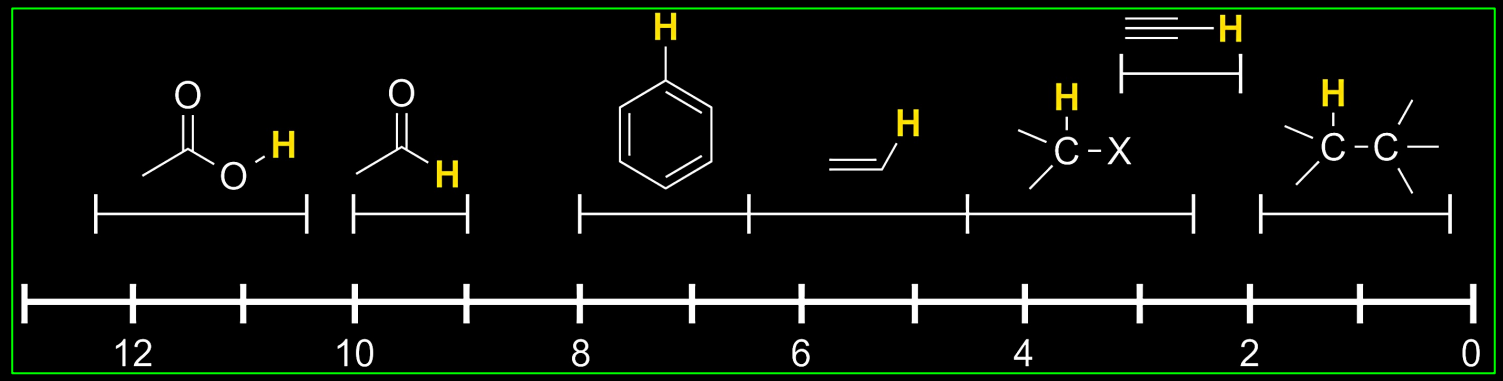
Summary of previous class

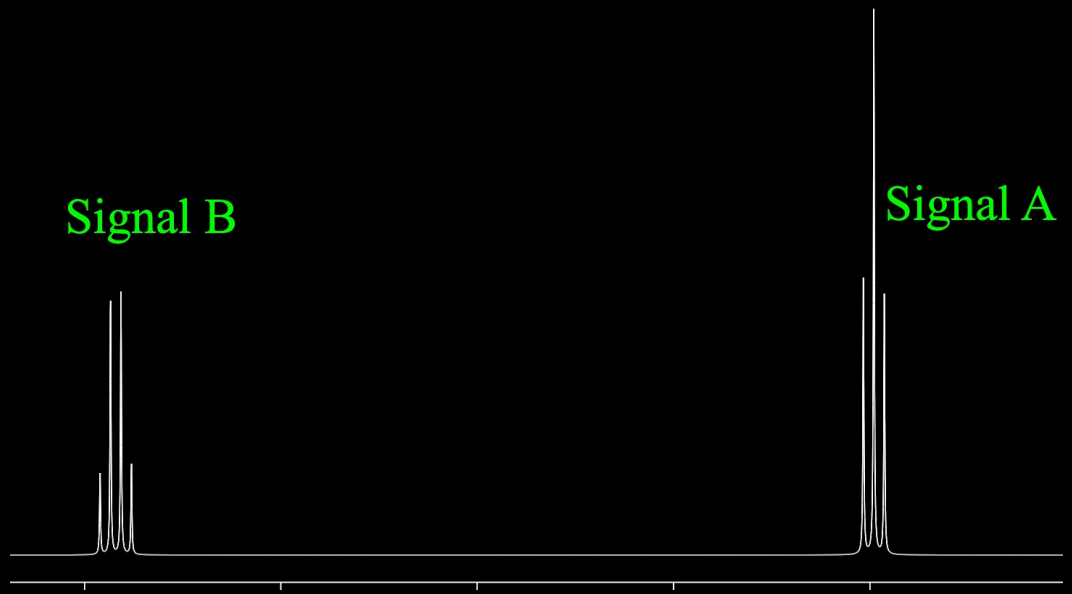
^{1}H NMR Spectroscopy

Your simple guide to chemical shifts



CH_3CH_2Cl

Signal A Signal B



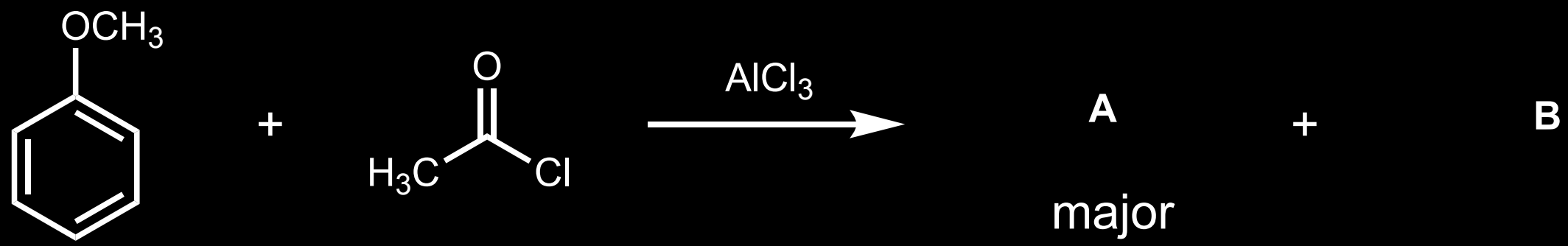
N+1 Rule

N= number of neighboring / different hydrogens

☆ Practice questions

^1H NMR Spectroscopy

Friedel crafts reaction of anisole using acetyl chloride in the presence of $AlCl_3$ gave products **A** and **B**. Using the ^1H NMR data identify the products **A** and **B**.



