6 things to know about $^{13}$C NMR

1. Signals weak ($\mu$ is 25% of $^1$H & only 1% abundant)
2. Signals almost always singlets:
   - no C-C splittings because 99% of neighbors are $^{12}$C
   - no C-H splittings due to “decoupling”
3. Large chemical shift range (0 to 230 ppm)
   - sp$^3$ and sp C are 0 – 100 ppm
   - sp$^2$ C are 100 – 230 ppm (C=O above 165 ppm, C=C below 165 ppm)
4. Integrations are unreliable, but ...
   - peak due to 2 equiv. carbon usually = 2x higher
   - C not bound to H (quaternary C = 4° C) are small (≈ 30 – 50% height)
5. DEPT (distortionless enhanced polarization transfer) give # of attached H:
   - DEPT 90 – see ONLY CH (3°)
   - DEPT 135 – CH (3°) and CH$_3$ (1°) are upright, CH$_2$ (2°) are upside down
6. “Accidental” peak overlap very rare → # of peaks = # of unique C atoms.
   - Using DEPTs → # of unique C atoms of each type (1°, 2°, 3° or 4°).

$^{13}$C NMR spectrum of tert-butyl acetate

[Diagram showing the NMR spectrum of tert-butyl acetate with peaks labeled a, b, c, d, and integration notes]

DEPT experiments can be used to identify resonances as due to C, CH, CH$_2$ or CH$_3$ (4°, 3°, 2° or 1° C).

The boxed parts of DEPT spectra were simulated (they were cut off in the published source).

Source: [http://www.chem.ox.ac.uk/spectroscopy/nmr/PDFs/Organic NMR 1.pdf](http://www.chem.ox.ac.uk/spectroscopy/nmr/PDFs/Organic NMR 1.pdf)

$^{13}$C NMR of cholesterol acetate (and showing how ChemDraw can predict the spectrum)

Chemical shift predictions from ChemDraw

from Duckett and Gilbert

Fig. 5.23 $^{13}$C n.m.r. spectrum (fully decoupled) of cholesterol acetate
NMR structure problem: C, 54.53; H, 9.15; O, 36.32. Name that compound (using 1H and 13C NMR)

Empirical formula
C₄H₈O₂

Identifying an unknown from NMR spectrum: example from http://www.chem.ucla.edu/~webspectra/

Elemental Analysis: C, 70.6%; H, 5.9%; O, 23.5%
Empirical Formula: C₄H₄O

1H NMR spectrum

13C NMR spectrum
CDCl₃ (77 ppm)
Expect predictions to be within ca. 0.3 ppm

ortho: 8.07
meta: 7.72

7.77
7.72

7.27 error avg 0.3 max 0.3
7.62 error avg 0.3 max 0.7