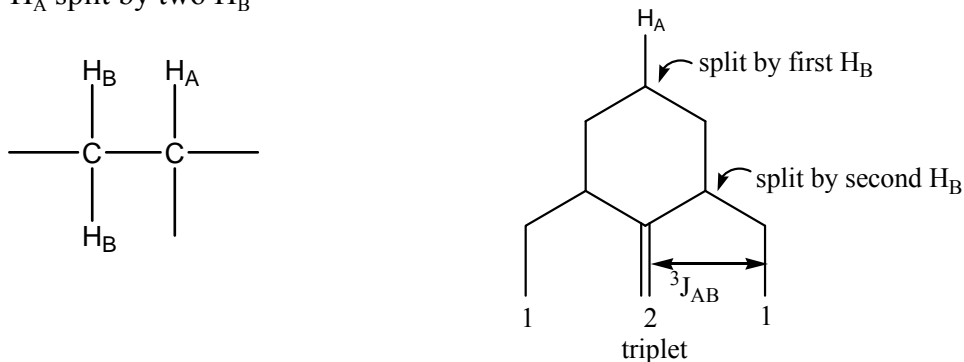


T4a Practice problems (Refer to pages C30-C34 in the online manual)

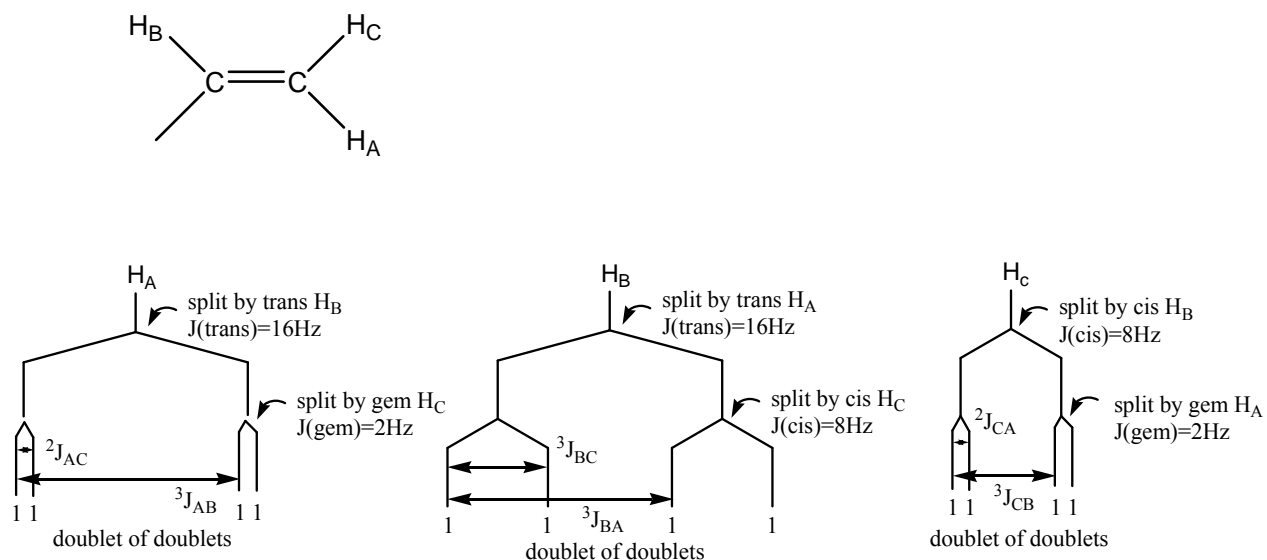
T4a Practice problems

1. Draw the tree diagrams for the following examples. Use the $2nI + 1$ rule and draw trees to show both # of lines *and* relative intensities. Determine where to measure coupling constants (J values) and the notation for the coupling constants.

