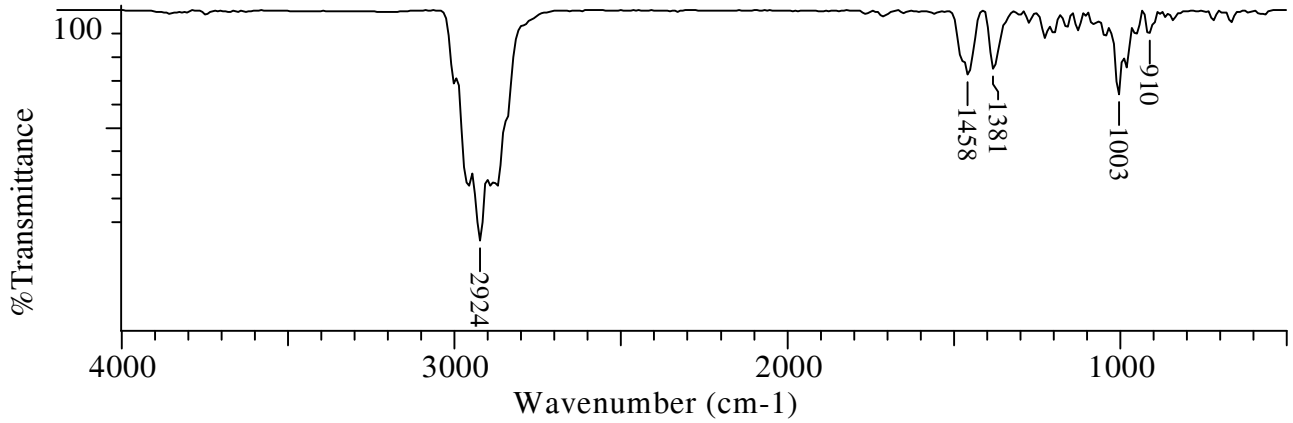
**INADEQUATE**



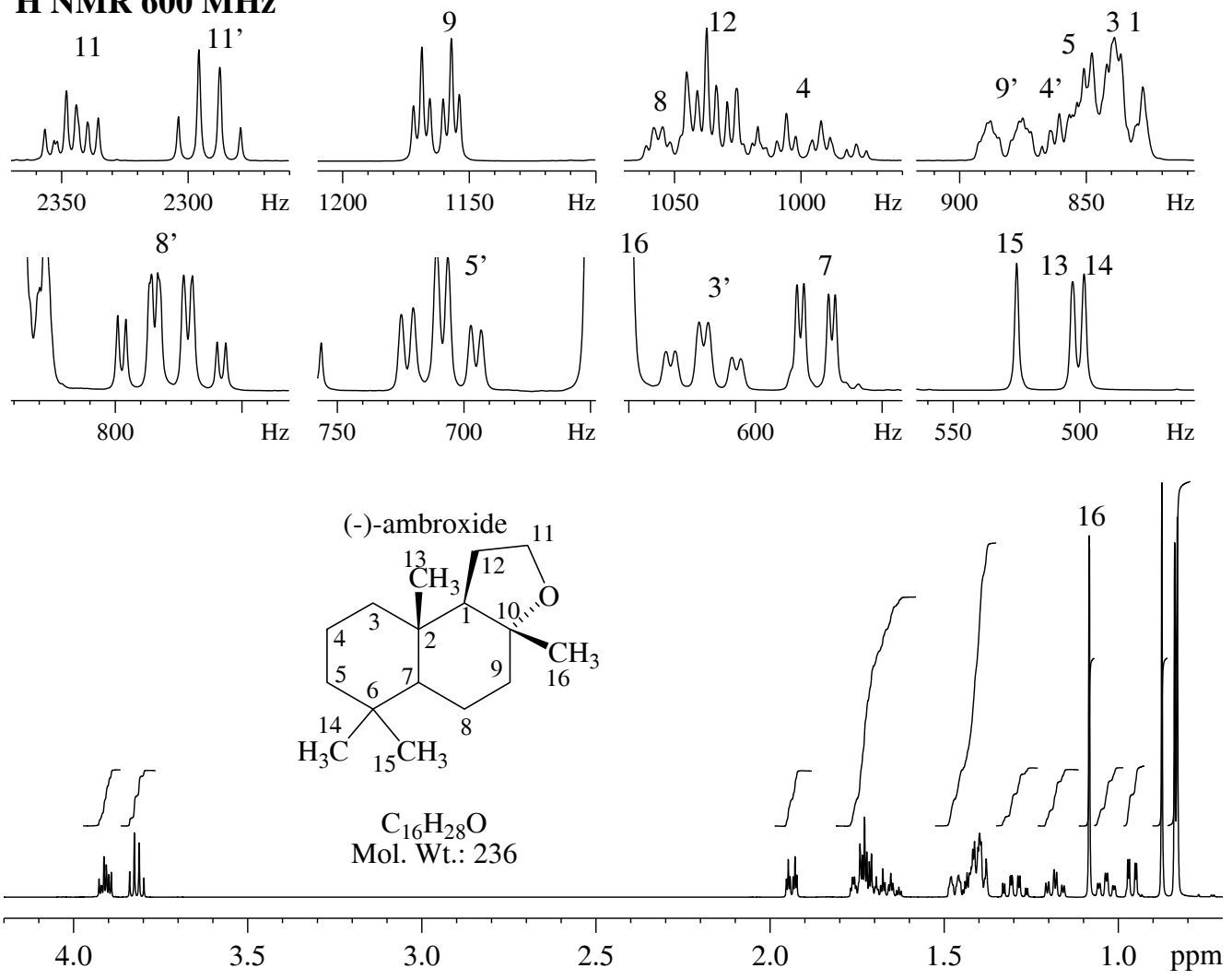
**MASS**




**IR**

