

12.11: CHEMICAL SHIFTS AND INTERPRETING ^{13}C NMR SPECTRA

^{13}C NMR CHEMICAL SHIFTS

The Carbon NMR is used for determining functional groups using characteristic shift values. ^{13}C chemical shift is affected by electronegative effect and steric effect. If an H atom in an alkane is replaced by substituent X, electronegative atoms (O, N, halogen), α -carbon and β -carbon shift to downfield (left; increase in ppm) while γ -carbon shifts to upfield. The steric effect is observed in acyclic and cyclic systems, which leads to downshifted chemical shifts. Figure 9 shows typical ^{13}C chemical shift regions of the major chemical class.

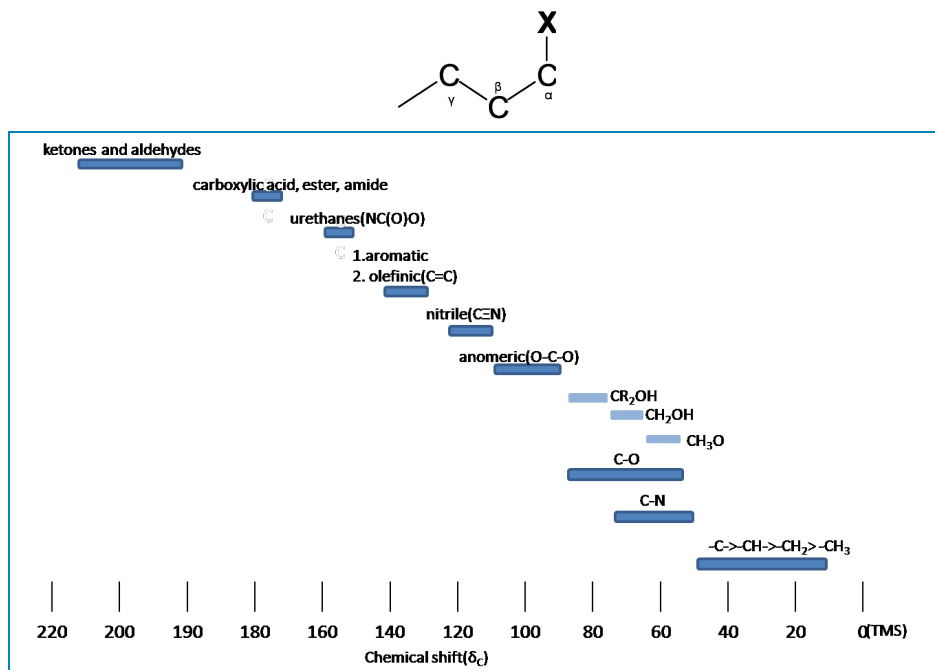


Figure 9: ^{13}C Chemical shift range for organic compound

SPIN-SPIN SPLITTING

Comparing the ^1H NMR, there is a big difference thing in the ^{13}C NMR. The ^{13}C - ^{13}C spin-spin splitting rarely exists between adjacent carbons because ^{13}C is naturally lower abundant (1.1%)

- ^{13}C - ^1H Spin coupling:** ^{13}C - ^1H Spin coupling provides useful information about the number of protons attached to a carbon atom. In case of one bond coupling ($^1J_{\text{CH}}$), $-\text{CH}$, $-\text{CH}_2$, and CH_3 have respectively doublet, triplet, quartets for the ^{13}C resonances in the spectrum. However, ^{13}C - ^1H Spin coupling has a disadvantage for ^{13}C spectrum interpretation. ^{13}C - ^1H Spin coupling is hard to analyze and reveal structure due to a forest of overlapping peaks that result from 100% abundance of ^1H .
- Decoupling:** Decoupling is the process of removing ^{13}C - ^1H coupling interaction to simplify a spectrum and identify which pair of nuclei is involved in the J coupling. The decoupled ^{13}C spectra shows only one peak (singlet) for each unique carbon in the molecule (Fig 10.). Decoupling is performed by irradiating at the frequency of one proton with continuous low-power RF.

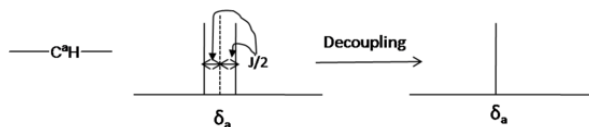


Fig 10. Decoupling in the ^{13}C NMR

CONTRIBUTORS AND ATTRIBUTIONS

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