B.Sc. Semester-VI
Paper CC-XIV
Organic Chemistry-V

III. Nuclear Magnetic Resonance Spectroscopy

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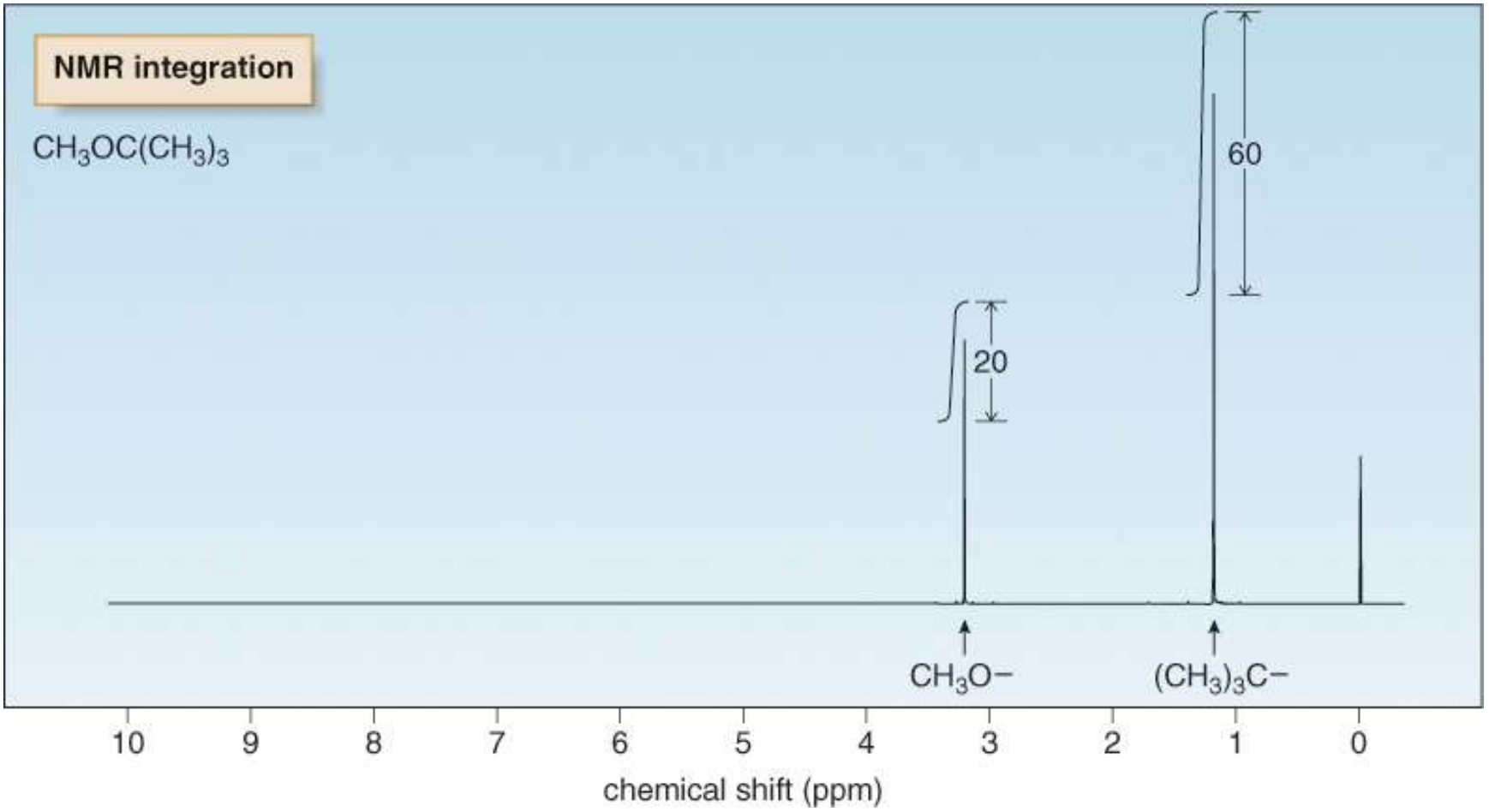
Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR—Intensity of Signals

