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# Calculating $^1$H NMR Chemical Shifts

If a carbon has more than one functional group directly attached to it, the following table can be used to estimate the chemical shift of an attached hydrogen.

**$-CH_2-$ Calculation** $\quad \delta\ (ppm)\ R_1-CH_2-R_2 = 1.2 + \Delta_{R1} + \Delta_{R2}$

Methylenes ($CH_2$) have <u>two</u> groups attached, so the starting chemical shift (1.2 ppm) will be adjusted using <u>two</u> values from the table (Δ values).

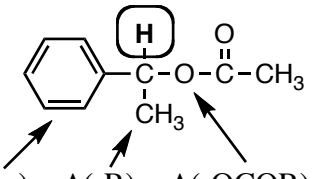
**$-CH-$ Calculation** $\quad \delta\ (ppm)\ R_2-\underset{R_3}{\overset{R_1}{C}}-H = 1.5 + \Delta_{R1} + \Delta_{R2} + \Delta_{R3}$

Methines (CH) have <u>three</u> groups attached, so the starting chemical shift (1.5 ppm) will be adjusted using <u>three</u> values from the table (Δ values).

## Protons on sp$^3$ Carbons: Chemical Shift Calculation Table

| –R | Δ | Description | –R | Δ | Description |
|---|---|---|---|---|---|
| $-CH_2R$ | 0.0 | alkyl | $-OH$ | 2.3 | α to alcohol O |
| $-CR=CR_2$ | 0.8 | allylic (next to alkene) | $-OR$ | 2.1 | α to ether O |
| $-C\equiv CR$ | 0.9 | propargylic (next to alkyne) | $-OAr$ | 2.8 | α to O of aromatic ether |
| $-C\equiv N$ | 1.2 | α to cyano | $-O-\overset{O}{\overset{\|\|}{C}}-R$ | 2.8 | α to O of ester |
| $-Ar$ | 1.4 | benzylic | $-O-\overset{O}{\overset{\|\|}{C}}-Ar$ | 3.1 | α to O of aromatic ester |
| $-\overset{O}{\overset{\|\|}{C}}-R$ | 1.2 | α to ketone or aldehyde C=O | $-NR_2$ | 1.5 | α to amine |
| $-\overset{O}{\overset{\|\|}{C}}-OR$ | 1.1 | α to ester or carb. acid C=O | $-NO_2$ | 3.2 | α to nitro |
| $-\overset{O}{\overset{\|\|}{C}}-Ar$ | 1.7 | α to C=O of aromatic ketone | $-SR$ | 1.3 | α to thiol or thioether |
| $-F$ | 3.2 | α to fluorine | | | |
| $-Cl$ | 2.2 | α to fluorine | | | |
| $-Br$ | 2.1 | α to bromine | | | |
| $-I$ | 2.0 | α to iodine | | | |

**Example:**
estimate the chemical shift of the selected proton



$\delta = 1.5 + \Delta(\text{-Ar}) + \Delta(\text{-R}) + \Delta(\text{-OCOR})$

$\delta = 1.5 + \quad 1.4 \quad + \quad 0.0 \quad + \quad 2.8$

$\delta =$ 5.7 ppm (*actual 5.4 ppm*)