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

III. Nuclear Magnetic Resonance Spectroscopy

L2: Chemical Shift

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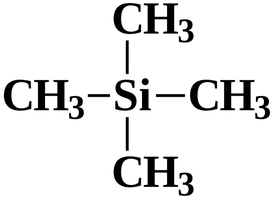
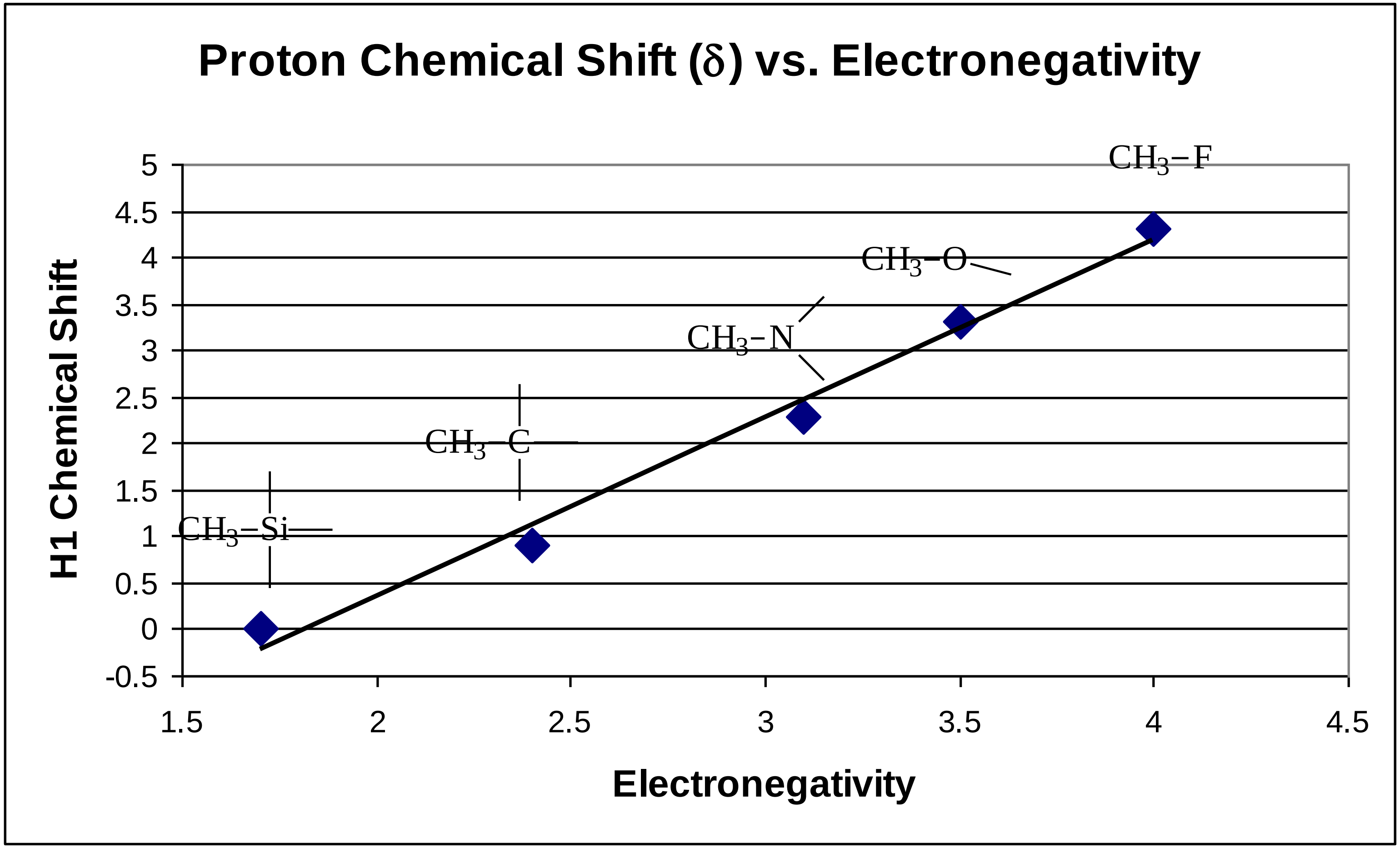
Chemical Shift

- We define the relative position of absorption in the NMR spectrum the **chemical shift**. It is a unitless number (actually a ratio, in which the units cancel), but we assign ‘units’ of ppm or δ (Greek letter delta) units.
- For ^{1}H, the usual scale of NMR spectra is 0 to 10 (or 12) ppm (or δ).
- The usual ^{13}C scale goes from 0 to about 220 ppm.
- The zero point is defined as the position of absorption of a standard, tetramethylsilane (TMS):
- This standard has only one type of C and only one type of H.



