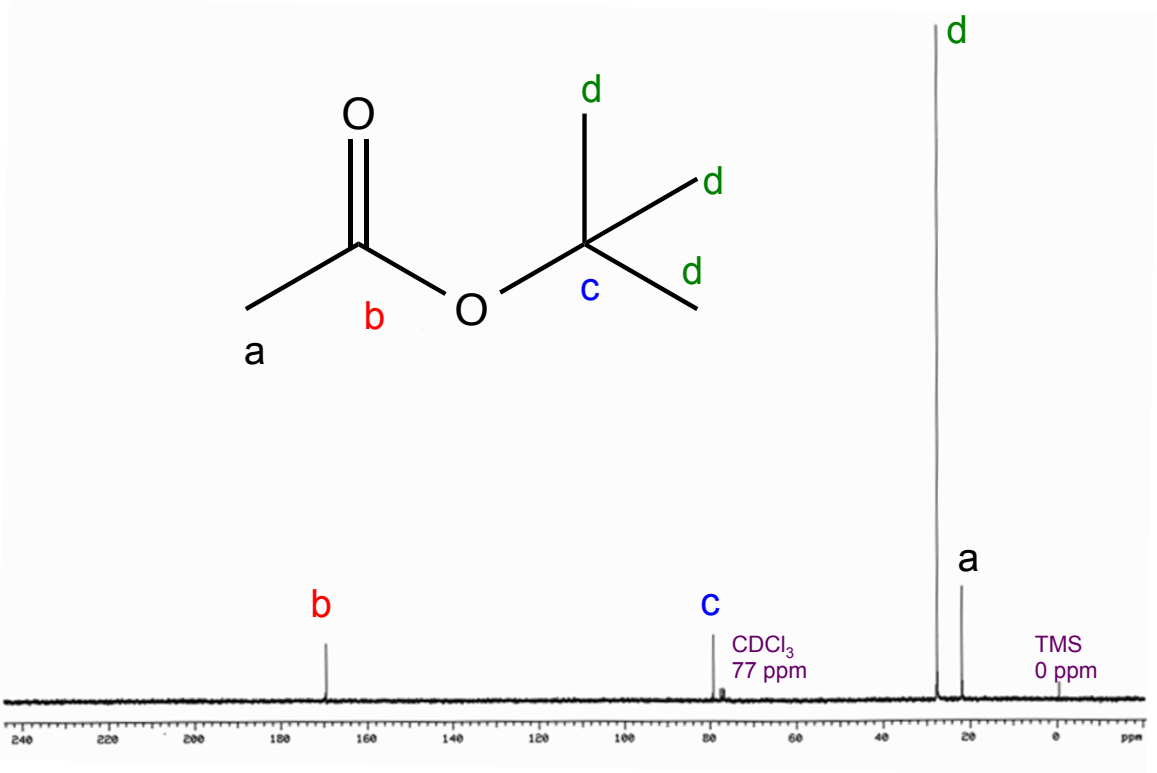
6 things to know about ^{13}C NMR

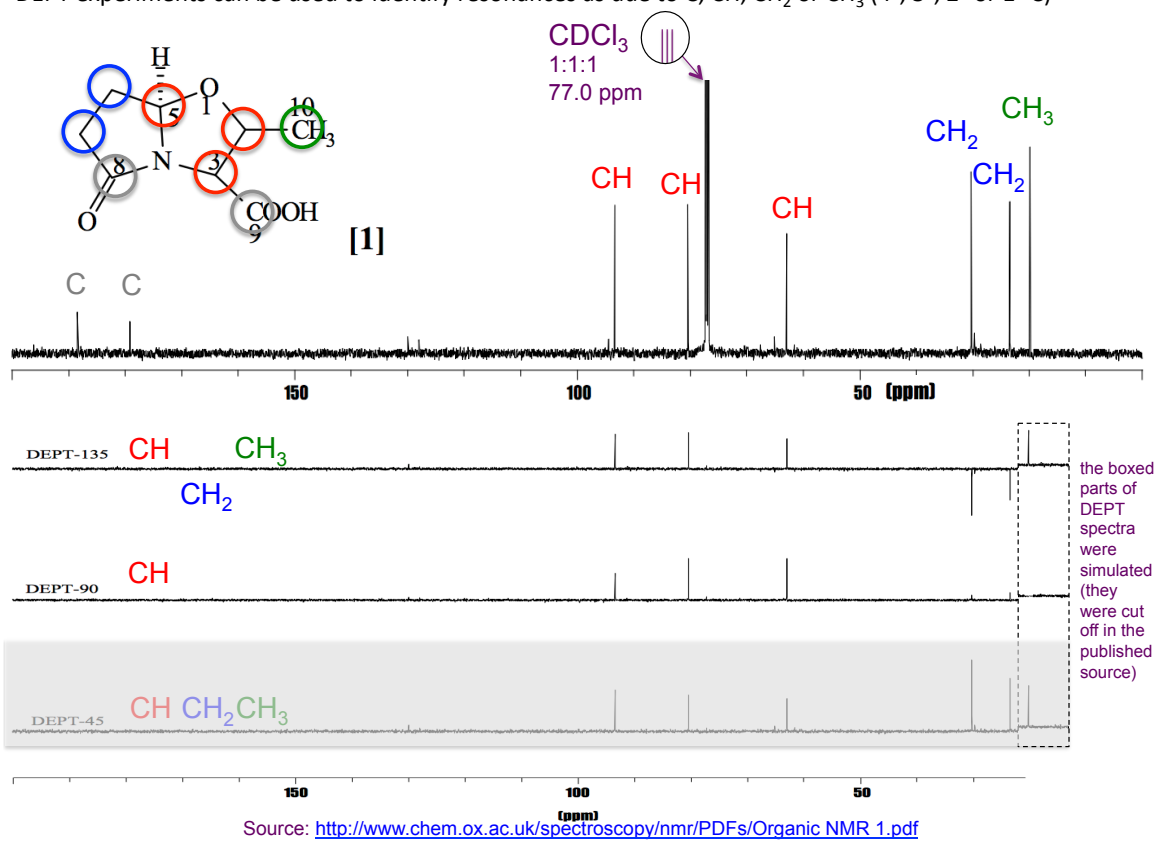
1. Signals weak (μ is 25% of ^{1}H & only 1% abundant)
2. Signals almost always singlets:
   - no C-C splittings because 99% of neighbors are ^{12}C
   - no C-H splittings due to "decoupling"