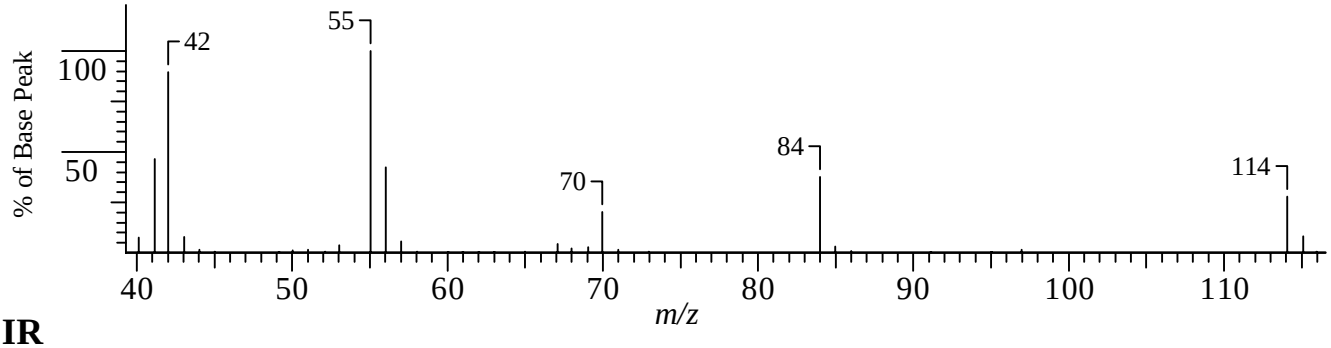



**$^1$H NMR 600 MHz**

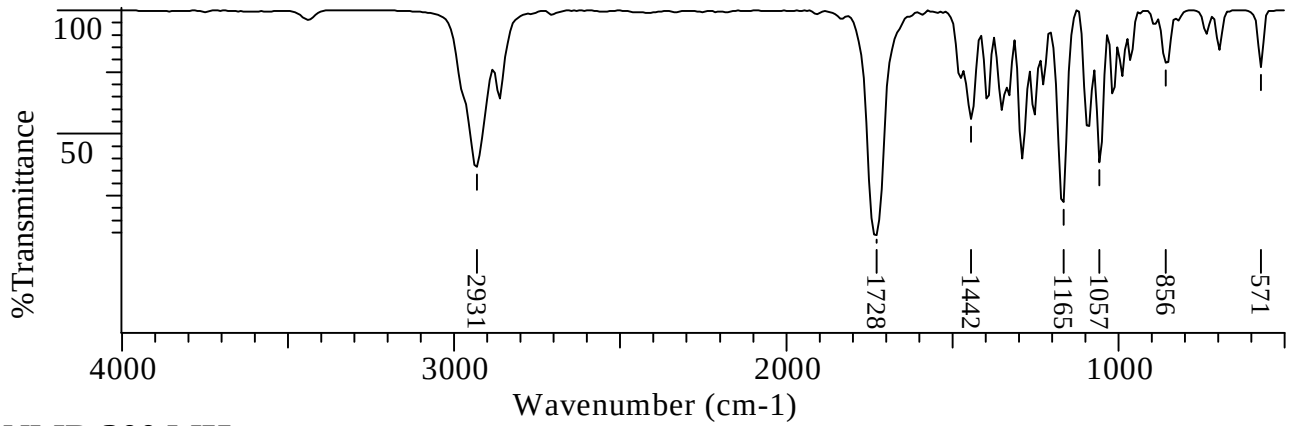


Problem 8.27A

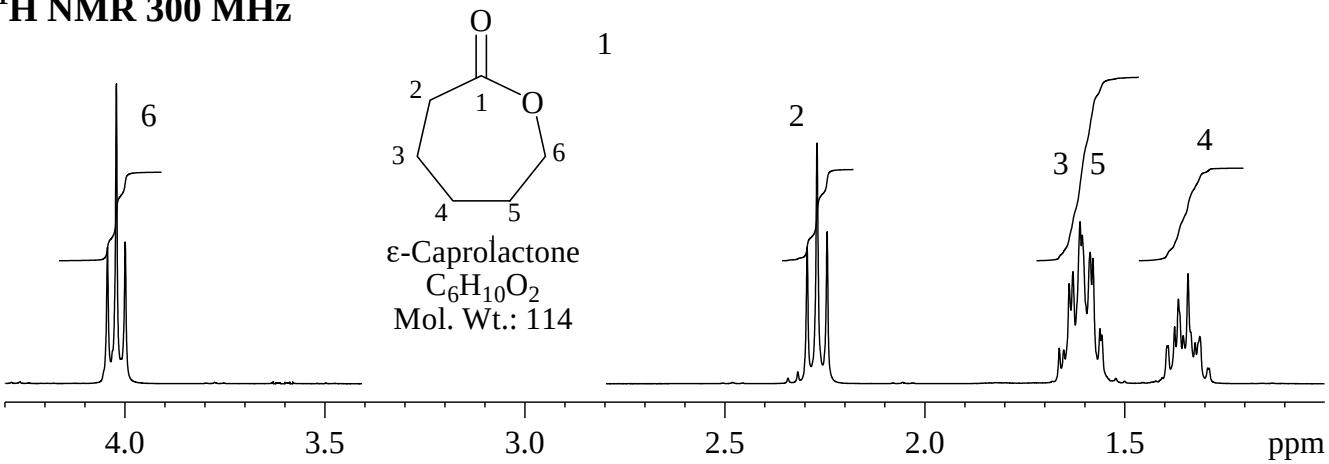