☆ Practice questions

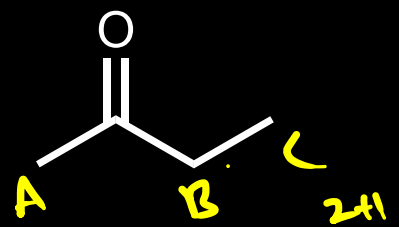
^1H NMR Spectroscopy

n+1 =

0+1 = 1

3+1 = 4

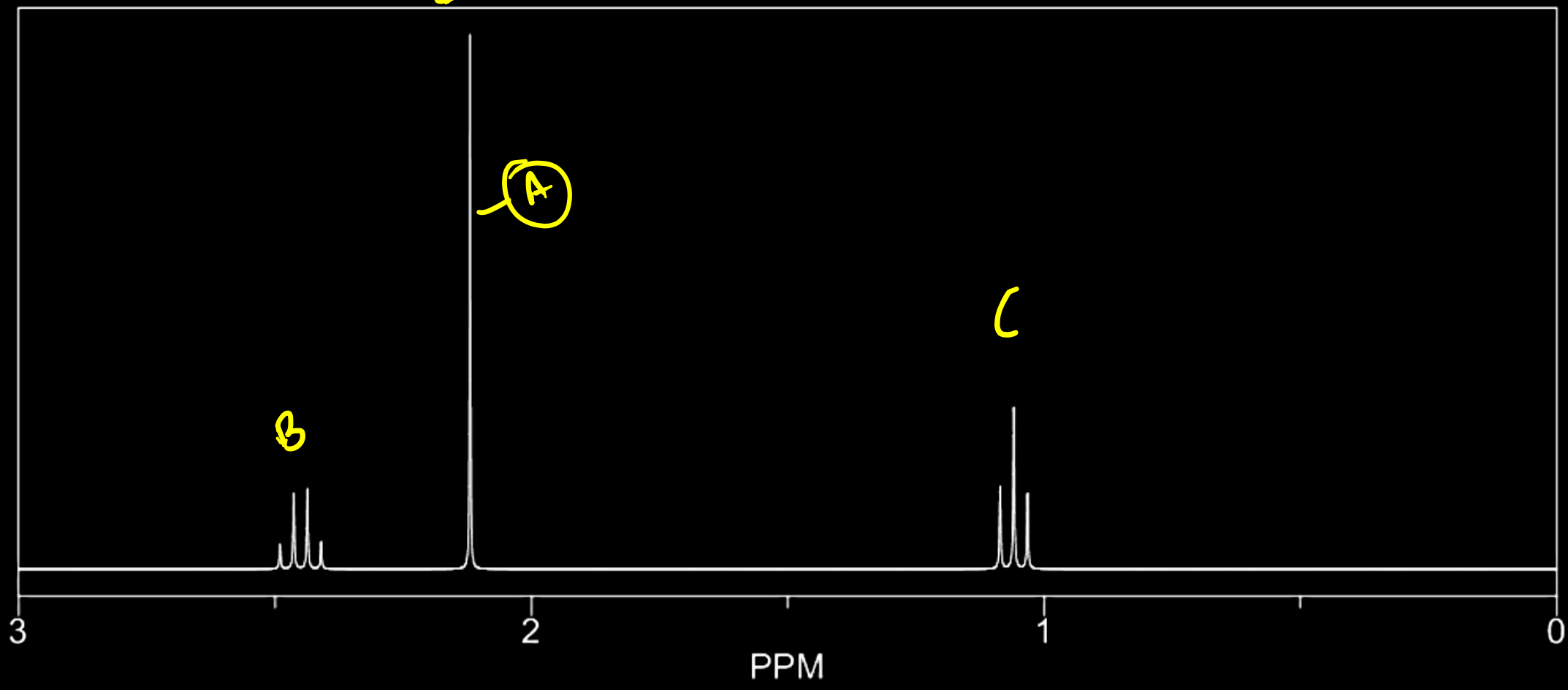
2+1



(s) A = 0.9 + 1.0 = 1.9

(q) B = 1.3 + 1.0 = 2.3

(t) C = 0.9 + 0.3 = 1.2



☆ Practice questions

^1H NMR Spectroscopy

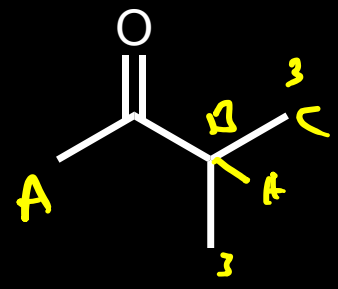
(d+1) = 1

1+1 = 2

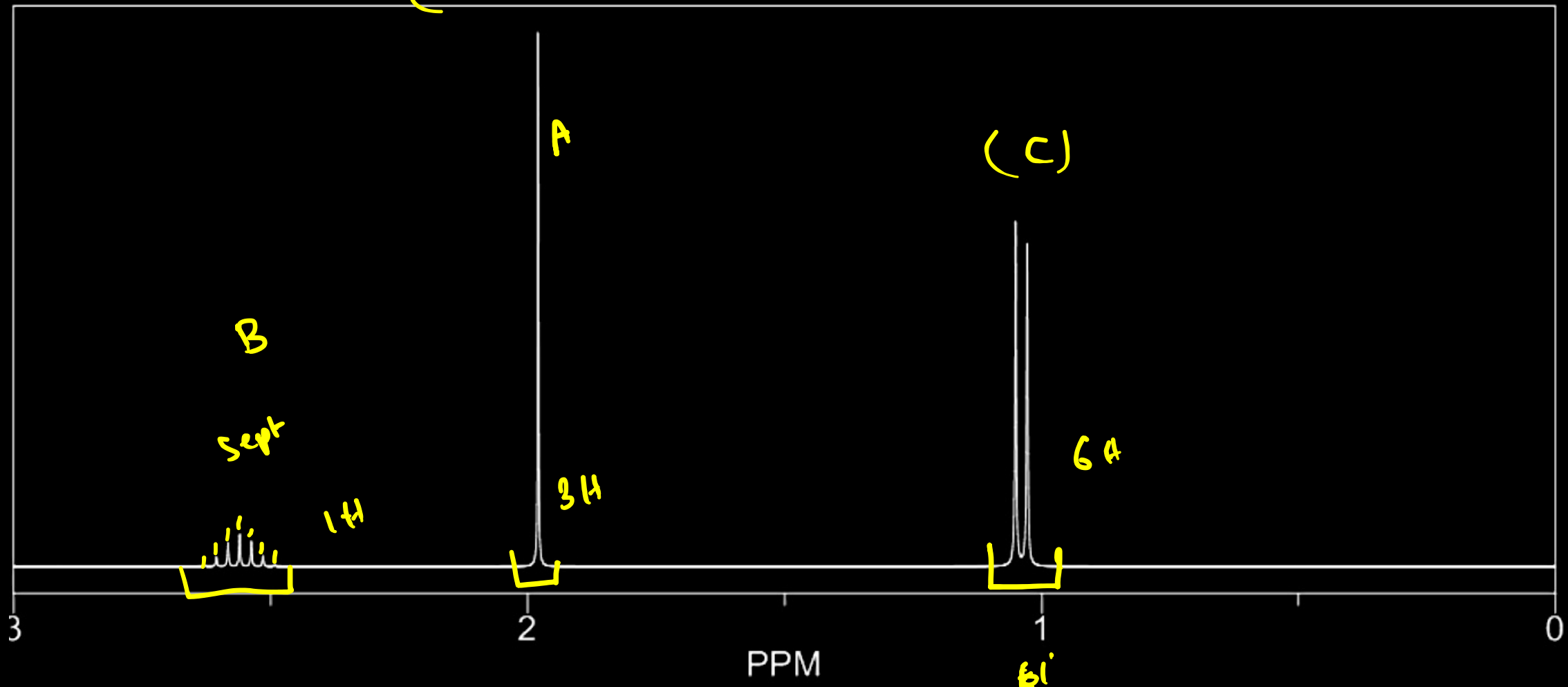