3. Large chemical shift range (0 to 230 ppm)
   - sp^3 and sp C are 0 – 100 ppm
   - sp^2 C are 100 – 230 ppm (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



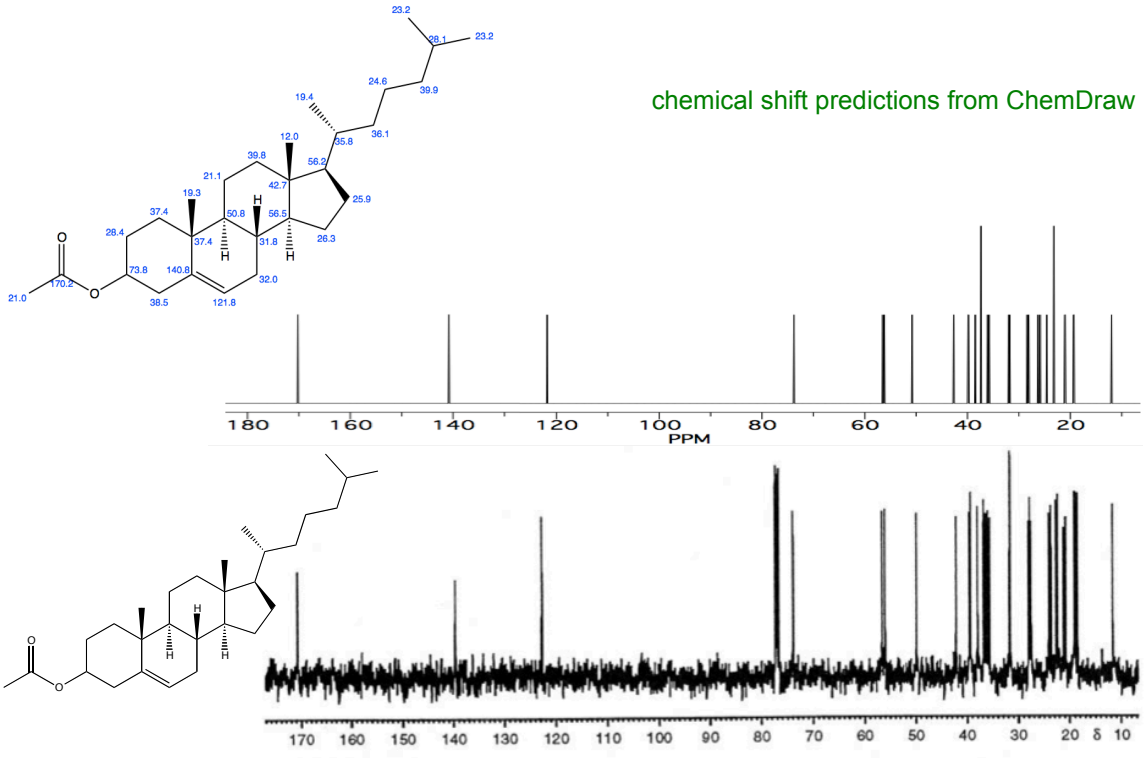
spectrumfrom http://www.wiredchemist.com/nmr/data/tbutylacetate-c13-full (11/22/13)

