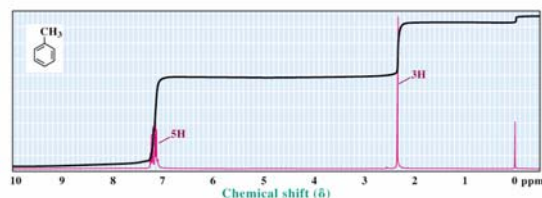


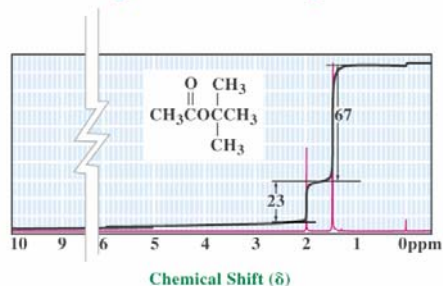
## Signal Areas

- ◆ Relative areas of signals are proportional to the number of hydrogens giving rise to each signal.
- ◆ All modern NMR spectrometers electronically integrate and record the area of each signal.

<sup>1</sup>H-NMR spectrum of toluene



<sup>1</sup>H-NMR spectrum of *tert*-butyl acetate



## Interpreting NMR spectra

- ◆ **Alkanes:** all <sup>1</sup>H-NMR signals fall in the narrow range of δ 0.8-1.7 (→ 4.5). <sup>13</sup>C signals fall in the considerably wider range of δ 0-60 (→ 85).
- ◆ **Alkenes:** vinylic hydrogens typically fall in the range δ 4.5-6.0
  - coupling constants are generally larger for *trans* vinylic hydrogens (*J*= 11-18 Hz) compared with *cis* vinylic hydrogens (*J*= 5-10 Hz).
  - the sp<sup>2</sup> hybridized carbons of alkenes give <sup>13</sup>C-NMR signals in the range δ 100-150 -- more typically 120-150 -- which is downfield from the signals of sp<sup>3</sup> hybridized carbons.

## Interpreting NMR spectra

- ◆ **Alkynes:**
  - Terminal alkynes appear between <sup>1</sup>H δ 2-3.
  - Alkyne carbons appear between δ 60-100.
  - Nitrile (C≡N) carbons appear downfield, δ 100-120.
- ◆ **Aromatic Compounds:**
  - Hydrogens attached to an aromatic ring appear downfield of vinylic protons, typically between δ 6.5 and 8.
  - Aromatic carbon atoms are almost always found between δ 120 and 160.

## Interpreting NMR spectra

- ◆ **Alcohols:**
  - the chemical shift of the hydroxyl hydrogen is variable. It normally falls in the range δ 3.0-4.5, but may be as low as δ 0.5.
  - hydrogens on an sp<sup>3</sup> hybridized carbon adjacent to the -OH group are deshielded by the electron-withdrawing inductive effect of the oxygen and their signals appear in the range δ 3.3-4.5.
- ◆ **Ethers:**
  - a distinctive feature in the <sup>1</sup>H-NMR spectra of ethers is the chemical shift, δ 3.3-4.5, of hydrogens on carbon attached to the ether oxygen. **This also appears in esters.**

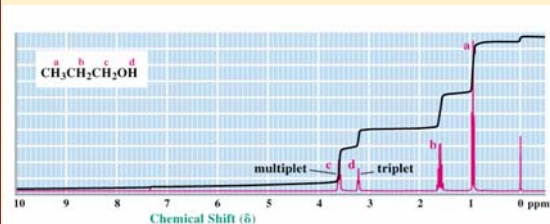
## Interpreting NMR spectra

- ◆ **Aldehydes:** the chemical shift of the aldehydic hydrogen is distinctive. It falls in the range  $\delta$  9-10. **Nothing else appears in that range.**
- ◆ **Acids:** the acid proton falls roughly into the range  $\delta$  11-12. However, it is often broadened, especially in concentrated solutions, and may not appear as a peak. The integration will still be there, though!
  - NMR is not the method of choice for identifying this functional group!

## Interpreting NMR spectra

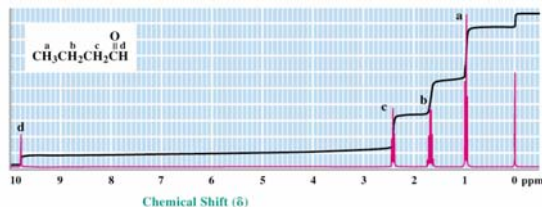
- ◆ **Carbonyl  $^{13}\text{C}$ :**
  - Non-conjugated aldehydes and ketones appear between  $\delta$  200 and 215.
  - Conjugated aldehydes and ketones appear upfield, between  $\delta$  180 and 200.
  - Acids, esters and amides appear at  $\delta$  160-185.

## 1-propanol



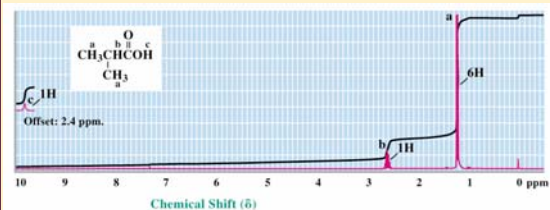
$^{13}\text{C-NMR}$ :  $\delta$  10.0 (a), 26.0 (b), 65.2 (c).

## butanal



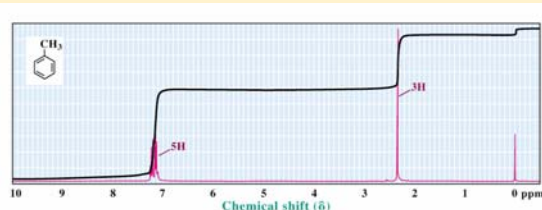
$^{13}\text{C-NMR}$ :  $\delta$  13.5 (a), 15.3 (b), 46.1 (c), 200.6 (d).

## 2-methylpropanoic acid



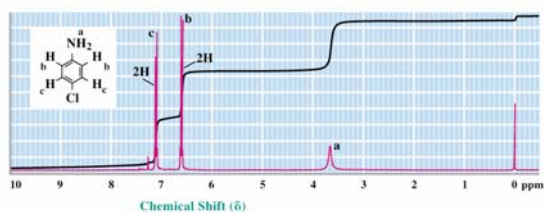
$^{13}\text{C-NMR}$ :  $\delta$  17.1 (a), 37.7 (b), 179.5 (C=O).

## toluene



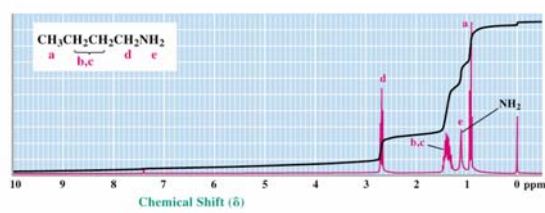
$^{13}\text{C-NMR}$ :  $\delta$  20.9, 125.5 (p), 128.4 (m), 129.2 (o), 137.7.

### 4-chloroaniline



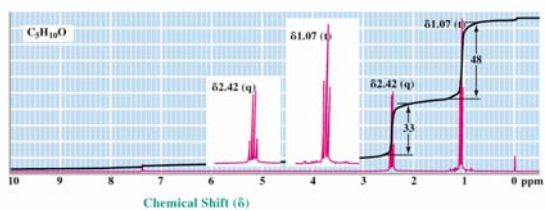
<sup>13</sup>C-NMR: δ 116.5 (b), 123.8 (C-Cl), 129.7 (c), 144.8 (C-N).

### 1-butanamine



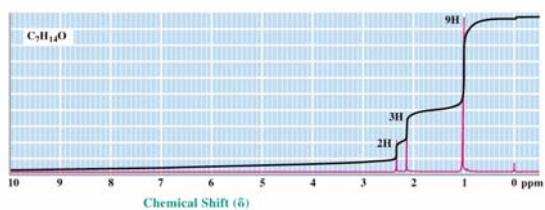
<sup>13</sup>C-NMR: δ 13.7 (a), 20.2 (b), 36.6 (c), 42.0 (d).

### NMR spectral problem



<sup>13</sup>C-NMR: δ 7.6, 33.6, 208.2.

### NMR Spectral problem



<sup>13</sup>C-NMR: δ 22.1, 25.4, 28.9, 58.3, 207.1.