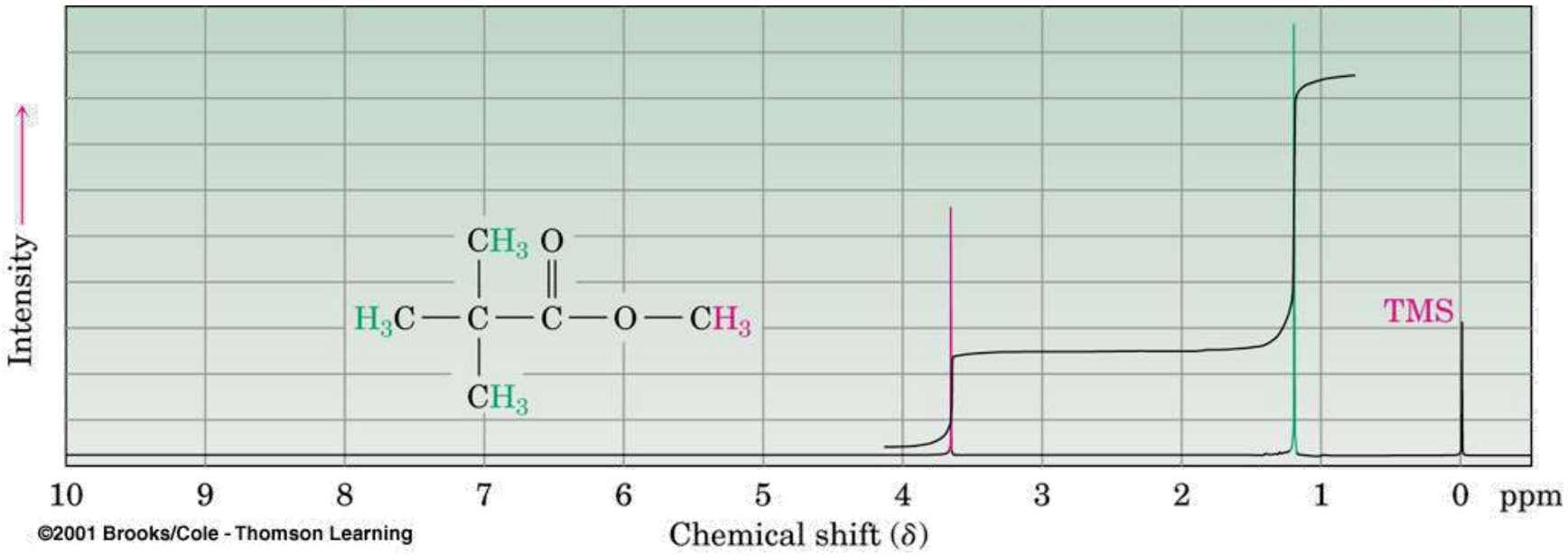
- The area under an NMR signal is proportional to the number of absorbing protons.
- An NMR spectrometer automatically integrates the area under the peaks, and prints out a stepped curve (integral) on the spectrum.
- The height of each step is proportional to the area under the peak, which in turn is proportional to the number of absorbing protons.
- Modern NMR spectrometers automatically calculate and plot the value of each integral in arbitrary units.
- The ratio of integrals to one another gives the ratio of absorbing protons in a spectrum. Note that this gives a ratio, and not the absolute number, of absorbing protons.

Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR—Intensity of Signals

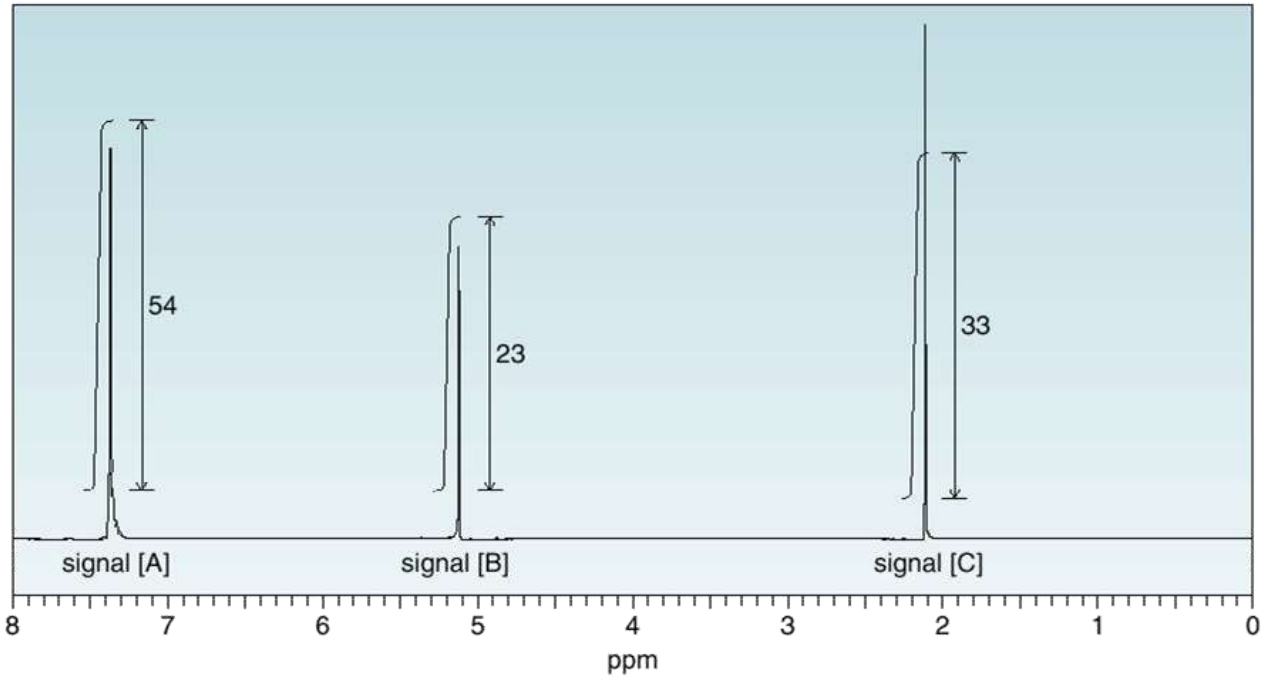


Methyl α,α-Dimethylpropionate



How To — Determine the Number of Protons Giving Rise to an NMR Signal

Example A compound of molecular formula $C_9H_{10}O_2$ gives the following integrated ^1H NMR spectrum. How many protons give rise to each signal?



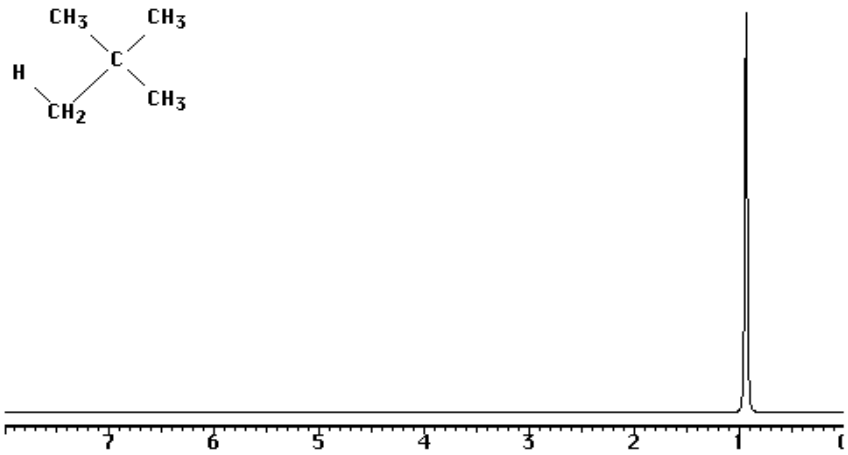
Step [1] **Determine the number of integration units per proton by dividing the total number of integration units by the total number of protons.**

