Nuclear Magnetic Resonance Imaging (NMR)
By: Nada Saab

Nuclear magnetic resonance (NMR) spectroscopy: The absorption of radio-frequency radiation by nuclei and the resulting transition between energy levels.

Resonance in NMR spectroscopy: The absorption of electromagnetic radiation by a precessing nucleus and the resulting flip of its nuclear spin from a lower energy state to a higher energy state.

Signal: A recording in an NMR spectrum of a nuclear magnetic resonance.

Equivalent Hydrogens: Hydrogens that have the same chemical environment.

Signal splitting: Splitting of an NMR signal into a set of peaks by the influence of nonequivalent nuclei on the same of adjacent atom (s).

(n+1) Rule: The ^{1}H-NMR signal of a hydrogen or a set of equivalent hydrogens is split into (n+1) peaks by a nonequivalent set of n equivalent neighboring hydrogens.

We have **three kinds of information** that can be driven from examination of a ^{1}H-NMR spectrum:
1- From the number of signals, we can determine the number of sets of equivalent hydrogens.
2- From integration of signal areas, we can determine the relative numbers of hydrogens giving rise to earth signal.
3- From the chemical shift of each signal, we drive information about the types of hydrogens in each set.

CHARACTERISTIC ^{1}H-NMR CHEMICAL SHIFTS

Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*	Type of Hydrogen (R = alkyl, Ar = aryl)	Chemical Shift (δ)*
$(CH_3)_4Si$	0 (by definition)	$RCOCH_3$	3.7–3.9
RCH_3	0.8–1.0	$RCOCH_2R$	4.1–4.7
RCH_2R	1.2–1.4	RCH_2I	3.1–3.3
R_3CH	1.4–1.7	RCH_2Br	3.4–3.6
$R_2C{=}CRCHR_2$	1.6–2.6	RCH_2Cl	3.6–3.8
$RC{\equiv}CH$	2.0–3.0	RCH_2F	4.4–4.5
$ArCH_3$	2.2–2.5	ArOH	4.5–4.7
$ArCH_2R$	2.3–2.8	$R_2C{=}CH_2$	4.6–5.0
ROH	0.5–6.0	$R_2C{=}CHR$	5.0–5.7
RCH_2OH	3.4–4.0	ArH	6.5–8.5
RCH_2OR	3.3–4.0	RCHO	9.5–10.1
R_2NH	0.5–5.0	RCOH	10–13
$RCCH_3$	2.1–2.3		
$RCCH_2R$	2.2–2.6		

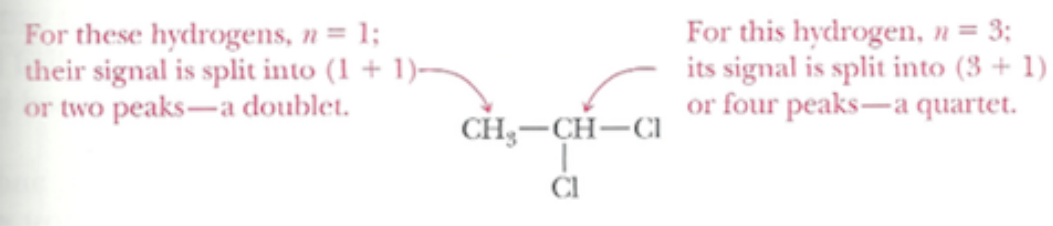
*Values are relative to tetramethylsilane. Other atoms within the molecule may cause the signal to appear outside these ranges.

