CH-314 Structural Analysis
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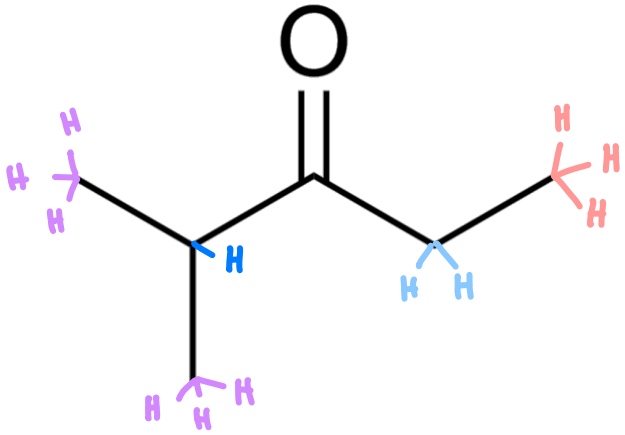
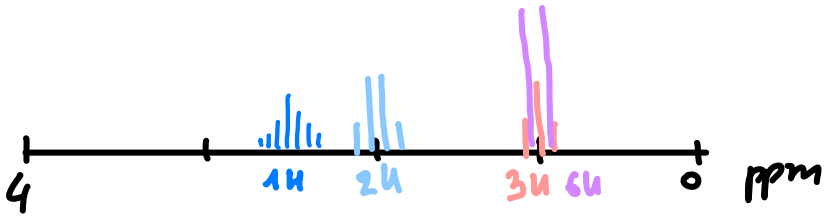
Jigsaw 2D

Combining your knowledge: Spectrum from a molecule
[Typical exam question]

The structure of 2-methyl-3-pentanone is given below.



1. Predict the ^{1}H spectrum. Show the relative intensities and the multiplicity expected from each hydrogen environment due to 3-bond couplings. Be sure to label the expected chemical shift of each peak.



2. How many signals would the ^{13}C spectrum of the molecule have if it was recorded (i) with and (ii) without proton decoupling?

1) With proton decoupling => 5 6 signals

2) without proton decoupling => 14 6 signals including multiplets giving us 18 total peaks.

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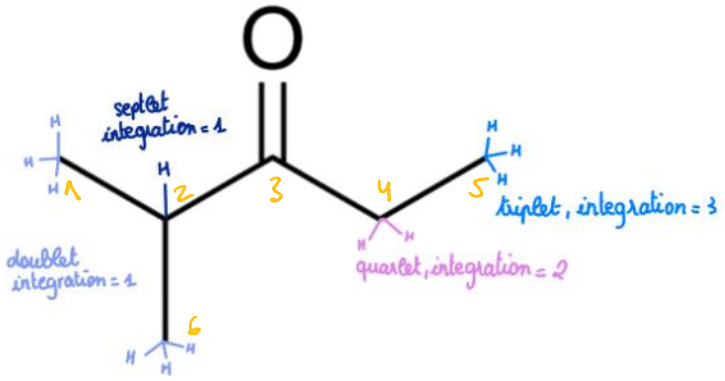
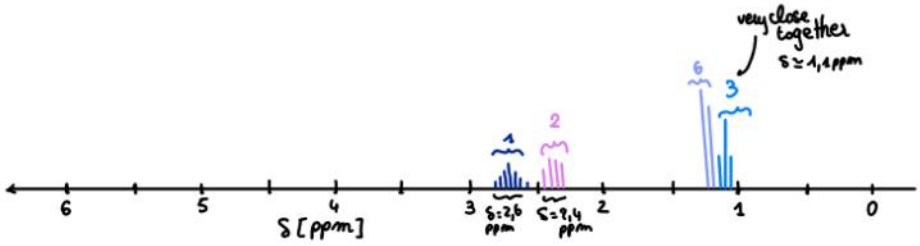


1. Predict the ^{1}H spectrum. Show the relative intensities and the multiplicity expected from each hydrogen environment due to 3-bond couplings. Be sure to label the expected chemical shift of each peak.



2. How many signals would the ^{13}C spectrum of the molecule have if it was recorded (i) with and (ii) without proton decoupling?

In practice we observe 5 as 1 and 6 are equivalent (there is a plane of symmetry in this molecule)

There's 6 carbons in the molecule.
(i) with proton decoupling, we will see 6 singlet peaks
(ii) without proton decoupling, it depends on the number of Hydrogen attached.
singlet for C without an H, doublet for one H attached, etc.
So here, there will be 6 multiplets: 3 quartet (C-1,5,6), 1 triplet (C-4), 1 doublet (C-2) and one singlet (C-3).

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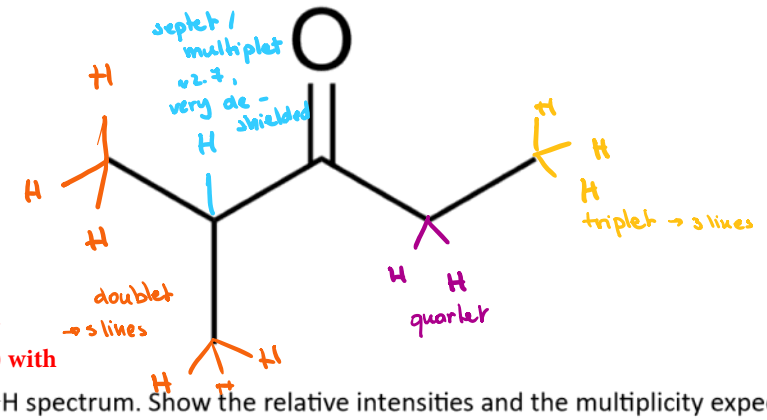


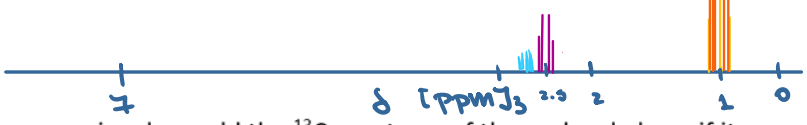
they are chemically equivalent, so they would all appear as a doublet (2 peaks) with intensity 6

1. Predict the ^{1}H spectrum. Show the relative intensities and the multiplicity expected from each hydrogen environment due to 3-bond couplings. Be sure to label the expected chemical shift of each peak.

The spectrum could be better qualitatively...

close in signal than they superpose (only around 0.2 ppm difference)

Septet with relative intensities of 1:6:15:20:15:6:1



2. How many signals would the ^{13}C spectrum of the molecule have if it was recorded (i) with and (ii) without proton decoupling?

ii) 5 : 2 of them are equivalent

i) 14 : for each carbon we add as many peaks as the amount of hydrogen it has
two quartets: CH_2-CH_3
$CH-CH_3$
doublet : CH
triplet : CH_2
singlet : C=O