M.Sc. Semester-III
Core Course - 7 (CC-7)
Application of Spectroscopy

III. Nuclear Magnetic Resonance Spectroscopy

L3: Classification of Protons and No of Signals

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Classification of Protons

- To interpret or predict NMR spectra, one must first be able to classify proton (or carbon) environments.
- Easiest to classify are those that are unrelated, or <u>different</u>. Replacement of each of those one at a time with some group (G) in separate models creates <u>**constitutional isomers**</u>.

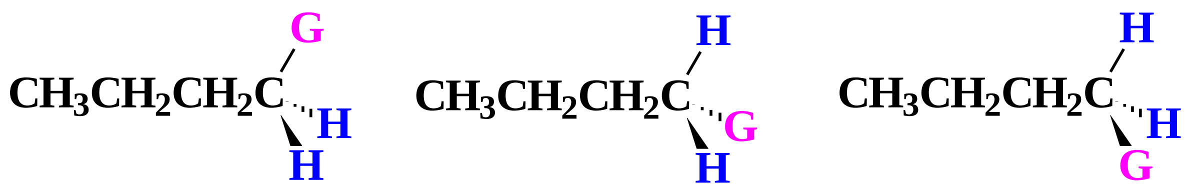
$$CH_3CH_2CH_2CH_3: \qquad CH_3CH_2\overset{G}{\overset{|}{C}}HCH_3 \qquad CH_3CH_2CH_2\overset{G}{\overset{|}{C}}H_2$$

These protons have <u>**different**</u> **chemical shifts.** This classification is usually the most obvious.

Classification of Protons

- **Homotopic** hydrogens are those that upon replacement one at a time with some group (**G**) in separate models creates **identical structures.**

$CH_3CH_2CH_2CH_3$:

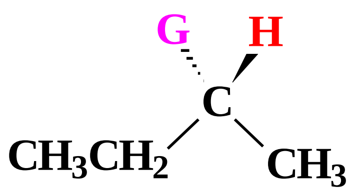


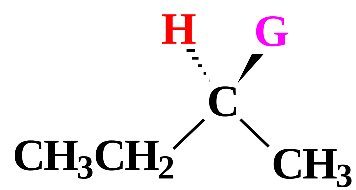
Homotopic protons have **the same chemical shifts.** We sometimes call them identical. Methyl hydrogens will always be in this category (because of free rotation around the bond to the methyl carbon). Molecular symmetry can also make protons homotopic.

Classification of Protons

- If replacement of one hydrogen at a time in separate models creates enantiomers, the hydrogens are **enantiotopic**.

$CH_3CH_2CH_2CH_3$:

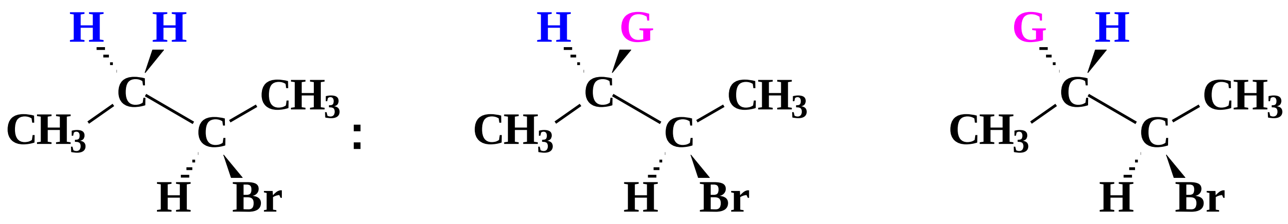




Enantiotopic protons have **the same chemical shifts.**

Classification of Protons

- If replacement of hydrogens in separate models creates diastereomers, the hydrogens are **diastereotopic**.