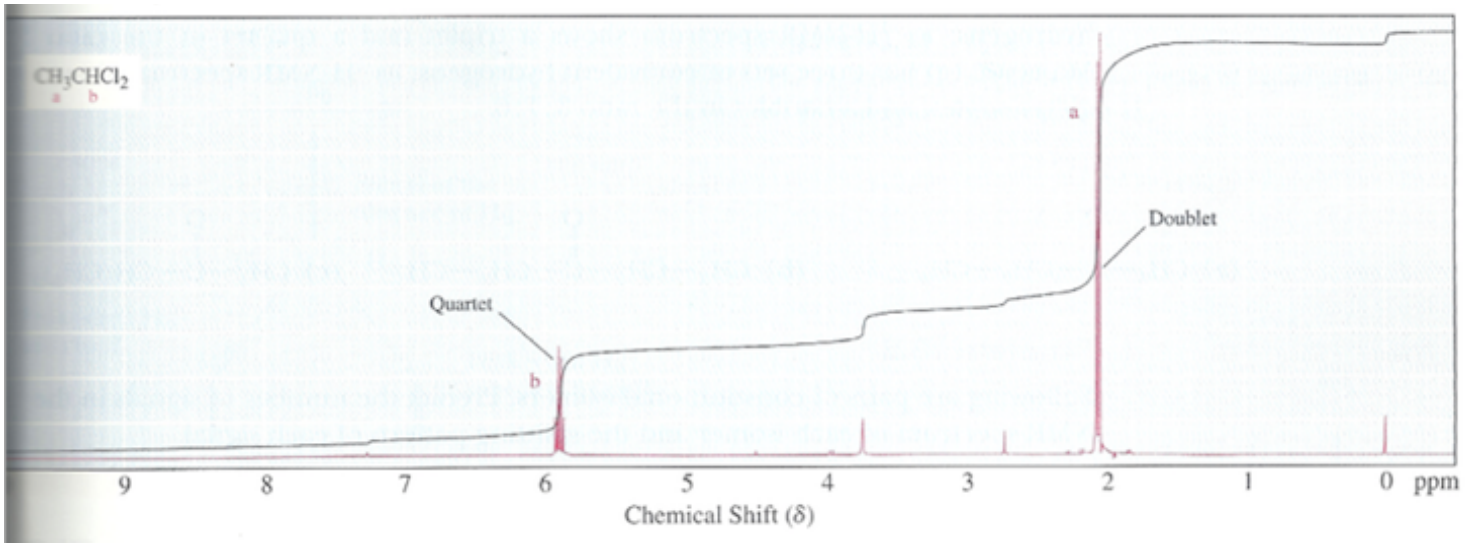
Exercise A:

Use the rules (signal splitting and (n+1) rule) below and explain with your own words the splitting of the hydrogen in the NMR spectrum:

Signal splitting: Splitting of an NMR signal into a set of peaks by the influence of nonequivalent nuclei on the same of adjacent atom (s).

(n+1) Rule: The ^{1}H-NMR signal of a hydrogen or a set of equivalent hydrogens is split into (n+1) peaks by a nonequivalent set of n equivalent neighboring hydrogens



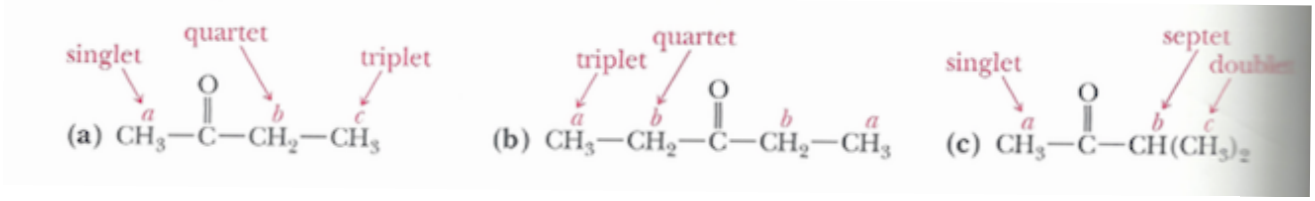


Exercise B:

Use the rules (signal splitting and (n+1) rule) below and explain with your own words the splitting of the hydrogen in the NMR spectrum:

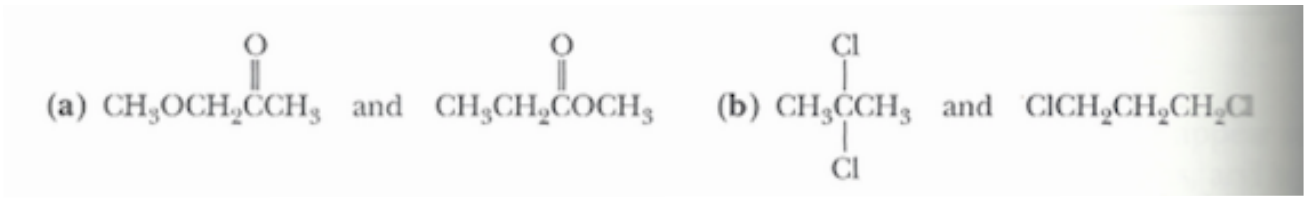
Signal splitting: Splitting of an NMR signal into a set of peaks by the influence of nonequivalent nuclei on the same of adjacent atom (s).

(n+1) Rule: The ^{1}H-NMR signal of a hydrogen or a set of equivalent hydrogens is split into (n+1) peaks by a nonequivalent set of n equivalent neighboring hydrogens.



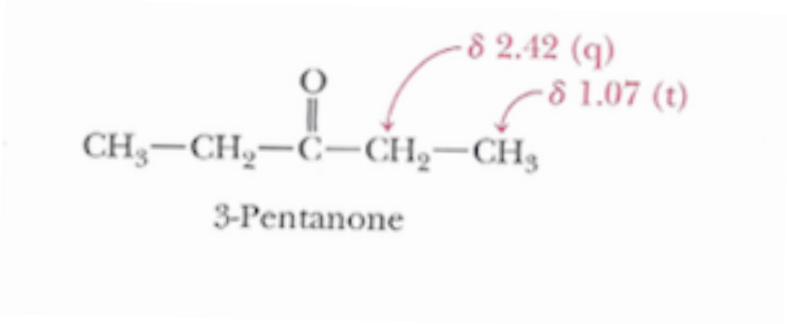
Exercise C:

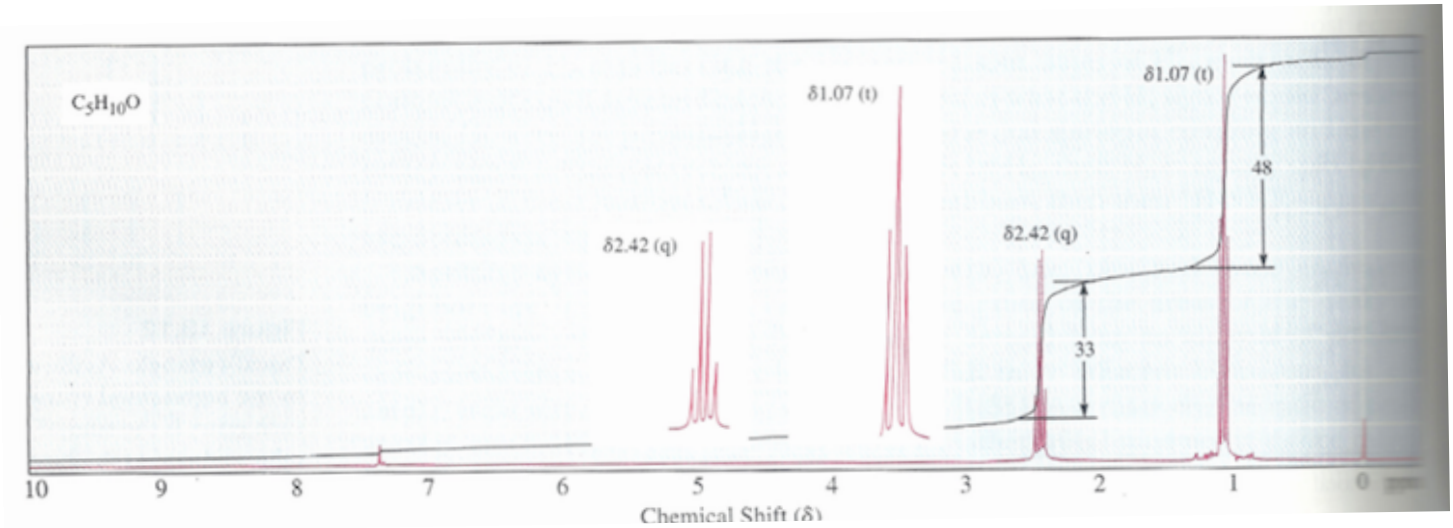
Follow the same rule for Exercises A and B and predict the splitting pattern of each signal of the NMR spectrum of each pair of constitutional isomers (a) and (b).



Exercise D:

Use the rules (signal splitting and (n+1) rule) and the table in page 2 " Characteristics of 1H-NMR Chemical Shifts" and explain with your own words and splitting and the location (shift) on each signal for 3-Pentanone.

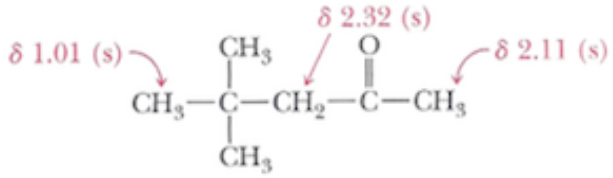




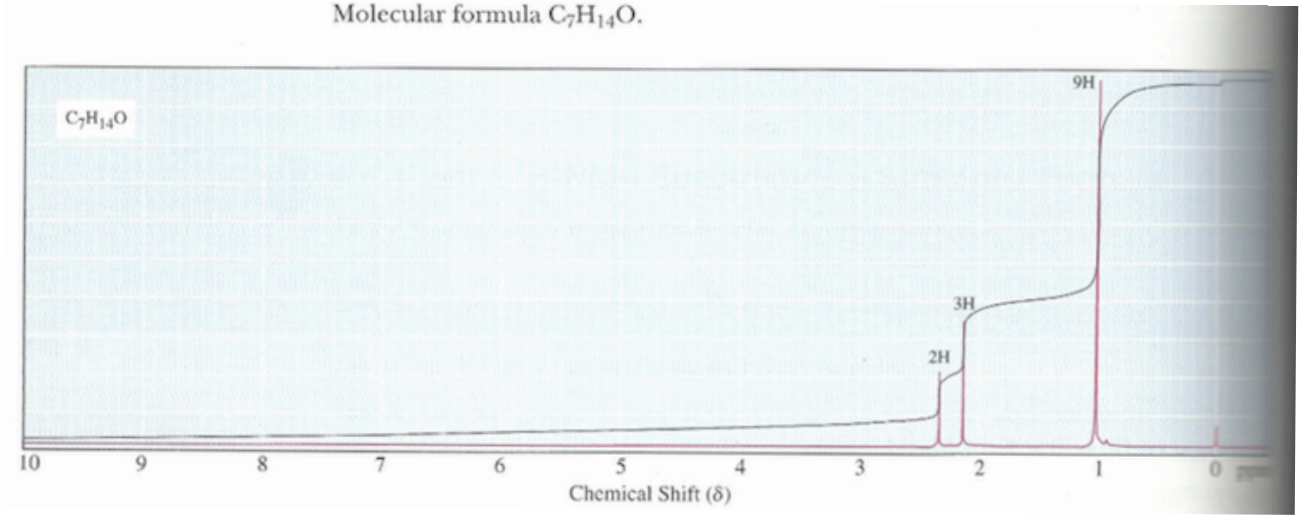
Exercise E:

Use the rules (signal splitting and (n+1) rule) and the table in page 2 " Characteristics of 1H-NMR Chemical Shifts" and explain with your own words and splitting and the location (shift) on each signal for 4,4 dimethyl-2-pentanone.

Structural formula. The compound is 4,4-dimethyl-2-pentanone.