- Total number of integration units: 54 + 23 + 33 = 110 units
- Total number of protons = 10
- Divide: 110 units/10 protons = **11 units per proton**

Step [2] **Determine the number of protons giving rise to each signal.**

- To determine the number of H atoms giving rise to each signal, divide each integration value by the answer of Step [1] and round to the nearest whole number.

Signal [A]:				Signal [B]:				Signal [C]:		
Answer: $\frac{54}{11}$	= 4.9 ≈	**5 H**		$\frac{23}{11}$	= 2.1 ≈	**2 H**		$\frac{33}{11}$	=	**3 H**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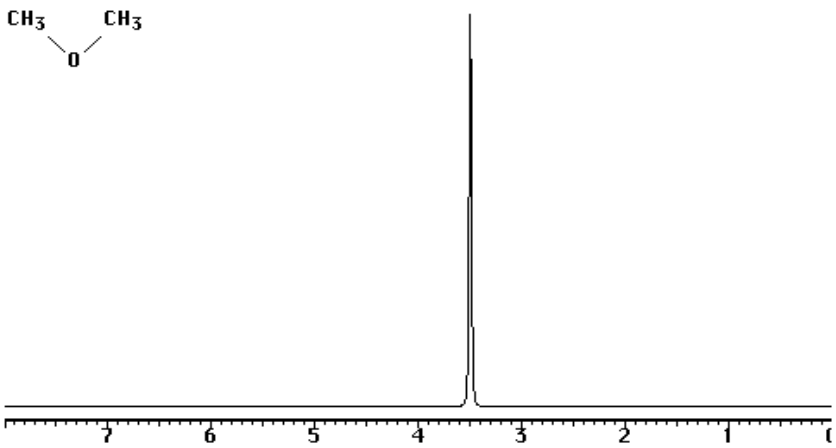
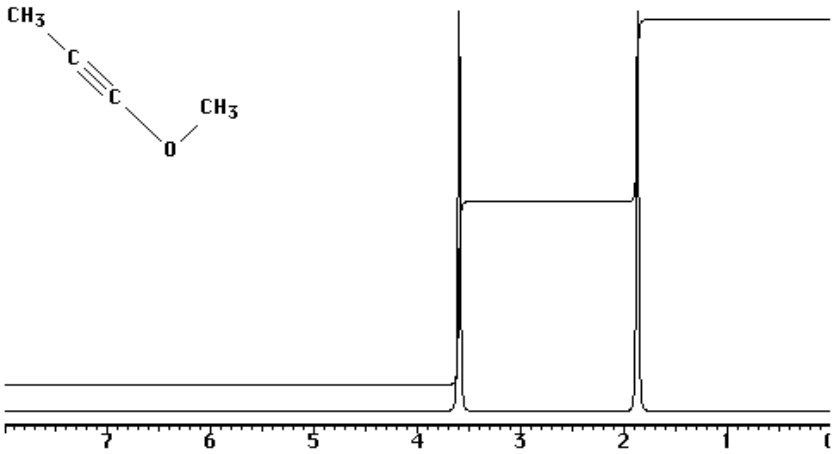
CH3
C
H
CH2
CH3
7
6
5
4
3
2
1