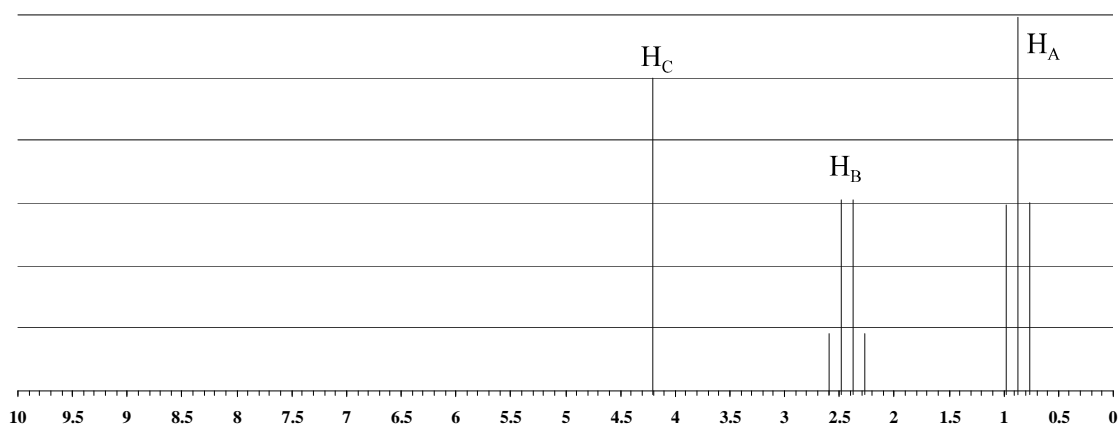
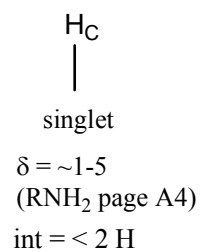
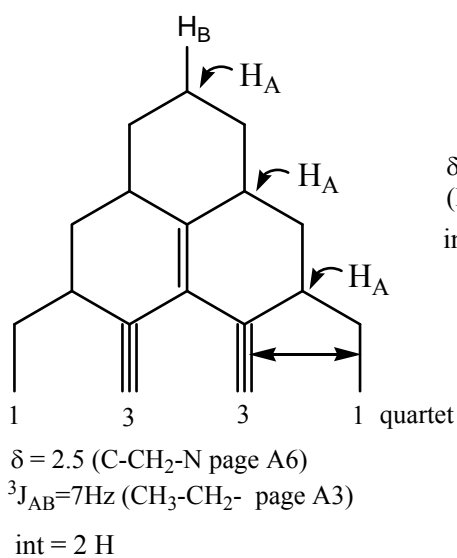
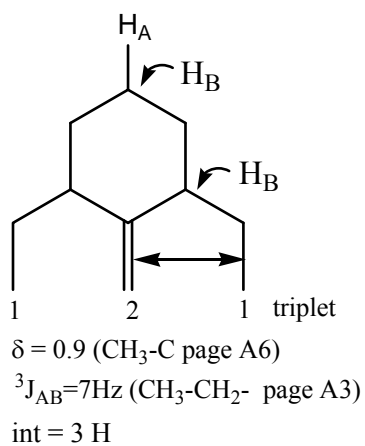
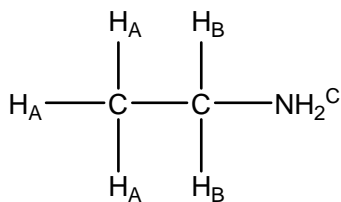
- a) H_A split by two H_B



- b) H_A , H_B and H_C , where $J_{HH(\text{trans})} = 16 \text{ Hz}$, $J_{HH(\text{cis})} = 8 \text{ Hz}$, $J_{HH(\text{gem})} = 2 \text{ Hz}$

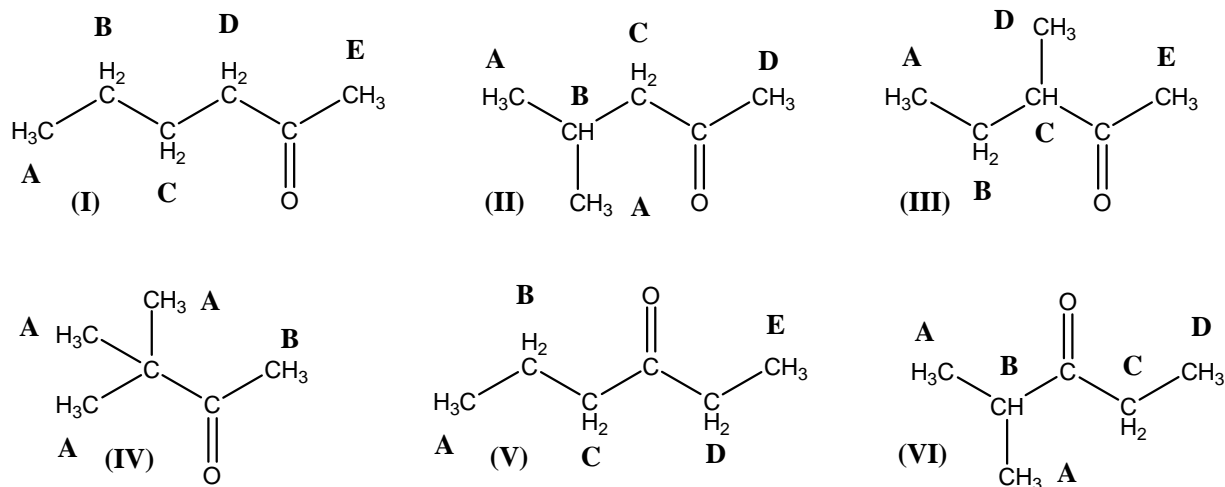


2. Predict the ^1H nmr spectrum of ethylamine, $\text{CH}_3\text{CH}_2\text{NH}_2$, by drawing tree diagrams and using the yellow data sheets to predict the chemical shift and coupling constants.