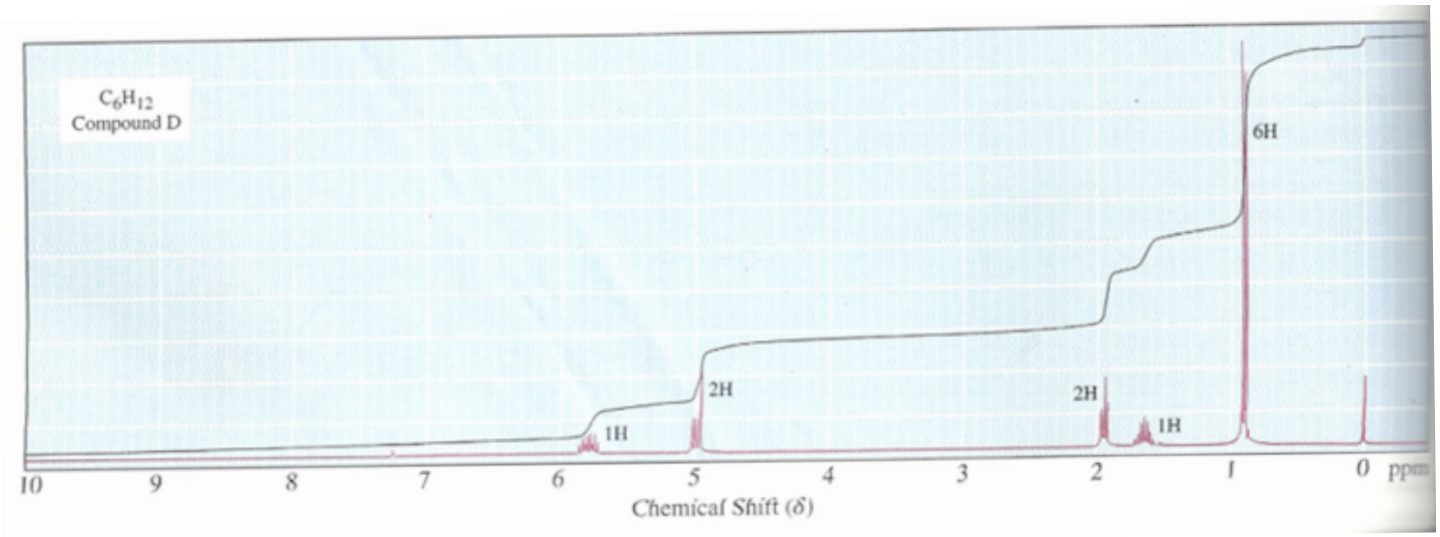


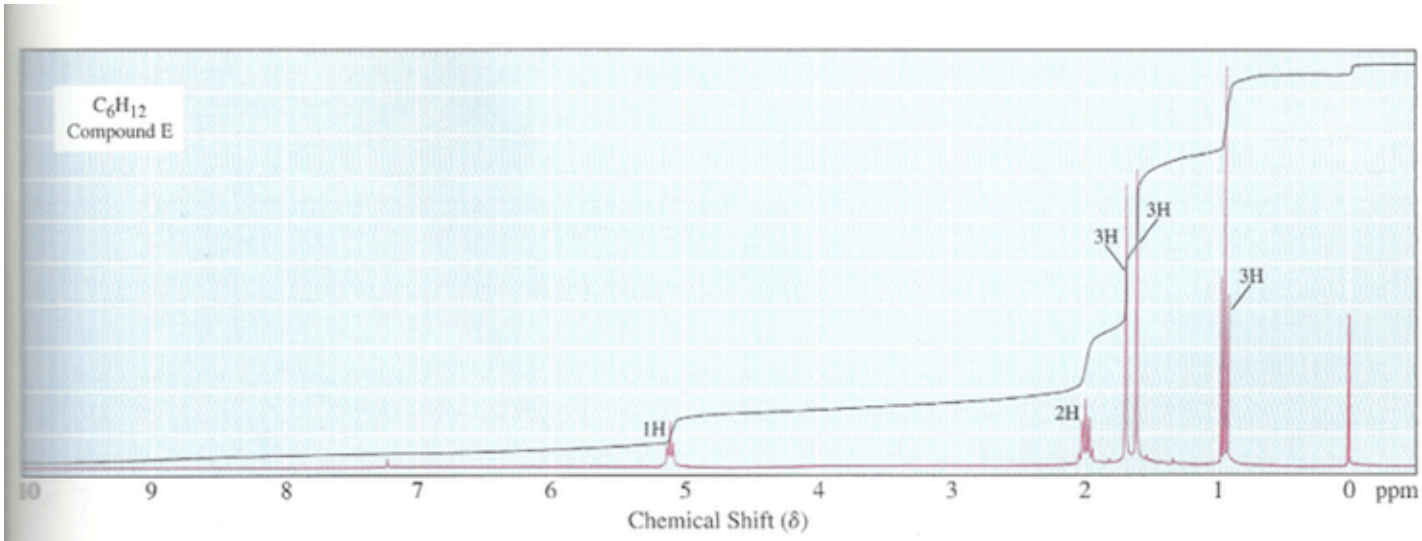
Molecular formula $C_7H_{14}O$.