CH3
CH3
O
7
6
5
4
3
2
1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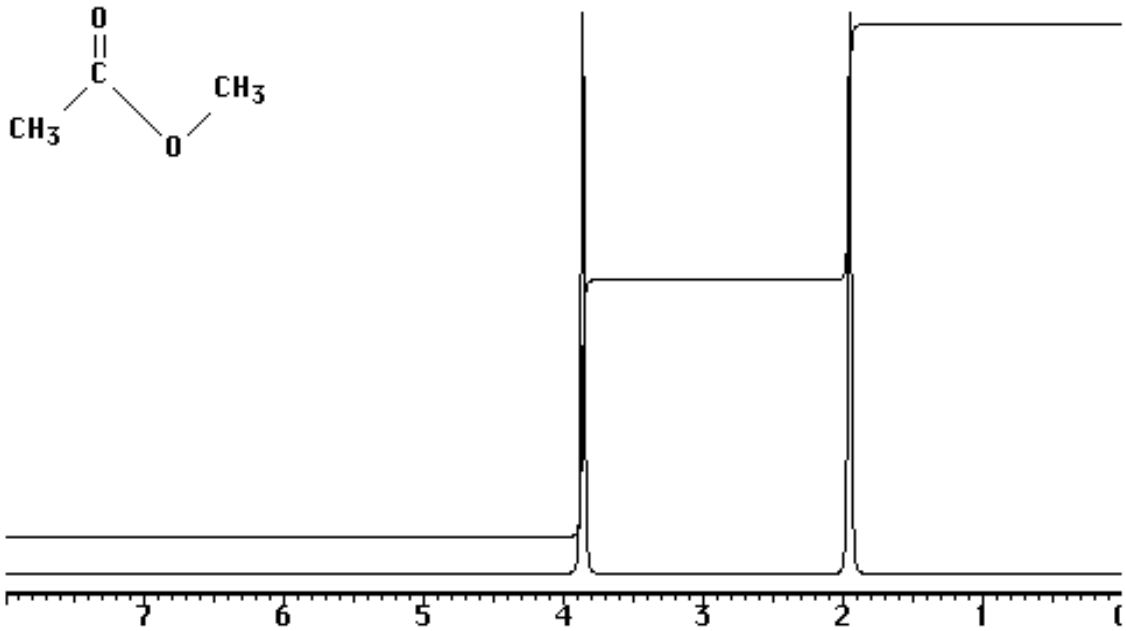
C
C
CH3
O
7
6
5
4
3
2
1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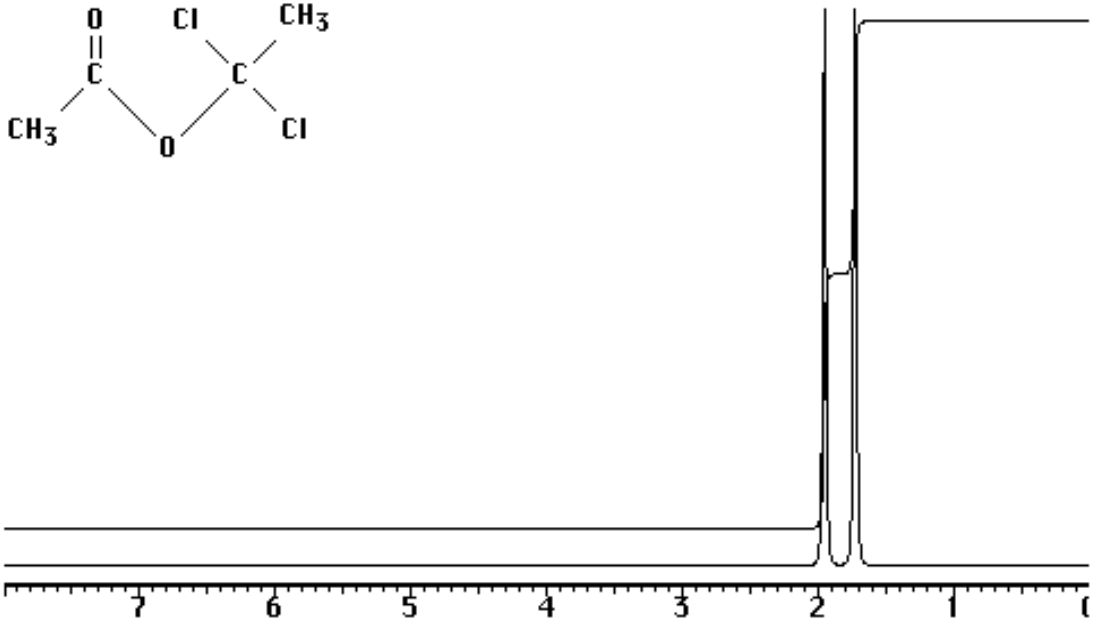