(s) A = 0.9 + 1.0 = 1.9

(sept) B = 1.7 + 1.0 = 2.7

(d) C = 0.9 + 0.3 = 1.2

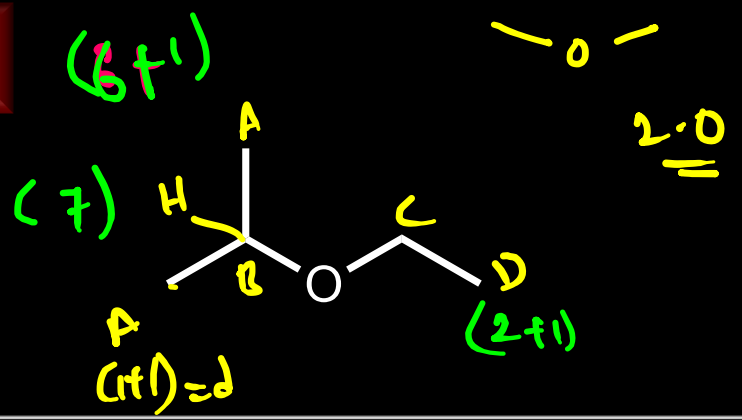


(n+1) = 7



☆ Practice questions

^1H NMR Spectroscopy

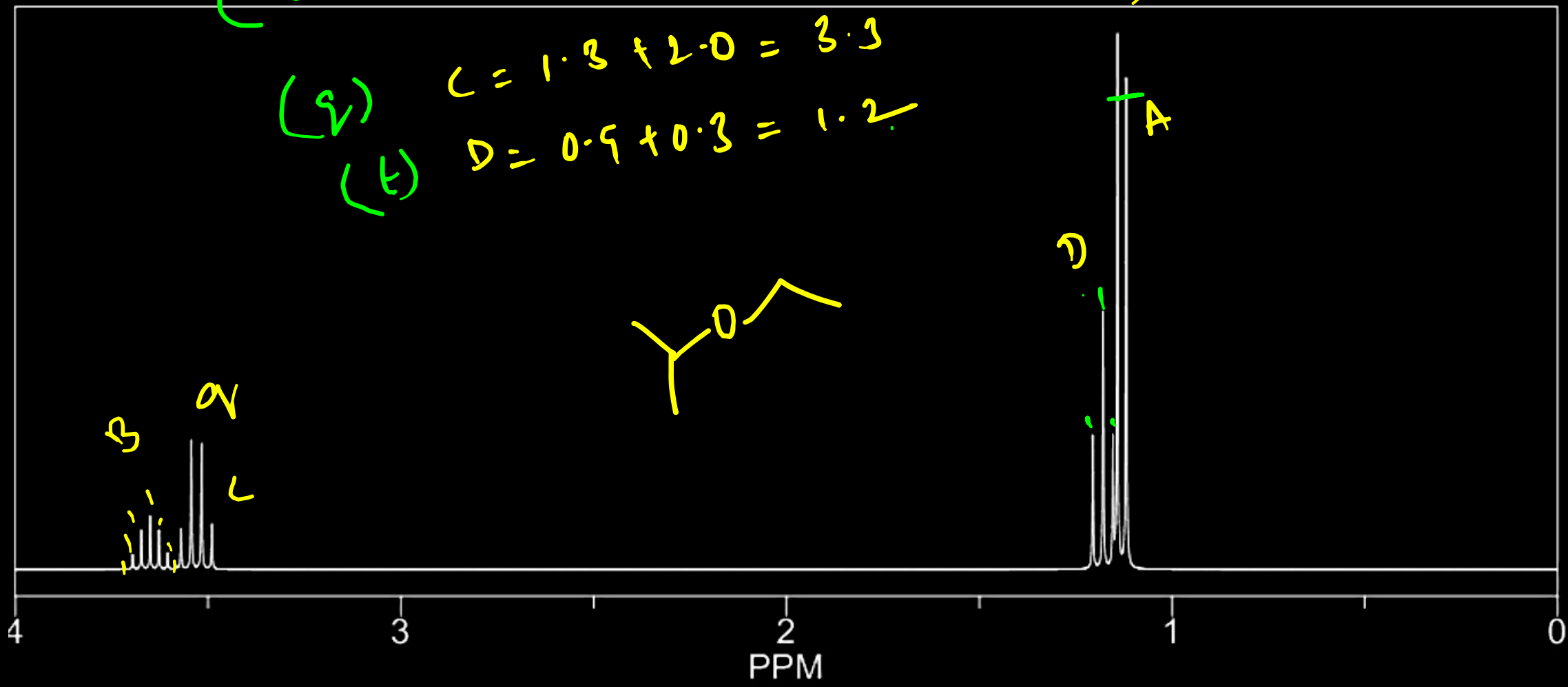


(d) A = 0.9 + 0.3 = 1.2

(Sept) B = 1.7 + 2.0 = 3.7

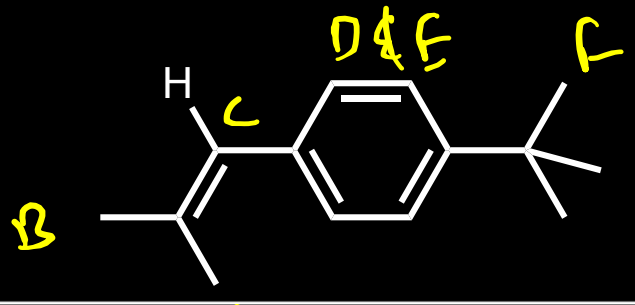
(q) C = 1.3 + 2.0 = 3.3

(t) D = 0.9 + 0.3 = 1.2



☆ Practice questions

^1H NMR Spectroscopy



4.5 - 2.5

A = 0.9 + 1.0 = 1.9

B = 0.9 + 1.0 = 1.9

C = 6.2

D & E = 7.7

F = 0.9 + 0.3 = 1.2

A&D

6H

F

D&E

C

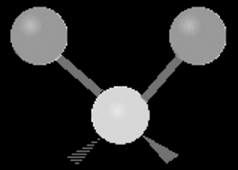
1H 1H 1H 9H

8 7 6 5 4 3 2 1 0

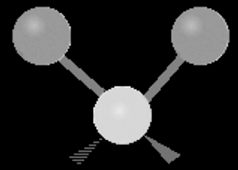
PPM

Infrared Spectroscopy

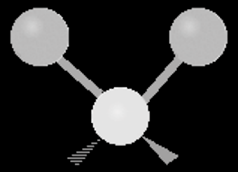
In **IR spectroscopy** we measure where molecules absorb photons of IR radiation.