Chemical Shifts

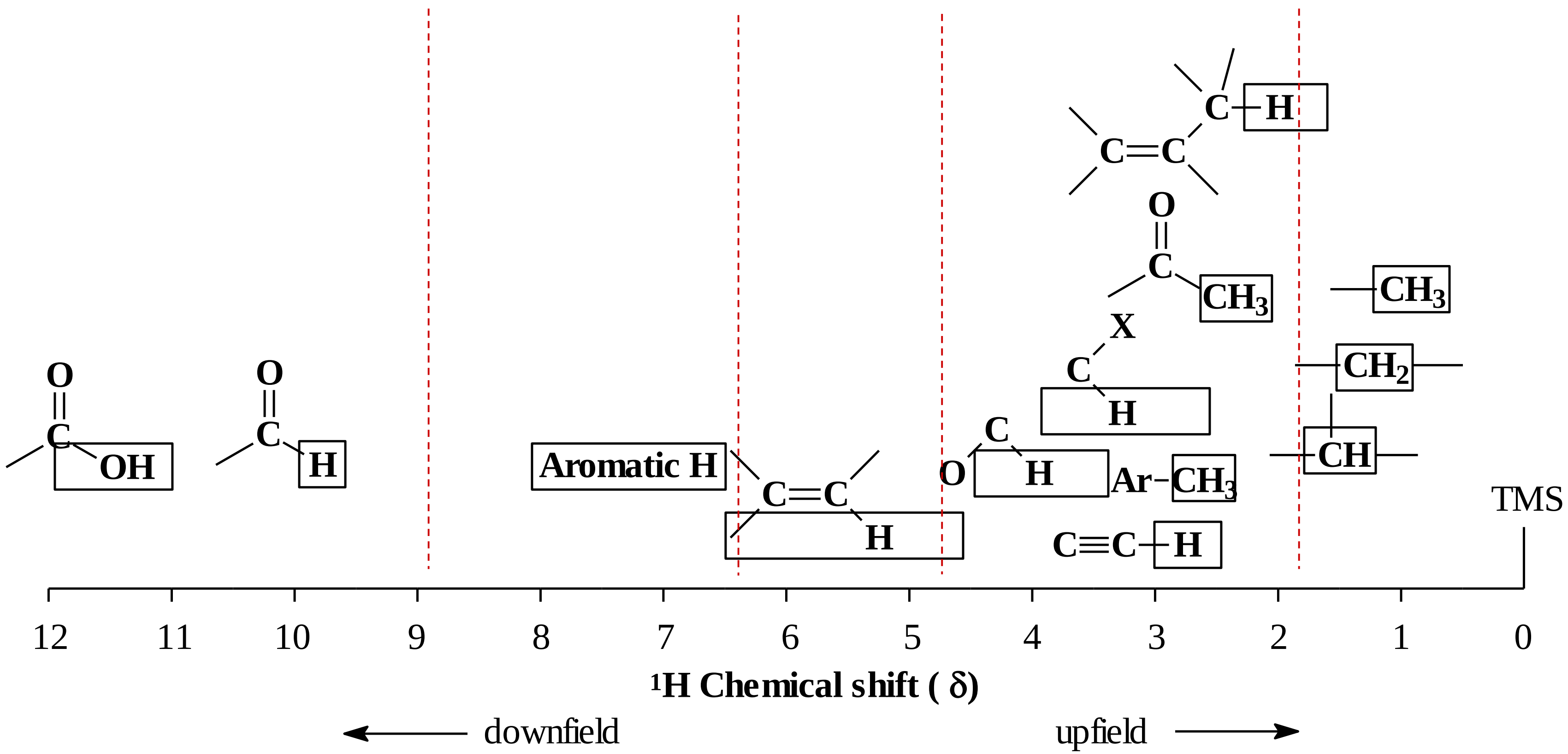


Chemical Shifts

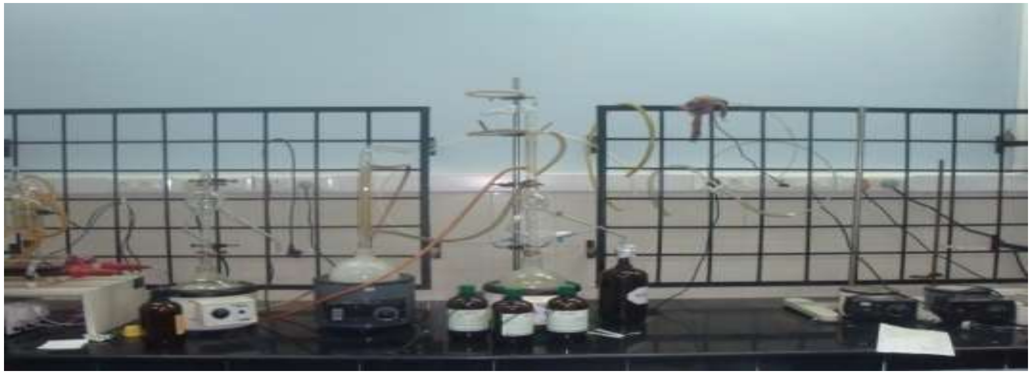
- Both ^{1}H and ^{13}C Chemical shifts are related to three major factors:
  - The hybridization (of carbon)
  - Presence of electronegative atoms or electron attracting groups
  - The degree of substitution (1º, 2º or 3º). These latter effects are most important in ^{13}C NMR, and in that context are usually called 'steric' effects.
- Now we'll turn our attention to ^{1}H NMR spectra

(they are more complex, but provide more structural information)

^{1}H Chemical Shifts



Thank You



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