Introduction to $^{13}$C-NMR Spectroscopy

Main topics

- $^{13}$C-atom chemical shift range
- $^1$H-coupled and decoupled $^{13}$C-NMR spectra
$^1$H-NMR Spectrum of $n$-pentane

300 MHz $^1$H NMR
In CDCl$_3$

three $^1$H-atom environments

$^1$H NMR spectrum of $n$-pentane showing three distinct environments at 5.94 and 6.00 ppm.
The ¹H-NMR spectrum of n-hexane shows three distinct environments. The spectrum was recorded at 300 MHz using CDCl₃ as the solvent.

The chemical shifts observed are at 8.00 and 6.00 ppm, indicating the presence of different types of hydrogen atoms in the molecule.
$^1$H-NMR Spectrum of $n$-docosane

300 MHz $^1$H NMR
In CDCl$_3$
$^{13}$C-NMR Spectroscopy

$^{13}$C is NMR active ($I = \frac{1}{2}$); $^{12}$C is NMR inactive ($I = 0$).

The natural abundance of $^{13}$C is $\sim 1.1\%$.

A greater chemical shift range provides greater differentiation of signals; reduced 2nd order effects.

Often the NMR experiment is performed in a $^1$H-decoupled manner to simplify the spectrum; removes coupling to H-atoms.
$^{13}$C-NMR Spectrum of $n$-Hexane

$^{13}$C-atom environments

75 MHz $^{13}$C NMR
In CDCl$_3$
$^{13}$C-NMR Spectrum of Methanol

$^1$H is > 99% abundant; it couples strongly to $^{13}$C – atom it is attached to ($^1$J$_{HC}$ = 100-210 Hz) with normal $n+1$ rule splitting.

512 scans
30 min
10 M concentration
$^{13}$C-NMR Spectrum of Ethanol

CDCl$_3$

CH$_3$CH$_2$OH

$^{1}$H – Coupled

$^{1}$H – Decoupled

512 scans
30 min
10 M concentration
$^{13}$C-NMR Spectrum of Ethyl Cyanoacetate

512 scans
30 min
0.35 M concentration
\[ ^{13}\text{C}-\text{NMR Spectrum of Ethyl Cyanoacetate} \]

75 MHz \[^{13}\text{C}\] NMR
In CDCl\(_3\)

Isotropic NMR Shifts relative to TMS calculated with WebMO/Gaussian09 at B3LYP/6-31G(d)
Determination of 4’-sulfamoylacetanilide Regiochemistry
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