DEPT experiments can be used to identify resonances as due to C, CH, CH_2 or CH_3 (4°, 3°, 2° or 1° C)



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

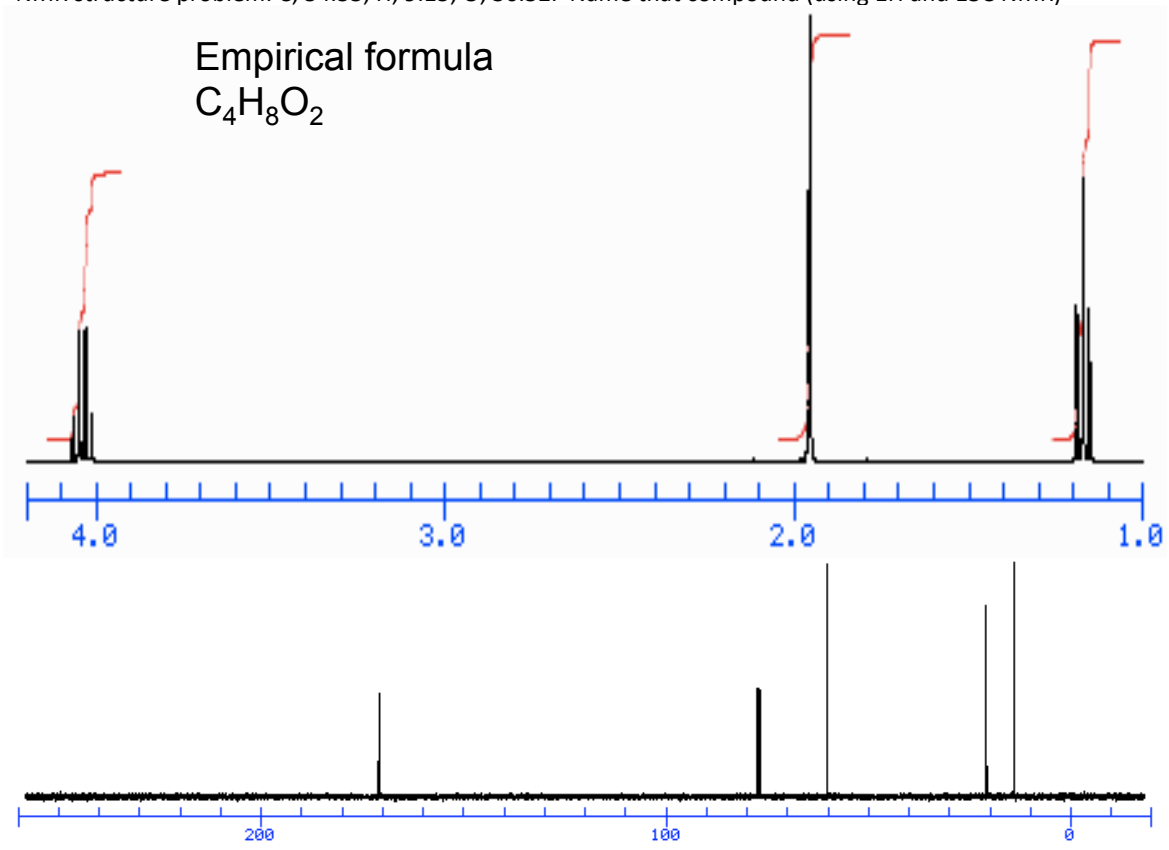
^{13}C NMR of cholesterol acetate (and showing how ChemDraw can predict the spectrum)