C
CH3
CH3
O
7
6
5
4
3
2
1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Cl
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C
C
CH3
O
Cl
7
6
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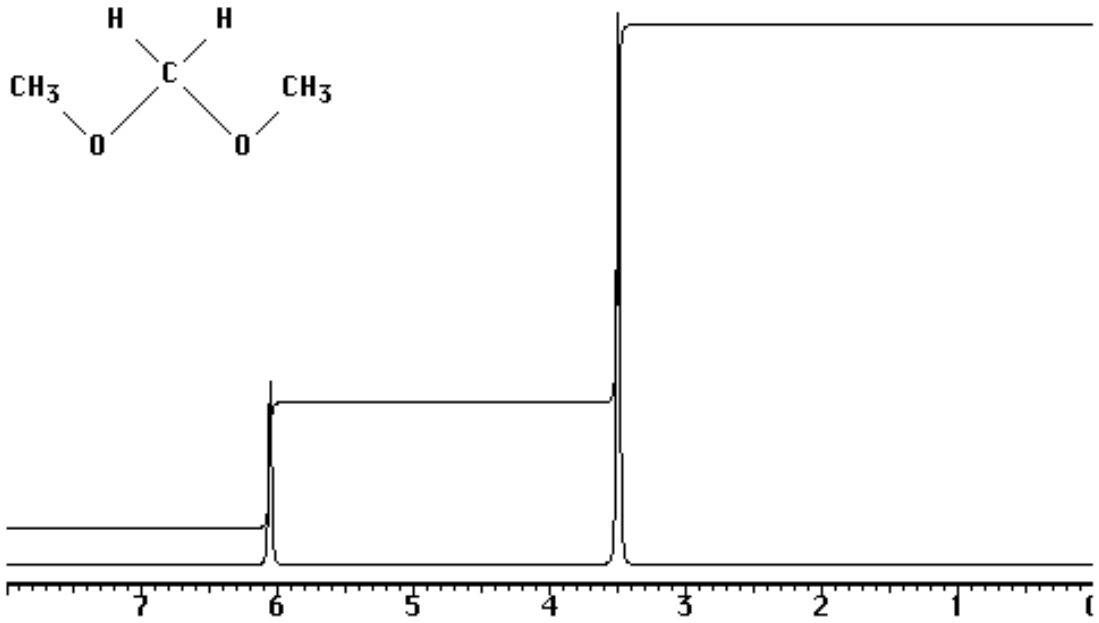
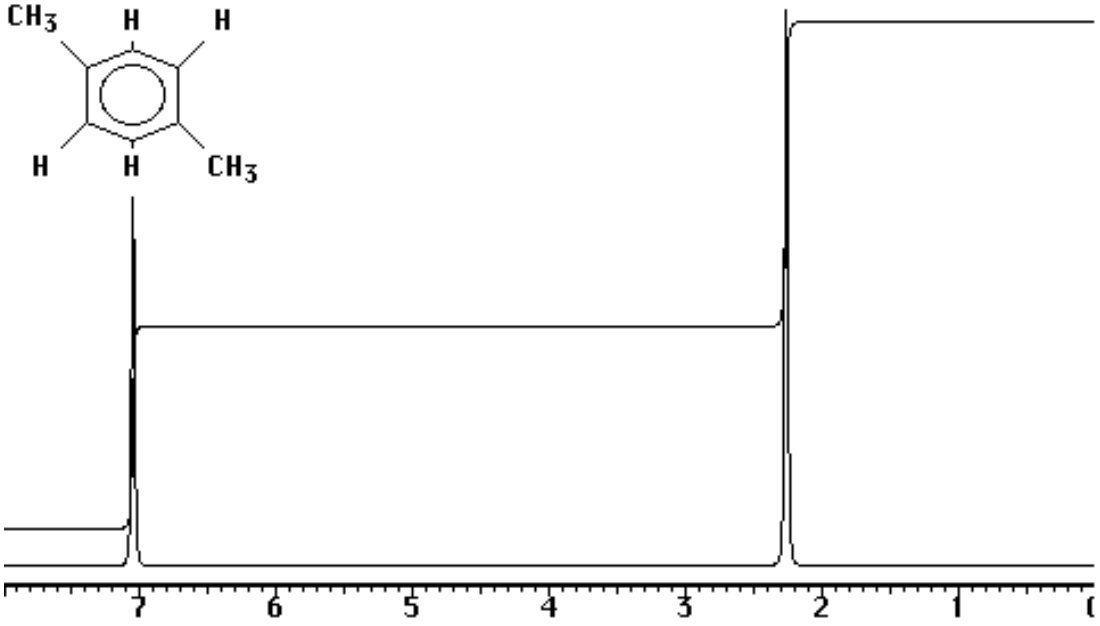
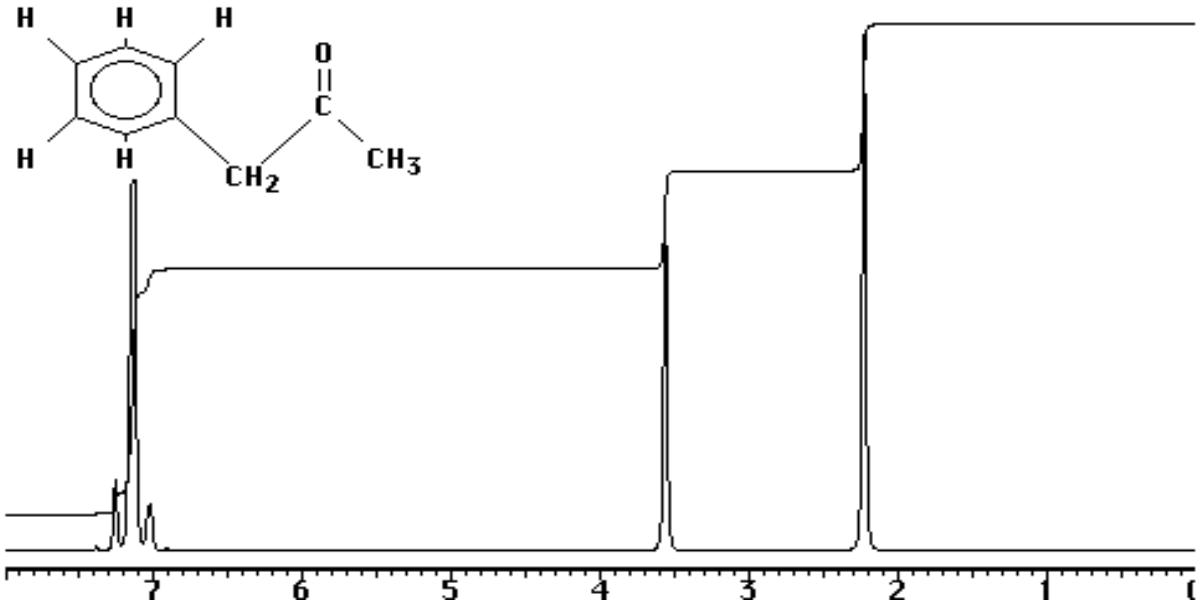
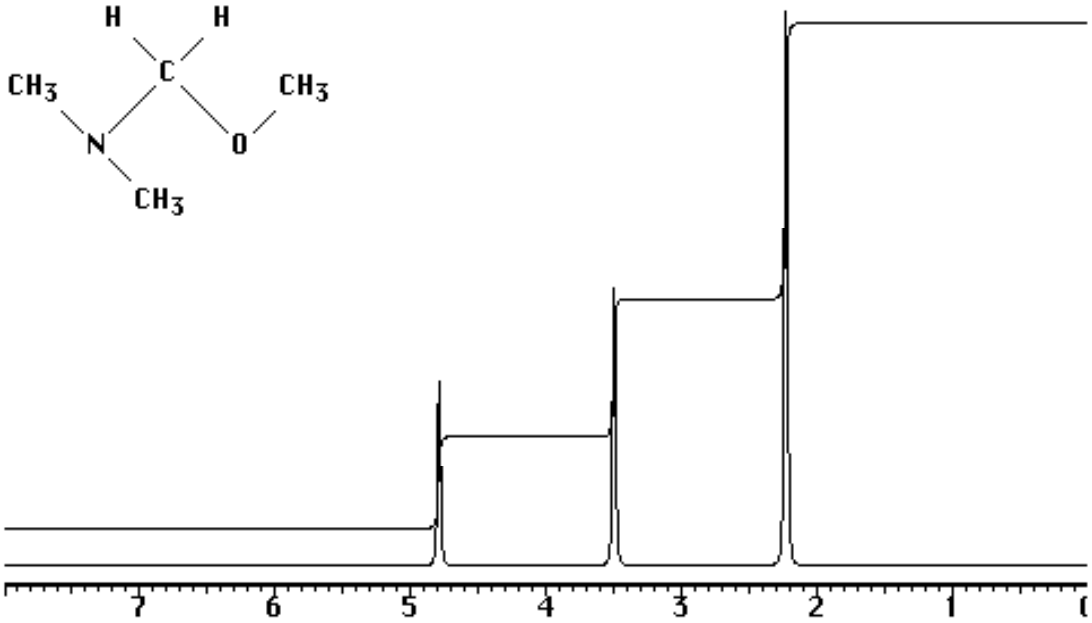
4
3
2
1