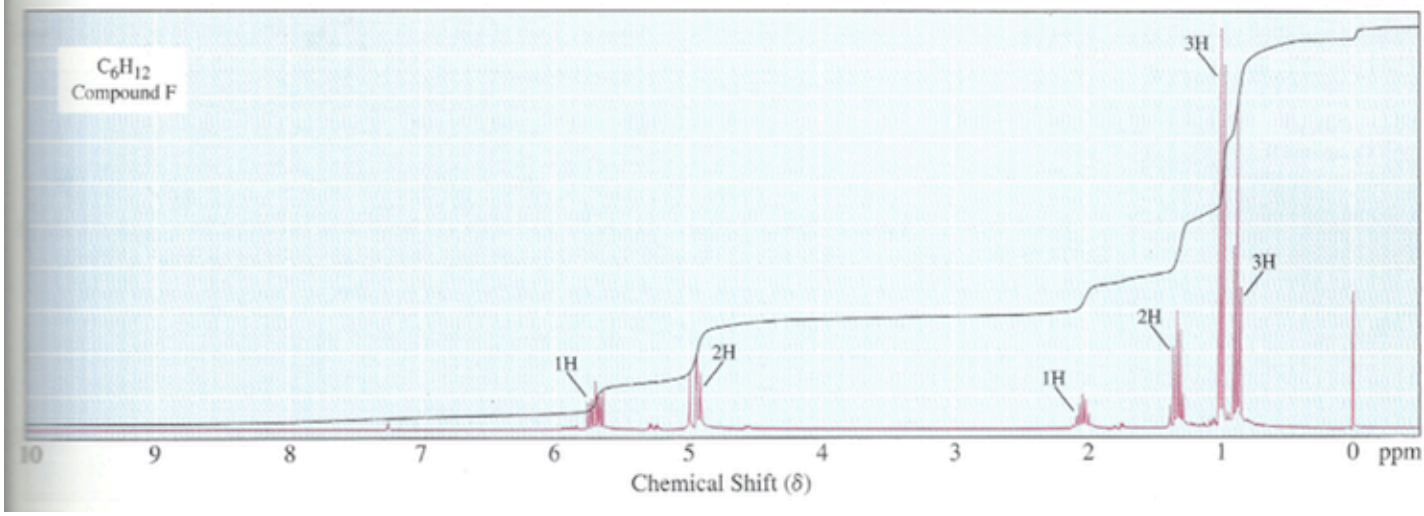


Exercise F:

Use the rules (signal splitting and (n+1) rule) and the table in page 2 " Characteristics of 1H-NMR Chemical Shifts" and determine the structure of the following spectrums.



