

SUBJECT - CHEMISTRY

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CLASS - B.Sc (Hons) PART - III

PAPER - V

TOPIC - The nmr spectra

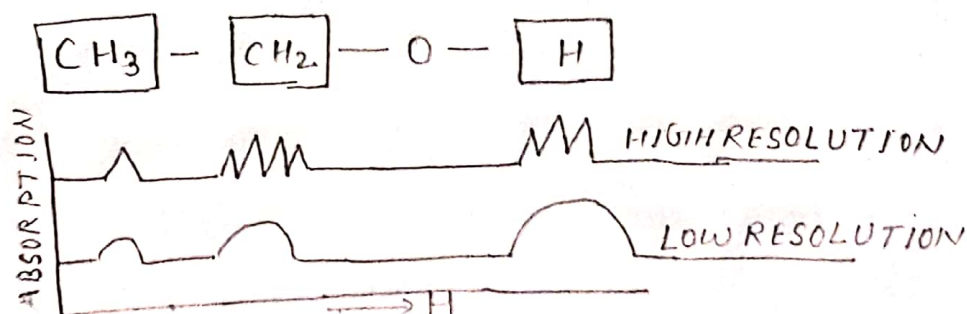
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Q Sketch the nmr spectra of ethanol solution both under high and low resolutions:

Ans $^{12}\text{C}_6$ and $^{16}\text{O}_6$ have no nuclear spin and hence they do not contribute to nmr spectrum. So the nmr spectrum of ethanol arises only due to the proton. Hence we expect only one peak but its nmr spectrum shows three peaks even at low resolution. In ethanol, protons have different environments and fields experienced are also different and hence absorption peaks are different.

When chemical environment is the same, peaks should be identical. The electrical surrounding of the proton in CH_3 group is not the same as that of CH_2 or OH group and hence three peaks are obtained. The areas under the curve 3:2:1 corresponds to CH_3 , CH_2 and OH protons respectively.



out of three, two peaks are split up under high resolution, though the areas under the curve remain the same. This splitting arises due to interaction between the spins of neighbouring nuclei.

The field faced by CH_3 protons is influenced by the proton spin arrangements of the adjacent carbon i.e. CH_2 . Two protons of CH_2 group can have three possible spin orientations that may affect the resonance frequencies of the protons of CH_3 group as shown below.

a $\uparrow\uparrow$

b $\uparrow\downarrow \downarrow\uparrow$

c $\downarrow\downarrow$

The intensity of the peaks a:b:c is in the ratio of 1:2:1. Obviously CH_3 group peak is split into three 1:2:1 ratio. Similarly CH_2 group is affected by possible orientations of three protons present in CH_3 group. These three protons can have four possible orientations. The intensity of peaks a:b:c:d is in the ratio of 1:3:3:1.

a $\uparrow\uparrow\uparrow$

b $\uparrow\downarrow\downarrow \downarrow\uparrow\downarrow \downarrow\downarrow\uparrow$

c $\downarrow\uparrow\uparrow \uparrow\downarrow\uparrow \uparrow\uparrow\downarrow$

d $\downarrow\downarrow\downarrow$

The CH_2 group peak is split into four in 1:3:3:1 ratio. Even under high resolution, the O-H peak does not split due to rapid proton transfer among many molecules. Such transfer is catalysed by acid or base. Moreover, the O-H peak is also expected to split into three and CH_2 into eight lines in the case of pure ethanol.