

Q Explain spin-spin interaction (or coupling) of nmr signals with a suitable example.

Ans The splitting of nmr signal into  $2nI+1$  peaks due to interaction of adjacent nuclear spins under high resolution is called spin-spin interaction, where  $n$  is the number of equivalent protons on the adjacent group. Though signal splits but the area under the curve remains the same. Unlike chemical shift ( $\delta$ ), it is independent of magnetic field. The relative peak intensities are given by coefficients of terms in the expansion of  $(\gamma+1)^n$ :

$$(\gamma+1)^1 = \gamma+1 \text{ i.e. } 1:1$$

$$(\gamma+1)^2 = \gamma^2 + 2\gamma + 1 \text{ i.e. } 1:2:1$$

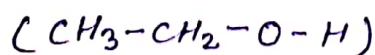
$$(\gamma+1)^3 = \gamma^3 + 3\gamma^2 + 3\gamma + 1 \text{ i.e. } 1:3:3:1$$

$$(\gamma+1)^4 = \gamma^4 + 4\gamma^3 + 6\gamma^2 + 4\gamma + 1 \text{ i.e. } 1:4:6:4:1$$

$$(\gamma+1)^5 = \gamma^5 + 5\gamma^4 + 10\gamma^3 + 10\gamma^2 + 5\gamma + 1 \text{ i.e. } 1:5:10:10:5:1$$

It is not operative beyond three bonds and so splitting occurs due to neighbouring H-atoms and no splitting is caused by protons of the same environment or equivalent protons.

Let us consider ethanol



$$\text{Number of peaks for } \text{CH}_2 = 2nI+1 = 2 \times 3 \times \frac{1}{2} + 1 = 4$$

$$\text{Number of peaks for } \text{CH}_3 = 2 \times 2 \times \frac{1}{2} + 1 = 3$$

The nuclear spin of two protons of CH<sub>2</sub> group can have three possible orientations that may affect the resonance frequencies of protons of CH<sub>3</sub> group:

Orientations	I	Peak intensity
↑↑	+1	1
↑↓ ↓↑	0	2
↓↓	-1	1

The nuclear spin of CH<sub>3</sub> protons interacts with I = +1, 0, -1 and thus splits into three peaks in the peak height i.e. intensity ratio 1:2:1

The nuclear spin of three protons of CH<sub>3</sub> group can have four possible orientations that may affect the resonance frequencies of protons of CH<sub>2</sub> group

Orientations	I	Peak intensity
↑↑↑	+3/2	1
↓↑↑ ↑↓↑ ↑↑↓	+1/2	3
↑↓↓ ↑↓↑ ↓↑↓	-1/2	3
↓↓↓	-3/2	1

The nuclear spin of CH<sub>2</sub> protons interacts with the nuclear spin of CH<sub>3</sub> protons and thus CH<sub>2</sub> signal splits into four peaks in the intensity ratio 1:3:3:1. The O-H peak does not split due to the presence of O-atom (I=0) between C & H-atoms. The <sup>1</sup>H nmr spectrum for ethanol under high and low resolution is shown as:

