

NMR Spectrum Processing Hints

NMR interpretation means 1) accounting for ALL signals in a spectrum and 2) accounting for ALL protons in a proposed structure. No significant omissions are allowed.

There is no “right” place to start in looking at a spectrum. Information and patterns of all sorts can leap out of the page and demand your attention.

If you are stumped, a methodical approach works best. A methodical approach is also required to make sure you account for ALL signals and protons (see above).

- Label all possibly confounding peaks.
 - NMR standard (TMS at 0 ppm)
 - NMR solvent (CDCl₃ contains CHCl₃ at ~7.24 ppm + HCl (sometimes) at ~1.6 ppm)
 - Impurities generated by your experiment (solvents, unconsumed reactants, side products)
- Work with chemical shifts first. This tells you
 - how many types of protons you have to worry about
 - their chemical environments
 - sort into “alkane H”, “alkene H”, “arene H”
 - sort “alkane H” by likely deshielding groups (X), as in X-C-H or X-C-C-H
- Work with integrals next. This tells you (roughly) what number of H there are of each type
- When working with coupling patterns,
 - *do* focus on J and peak spacing (peaks must be equally spaced)
 - *don't* worry about small deviations from expected peak intensities (many factors distort intensities), but *do* worry about large deviations (a 1:1:1 triplet is impossible)
 - remember (and use) this fact: coupling is a process involving (and affecting) *two* groups of protons. Suppose you notice a quartet that integrates to 2H. You might think, “I have found a CH₂ in –CH₂CH₃” because this group contains 2H and has 3 neighbors. You should then think, “this same coupling must affect the CH₃ group too.” Is there a 3H triplet? Do the quartet and triplet have the same J?