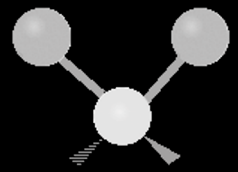
Symmetric stretching



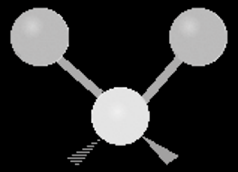
Antisymmetric stretching



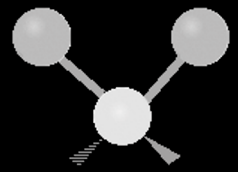
Scissoring



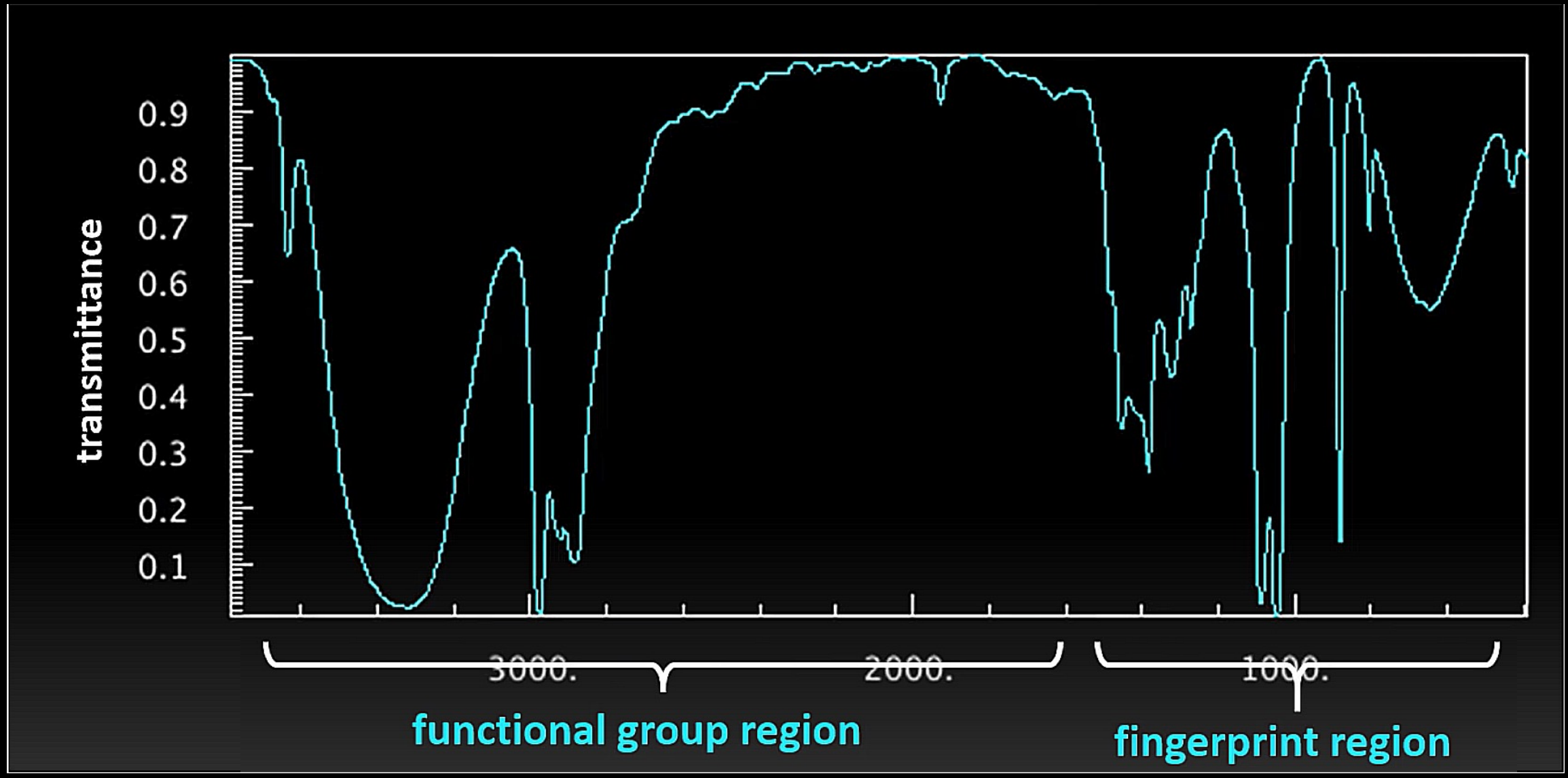
Rocking

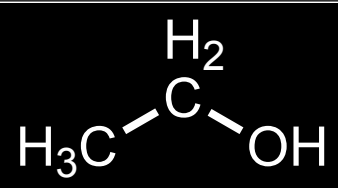


Wagging



Twisting


transmittance
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
3000.
2000.
1000.
functional group region
fingerprint region

