

## General Procedure for Structure Determination

1. Use the formula to write down:
  - \* structures of all possible functional groups; for example, a molecule containing a single oxygen could be an alcohol, ether, aldehyde, or ketone, but not a carboxylic acid or ester;
  - \* the number of possible rings, double bonds, and triple bonds (called the unsaturation number, or index of hydrogen deficiency). This is obtained by comparing the formula to that for an alkane having the same number of carbons.
2. Look in the three "windows" in the **infrared spectrum** (around 3000, 2700–2000, 1800–1600, and below 1200  $\text{cm}^{-1}$ ) to:
  - \* identify functional groups ( $-\text{OH}$ ,  $\text{C}=\text{O}$ ,  $\text{NO}_2$ , etc);
  - \* get skeletal information, such as:
    - o substitution pattern and stereochemistry of double bonds (CH out-of-plane);
    - o substitution pattern of benzene rings (CH out-of-plane);
    - o presence of C–O stretch (ether, ester, alcohol)
3. Check the  $^1\text{H}$  nmr for familiar patterns, such as the 6H doublet/1H septet that signals an isopropyl group, or the 2H quartet/3H triplet of an ethyl. These will not always be present, of course, but if they are, they help enormously.
4. Write down structure fragments as they are identified, and subtract their formulas from the molecular formula. This informs you about how much remains to be learned.
5. Use  $^1\text{H}$  and  $^{13}\text{C}$  NMR data to:
  - \* find/confirm functional groups (e.g., carbonyl carbons, benzene hydrogens);
  - \* get the numbers of different kinds of C and H;
  - \* get the actual numbers of H by comparing the integration to the formula;
  - \* get skeletal information from H–H and H–C coupling.
6. Write plausible structures as soon as possible!
7. Use data from spectra to accept or reject those structures.
8. When you think you know what the molecule is, match every prominent ir and nmr peak with the corresponding structural features, comparing frequencies and chemical shifts to your Tables. Also make sure the integration matches. Every bit of spectral data must fit your proposed structure. This is an important check on the correctness of your result!