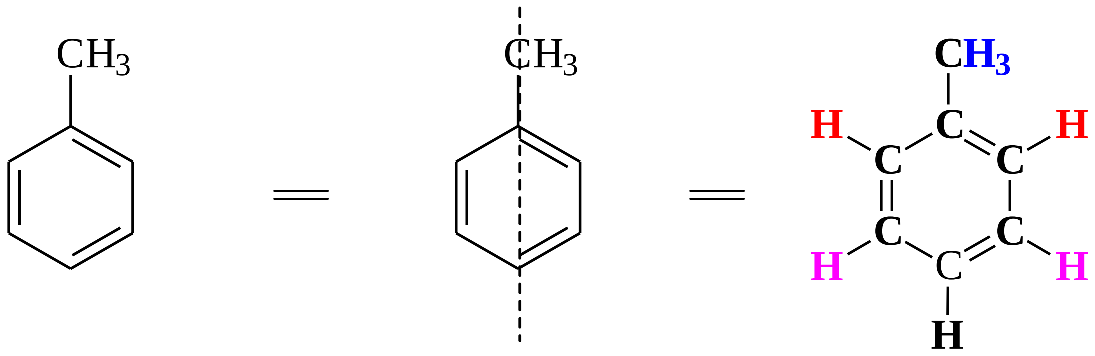
Diastereotopic protons have **different chemical shifts.** Usually, in order to have diastereotopic protons, there has to be a stereocenter somewhere in the molecule. However, cis-trans alkene stereoisomers may also have diastereotopic protons.

^{1}H NMR Problems

- How many unique proton environments are there in:

CH_3CH_2Br = CH_3CH_2Br **2 environments**

$CH_3OCH_2CH_2CH(CH_3)CH_3$ = $CH_3OCH_2CH_2CH(CH_3)CH_3$ **5 environments**



4 environments

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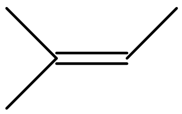
^{1}H NMR Problems



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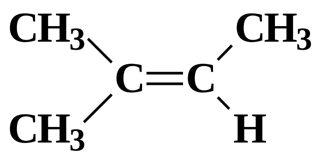

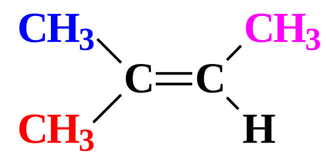

4 environments

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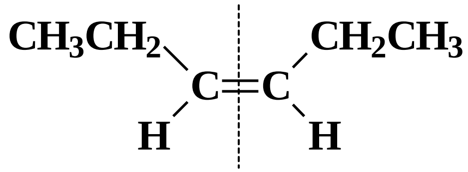
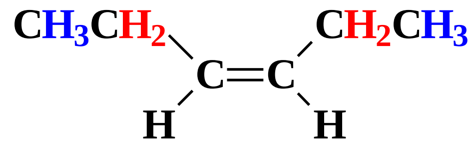
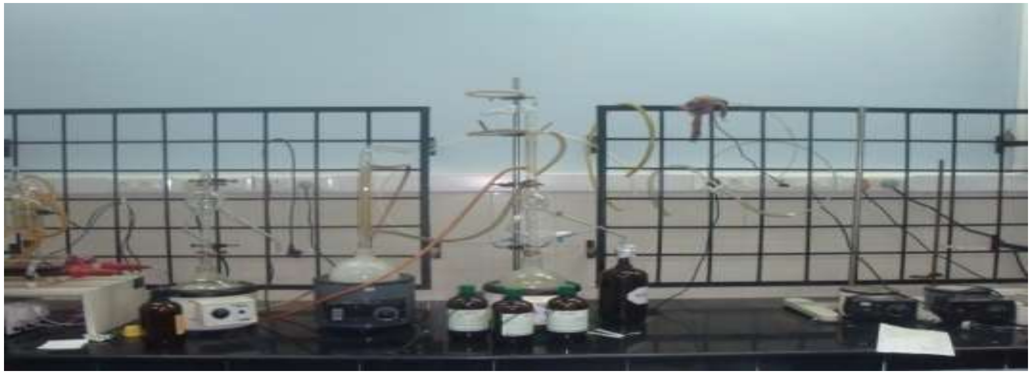




3 environments

Symmetry Simplifies Spectra!!!

Thank You



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