from Duckett and Gilbert

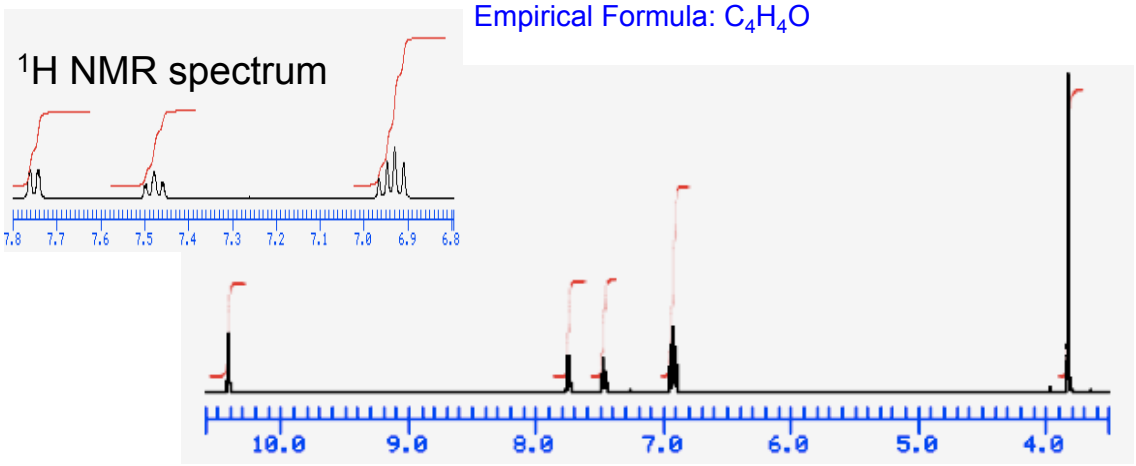
Fig. 5.23 ^{13}C n.m.r. spectrum (fully decoupled) of cholesterol acetate

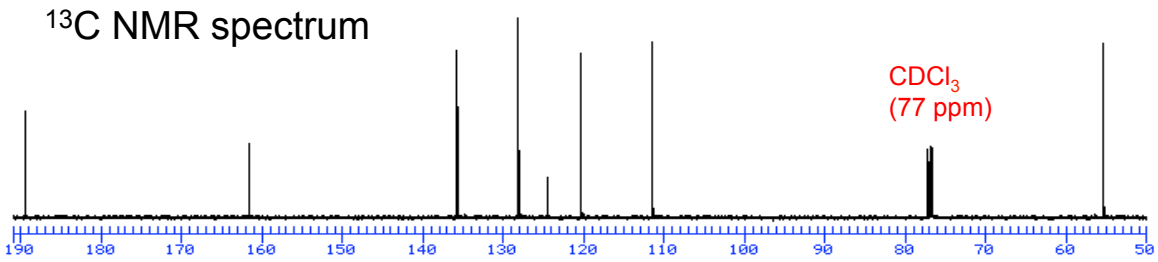
NMR structure problem: C, 54.53; H, 9.15; O, 36.32. Name that compound (using 1H and 13C NMR)



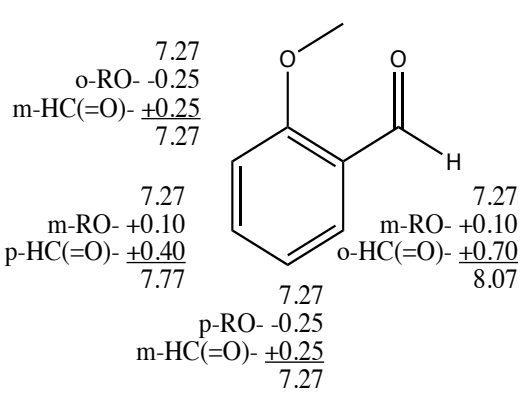
Identifying an unknown from NMR spectrum: example from http://www.chem.ucla.edu/~webspectra/

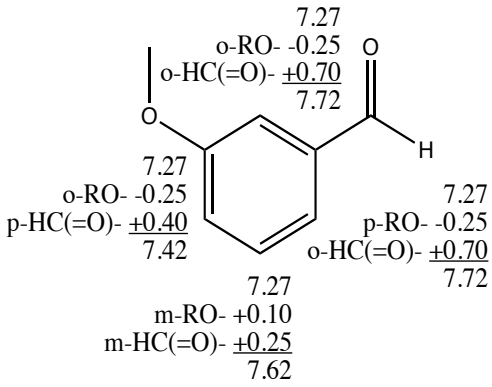
Elemental Analysis: C, 70.6%; H, 5.9%; O, 23.5%
Empirical Formula: C_4H_4O





Expect predictions to be within ca. 0.3 ppm





ortho: 8.07 7.77 7.27 7.27 error avg 0.3 max 0.3

meta: 7.72 7.72 7.62 7.27 error avg 0.3 max 0.7