The (n+1) Rule, an empirical rule used to predict the multiplicity and, in conjunction with Pascal's triangle, splitting pattern of peaks in $^1$H and $^{13}$C NMR spectra, states that if a given nucleus is coupled (see spin coupling) to n number of nuclei that are equivalent (see equivalent ligands), the multiplicity of the peak is $n+1$. eg. 1:

![Diagram](image1.png)

1

The three hydrogen nuclei in 1, \(\text{H}_a\), \(\text{H}_b\), and \(\text{H}_c\), are equivalent. Thus, 1H NMR spectrum of 1 \(\text{H}_a\)s only one peak. \(\text{H}_a\), \(\text{H}_b\), and \(\text{H}_c\) are coupled to no hydrogen nuclei. Thus, for \(\text{H}_a\), \(\text{H}_b\), and \(\text{H}_c\), n=0; \((n+1) = (0+1) = 1. The multiplicity of the peak of \(\text{H}_a\), \(\text{H}_b\), and \(\text{H}_c\) is one. The peak \(\text{H}_a\)s one line; it is a singlet. eg. 2:

![Diagram](image2.png)

2

There are two sets of equivalent hydrogen nuclei in 2:

- Set 1: \(\text{H}_a\)
- Set 2: \(\text{H}_b\), \(\text{H}_c\)

Thus, the 1H NMR spectrum of 2 \(\text{H}_a\)s two peaks, one due to \(\text{H}_a\) and the other to \(\text{H}_b\) and \(\text{H}_c\).

The peak of \(\text{H}_a\): There are two vicinal hydrogens to \(\text{H}_a\): \(\text{H}_b\) and \(\text{H}_c\). \(\text{H}_b\) and \(\text{H}_c\) are equivalent to each other but not to \(\text{H}_a\). Thus, for \(\text{H}_a\), n=2; \((n+1) = (2+1) = 3. The multiplicity of the peak of \(\text{H}_a\) is three.
The peak $\{H_a\}$'s three lines; from the Pascal's triangle, it is a triplet.

The peak of $\{H_b\}$ and $\{H_c\}$: There is only one vicinal hydrogen to $\{H_b\}$ and $\{H_c\}$: $\{H_a\}$. $\{H_a\}$ is not equivalent to $\{H_b\}$ and $\{H_c\}$. Thus, for $\{H_b\}$ and $\{H_c\}$, $n=1$; $(n+1) = (1+1) = 2$. The multiplicity of the peak of $\{H_b\}$ and $\{H_c\}$ is two. The peak $\{H_a\}$'s two lines, from the Pascal's triangle, it is a doublet.

To determine the multiplicity of a peak of a nucleus coupled to more than one set of equivalent nuclei, apply the $(n+1)$ Rule independently to each other.

**eg:**

![Chemical Structure](image)

There are three set of equivalent hydrogen nuclei in 3:

- Set 1: $\{H_a\}$
- Set 2: $\{H_b\}$
- Set 3: $\{H_c\}$

<table>
<thead>
<tr>
<th></th>
<th>$H_a$</th>
<th>$H_b$</th>
<th>$H_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_a$</td>
<td>geminal; coupling occurs</td>
<td>vicinal; coupling occurs</td>
<td></td>
</tr>
<tr>
<td>$H_b$</td>
<td>geminal; coupling occurs</td>
<td></td>
<td>vicinal; coupling occurs</td>
</tr>
<tr>
<td>$H_c$</td>
<td>vicinal; coupling occurs</td>
<td>vicinal; coupling occurs</td>
<td></td>
</tr>
</tbody>
</table>

peak of $\{H_a\}$:
multiplicity of the peak of $H_a = 2 \times 2 = 4$. To determine the splitting pattern of the peak of $H_a$, use the Pascal's triangle, based on the observation that, for alkenyl hydrogens, $J_{\text{cis}} > J_{\text{gem}}$.

The peak of $H_a$ is a doublet of a doublet.

peak of $H_b$:

multiplicity of the peak of $H_b = 2 \times 2 = 4$. To determine the splitting pattern of the peak of $H_b$, use the Pascal's triangle, based on the observation that, for alkenyl hydrogens, $J_{\text{trans}} > J_{\text{gem}}$.

The peak of $H_b$ is a doublet of a doublet.
The peak of $H_b$ is a doublet of a doublet.

peak of $H_c$:

\[(n+1) = (1+1) = 2\]

multiplicity of the peak of $H_c = 2 \times 2 = 4$. To determine the splitting pattern of the peak of $H_c$, use the Pascal’s triangle based on the observation that, for alkenyl hydrogens, $J_{\text{trans}} > J_{\text{cis}}$).

The peak of $H_c$ is a doublet of a doublet.
Contributors and Attributions

- Gamini Gunawardena from the OChemPal site (Utah Valley University)