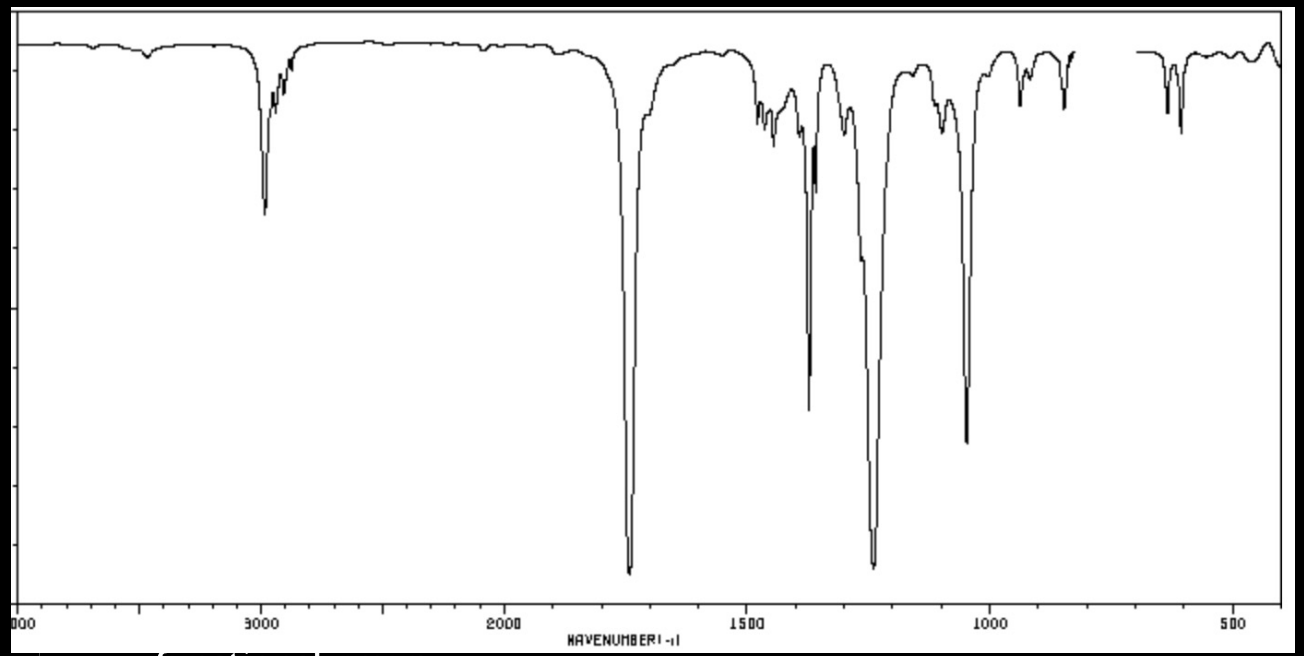

H2
C
H3C
OH

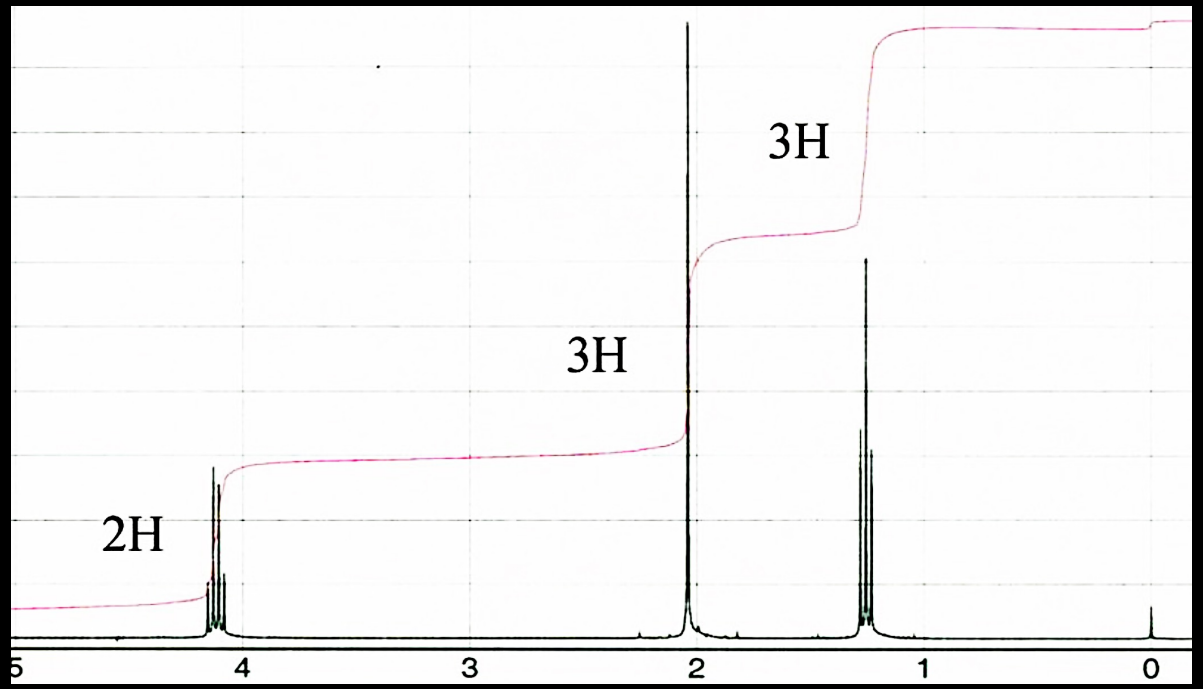
functional group wavenumbers

bond	wave#	intensity
O—H	3650-3200	strong, broad
C—H	3300-2700	medium
N—H	3500-3300	medium, broad
C≡N	2260-2220	medium
C≡C	2260-2100	weak-medium
C=C	1680-1600	medium
C=N	1650-1550	medium
C=O	1780-1650	strong
C—O	1250-1050	strong

Determining structure in organic chemistry

5) An organic compound ($C_4H_8O_2$) shows IR and 1H NMR spectrum as below. Identify the compound?





functional group wavenumbers

bond	wave#	intensity
O—H	3650-3200	strong, broad
C—H	3300-2700	medium
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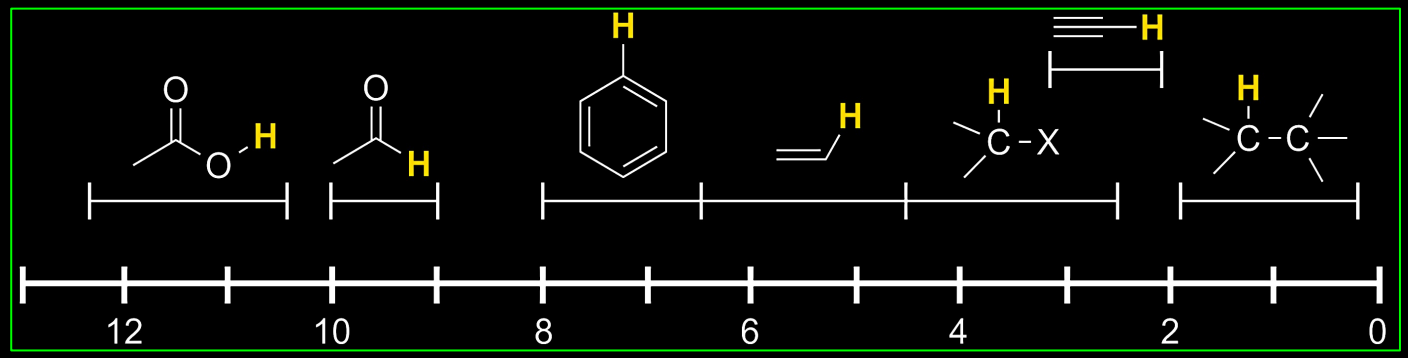
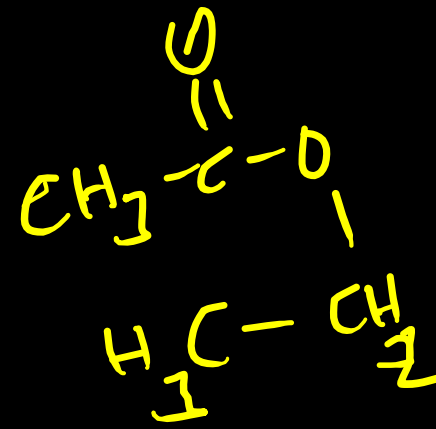
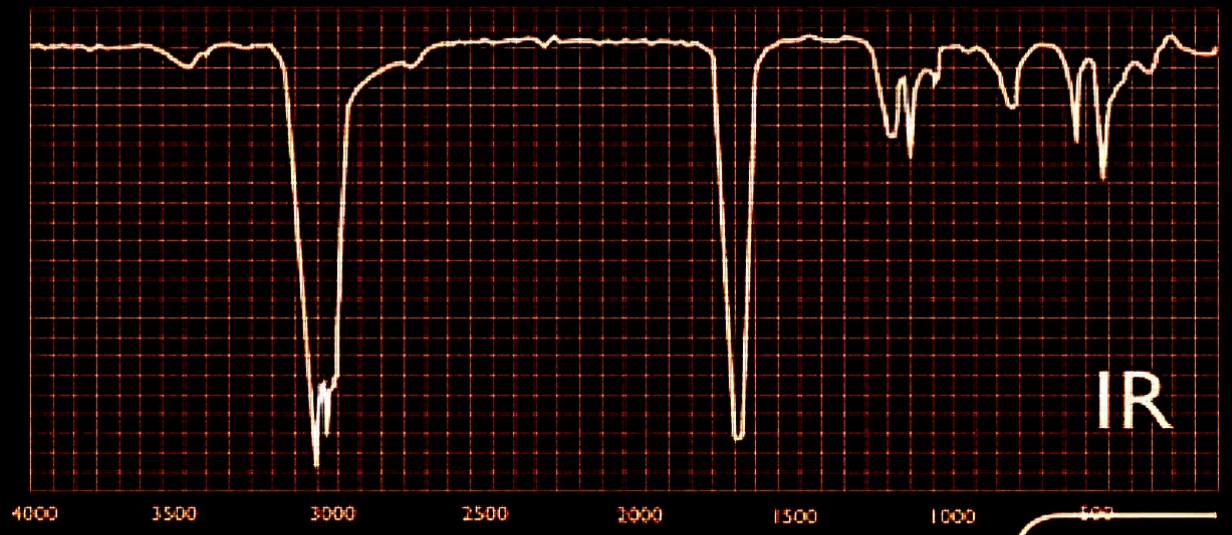
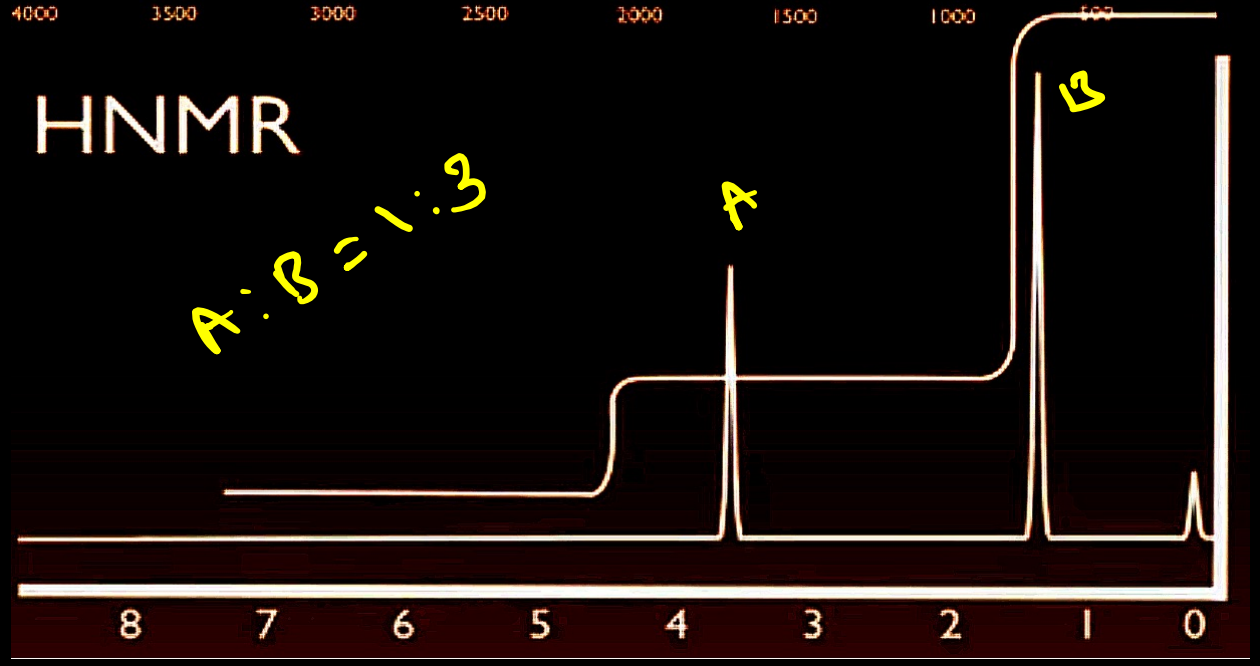
C≡N	2260-2220	medium
C≡C	2260-2100	weak-medium
C=C	1680-1600	medium
C=N	1650-1550	medium
C=O	1780-1650	strong
C—O	1250-1050	strong



