

NMR Chemical Shift Data

| ¹H NMR (δ) | | ¹³C NMR δ | |
|--|---------------|---|-----------------|
| Primary alkyl CH₃ | 0.9 ppm | Aldehyde/Ketone Carbonyl C=O | 220 - 190 ppm |
| Secondary alkyl CH₂ | 1.3 ppm | Acid/Ester/Amide Carbonyl C=O | 180 - 150 ppm |
| Tertiary alkyl CH | 1.5 ppm | Alkene C=C | 150 - 100 ppm |
| Alkene = CH | 4.6 - 5.9 ppm | Aromatic C=C | 140 - 110 ppm |
| Alkyne ≡ CH | 2 - 3 ppm | Alkyne C≡C | 100 - 75 ppm |
| Aromatic Ar- H | 6 - 8.5 ppm | Alcohol C-O | 95 - 35 ppm |
| Benzylic Ar CH₃ | 2 - 2.3 ppm | Ester C-OC(O) | 95 - 35 ppm |
| Allylic = C-CH₃ | 1.7 ppm | Amine/Amide C-N | 95 - 35 ppm |
| Alkyl Fluoride R- CH₂-F | 4 - 4.5 ppm | Alkyl R- C-R | 60 - 0 ppm |
| Alkyl Chloride R- CH₂-Cl | 3 - 4 ppm | Splitting patterns in spin 1/2 nuclei (¹H, ¹³C, ¹⁹F ³¹P etc) | |
| Alkyl Bromide R- CH₂-Br | 2.5 - 4 ppm | singlet (s) | none |
| Alkyl Iodide R- CH₂-I | 2 - 4 ppm | 1:1 doublet (d) | one |
| Hydroxyl RO H | 1 - 6 ppm | 1:2:1 triplet (t) | two identical |
| Alcohol R- CH₂-OH | 3.4 - 4 ppm | 1:3:3:1 quartet (q) | three identical |
| Ether R- CH₂-OR | 3.3 - 4 ppm | 1:4:6:4:1 quintet | four identical |
| Ester R- CH₂-OC(O)R | 3.7 - 4.1 ppm | septet | six identical |
| Ester RO C(O)CH₂-R | 2 - 2.2 ppm | 1:1:1:1 doublet of doublets (dd) | two different |
| Aldehyde R CHO | 9 - 10 ppm | doublet of doublet of doublets (ddd) | three different |
| Aldehyde R- CH₂-CHO | 2 - 2.7 ppm | Unsaturation Number, U.N. = # of rings and/or double bonds | |
| Ketone R- CH₂-C(O)-R | 2 - 2.7 ppm | U.N. = {[#C - 1/2 (#H)] + 1/2(#N)} + 0(#O) + 1 | |
| Phenol Ar OH | 4 - 12 ppm | #C = number of Carbon atoms | |
| Carboxyl R- CO₂H | 10 - 12 ppm | #H = number of Hydrogen atoms (and Halogens) | |
| Amino R- NH₂ | 1 - 5 ppm | #N = number of Nitrogen atoms | |
| | | #O = number of Oxygen atoms | |