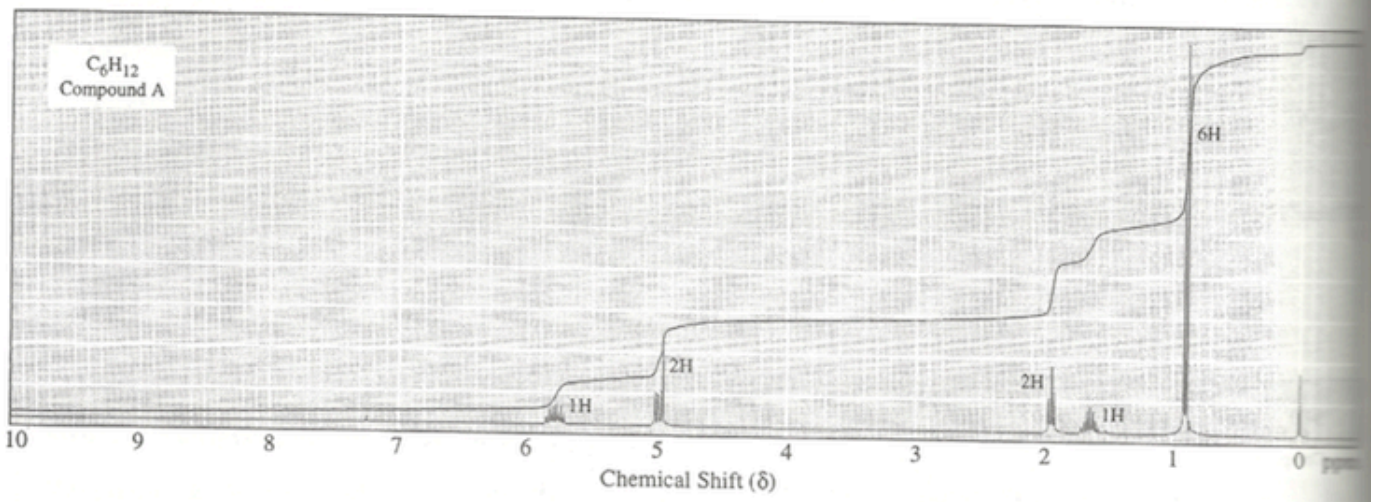


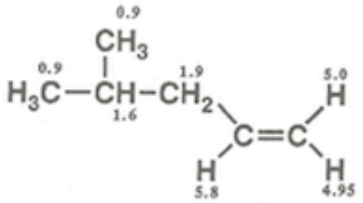


Exercise G:

Study the ^{1}H-NMR spectrum of each compound A, B and C. Explain the structure and rewrite the solution with your own explanation.

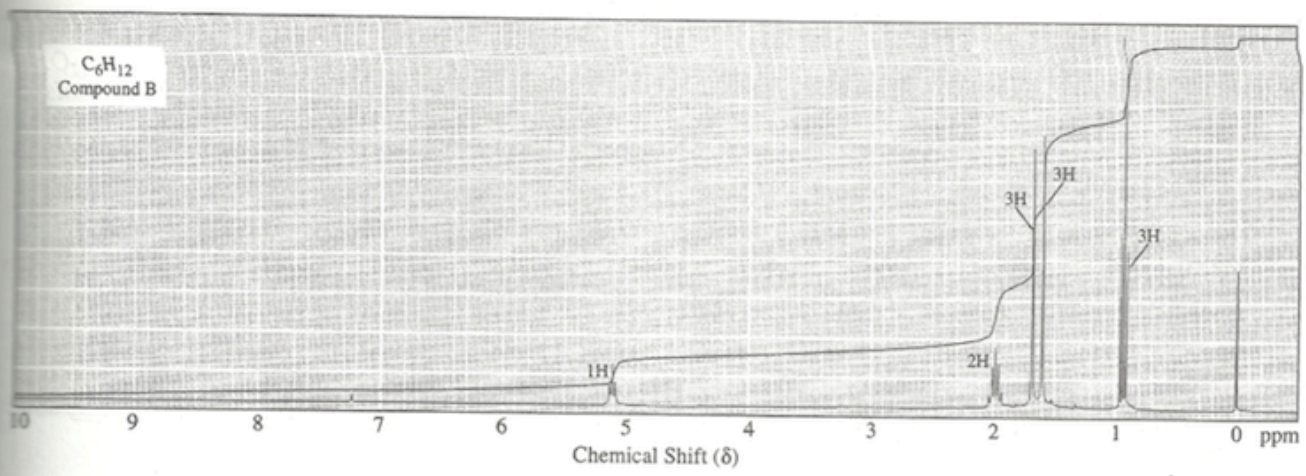
Compound A:

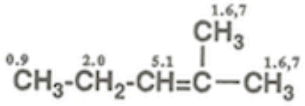




^{1}H-NMR δ 5.8 (1H, multiplet; this is more complex than expected because the adjacent vinylic hydrogens are not equivalent, -CH=), 4.95-5.0 (2H, multiplet, $=CH_2$; this is asymmetric because these two vinylic hydrogens are not equivalent and the hydrogen *trans* to the hydrogen on the other vinylogous carbon has the larger signal splitting so it is the signal at 5.0), 1.9 (2H, multiplet; doublet of doublets, $-CH_2-$), 1.6 (1H, multiplet; a triplet of septets, -CH-), 0.9 (6H, one doublet, $-CH_3$).

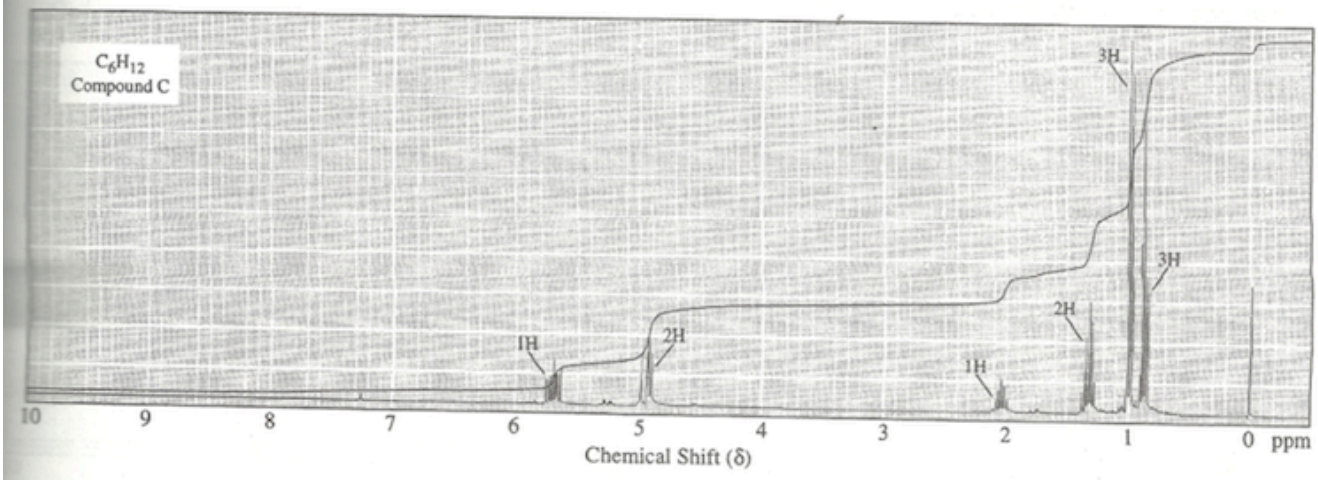
Compound B:

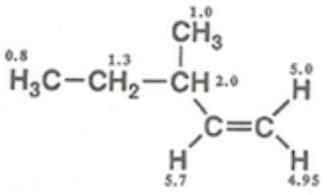




^{1}H-NMR δ 5.1 (1H, triplet, -CH=), 2.0 (2H, multiplet; a doublet of quartets, -CH_2-), 1.6 and 1.7 (6H, two singlets, =$C(CH_3)_2$), 0.9 (3H, triplet, -CH_3)

Compound C:





^{1}H-NMR δ 5.7 (1H, multiplet; this is more complex than expected because the adjacent vinylic hydrogens are not equivalent, -CH=), 4.9-5.0 (2H, multiplet, =CH_2; this is asymmetric because these two vinylic hydrogens are not equivalent and the hydrogen *trans* to the hydrogen

13.19 Following are three compounds of molecular formula $C_4H_8O_2$, and three ^{1}H-NMR spectra. Assign each compound its correct spectrum and assign all signals to their corresponding hydrogens.

(1) (2) (3)