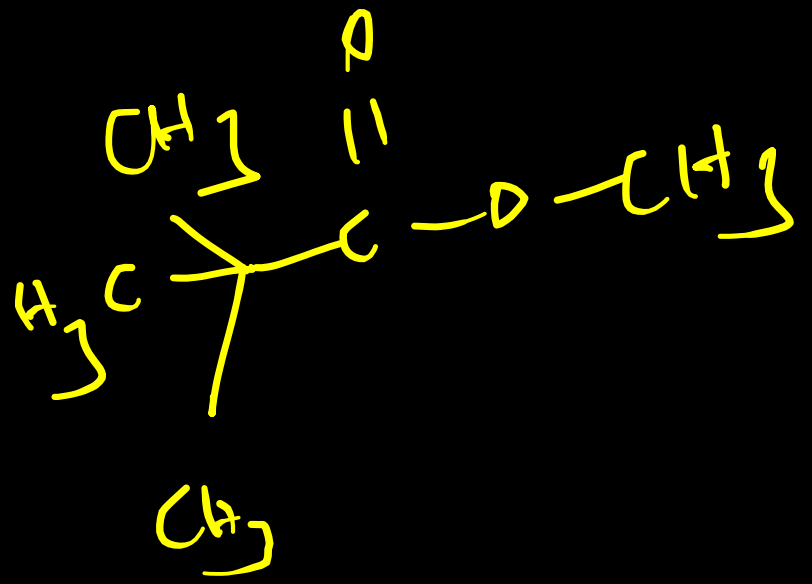


Determining structure in organic chemistry





Molecular formula: $C_6H_{12}O_2$



Thank You

For any queries related to CML101-Organic Chemistry:

Send a mail to vaitla@chemistry.iitd.ac.in

(or) you can send a message in MS teams