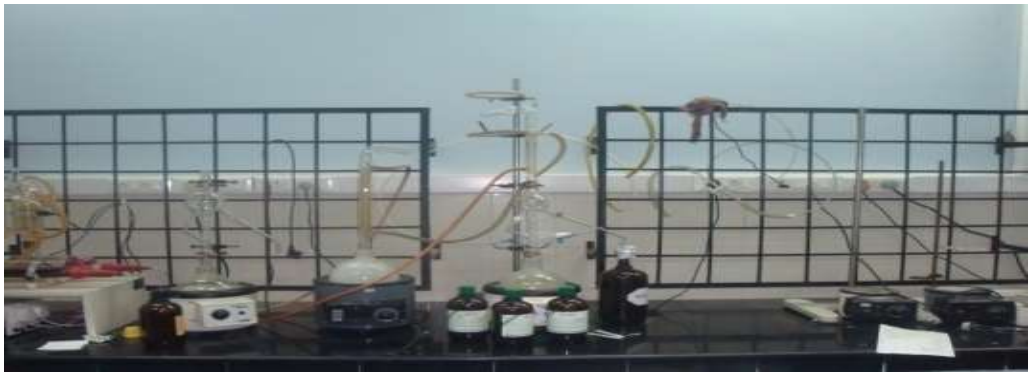

H
H
C
CH3
CH3
O
O
7
6
5
4
3
2
1


CH3
H
H
H
H
CH3
7
6
5
4
3
2
1


H
H
H
H
H
O
C
CH2
CH3
7
6
5
4
3
2
1


H
H
C
CH3
CH3
N
O
CH3
7
6
5
4
3
2
1

Thank You



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