**MASS**



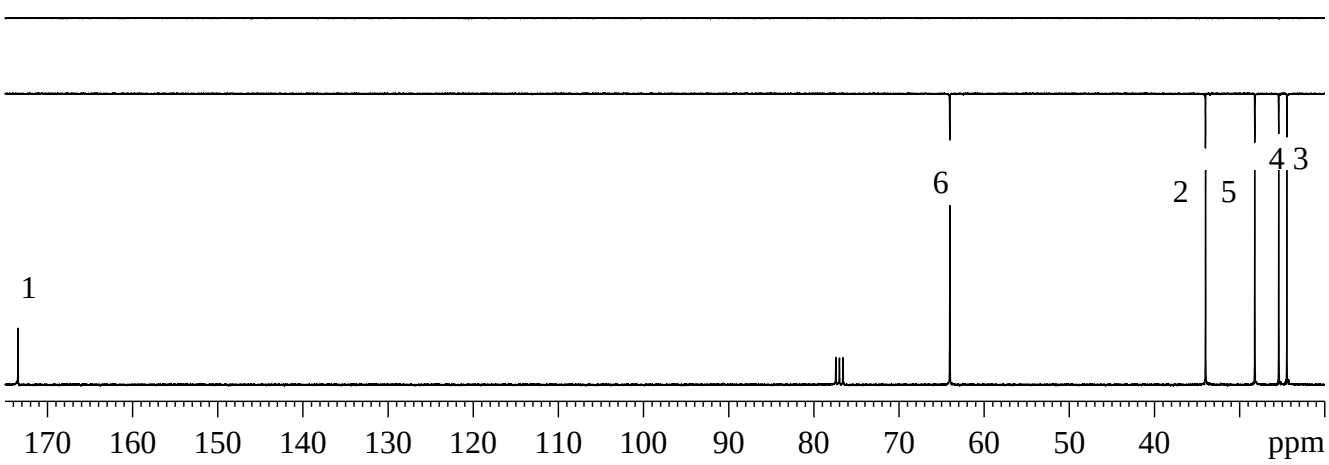

**IR**




**$^{1}$H NMR 300 MHz**




**$^{13}$C/DEPT NMR 75.5 MHz**



Problem 8.44B