*note: predicted spectrum is not to scale

3. Match the ketone isomer of $C_6H_{12}O$ to the 1H nmr pattern. Label the protons on the molecule and assign each signal using those letters to complete the table. Use the yellow data sheets (page A6) to predict the chemical shifts for the last molecule in the table to see how well these values agree with the actual results.

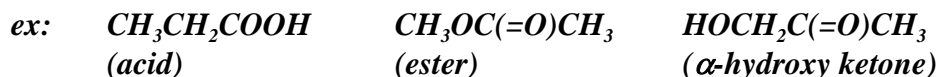


| Molecule | 1H signals | | | | | |
|------------|---|--|--|--|---|--|
| V | actual δ (ppm) | 0.9 t | 1.1 t | 1.6 sextet | 2.3 q | 2.4 t |
| | assignment | A | E | B | D | C |
| II | actual δ (ppm) | 0.9 d | 2.2 nonet | 2.2 s | 2.3 d | - |
| | assignment | A | B | D | C | |
| III | actual δ (ppm) | 0.9 t | 1.1 d | 1.7 pentet | 2.1 s | 2.4 sextet |
| | assignment | A | D | B | E | C |
| IV | actual δ | 1.1 s | 2.2 s | - | - | - |
| | assignment | A | B | | | |
| VI | actual δ (ppm) | 1.1 t | 1.2 d | 2.5 q | 2.6 septet | - |
| | assignment | D | A | C | B | |
| I | actual δ (ppm) | 0.9 t | 1.4 sextet | 1.6 pentet | 2.1 s | 2.4 t |
| | predicted δ (ppm) <i>page A6 data</i> | 0.9 CH_3-C | 1.4 $-C-CH_2-C-$ | 1.4 $-C-CH_2-C-$ | 2.2 CH_3-CO-R | 2.4 $-C-CH_2-CO-R$ |
| | assignment | A | B | C | E | D |

4. Molecular formula = C₃H₆O₂ (Refer to Figures 4-1 and 4-2)
 a) Calculate the DBE.

$$DBE = [2(3)+2]-6 = 2 \div 2 = 1$$

- b) Draw two possible structures for this molecule based only on the molecular formula (not the IR or ¹H nmr).

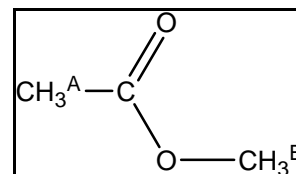


- c) Which band in the IR is most diagnostic? What functional group does this band indicate?

1747 cm^{-1} (s)
 C=O str., ester

- d) Tabulate the ¹H nmr data and assign all of the peaks using a diagram of the proposed structure.

| chemical shift, δ (ppm) | multiplicity | integration | | assignment |
|-----------------------------------|--------------|-------------|----------|--|
| | | actual | relative | |
| 7.24 | singlet | - | - | CHCl ₃ in CDCl ₃ |
| 3.60 | singlet | 10.670 | 1 H | H _B |
| 2.00 | singlet | 10.704 | 1 H | H _A (carbonyl methyl) |



- e) How did you rule out the other possible structure(s) proposed in 1b, using **both** the IR and nmr spectra?

Answers must reflect proposed structures in question (b)...

ex: IR: no 2400-3400 cm⁻¹ O-H str. ∴ not acid OR
 no 3200-3400 cm⁻¹ O-H str. ∴ not α -hydroxy ketone

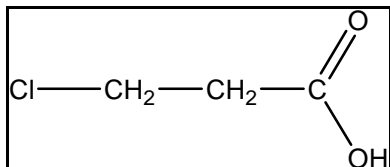
¹H nmr: only two signals ∴ not acid or enol OR
 no coupling ∴ not acid

Molecular formula = $C_3H_5ClO_2$

(Refer to Figures 4-3 A and B)

5. Using only the 1H nmr spectra shown, determine the structure of both isomers of $C_3H_5ClO_2$.

a)



b)

