

**Strategy**

1. Try to get a molecular formula.
  - a. more than likely, the molecular weight of our unknown is 94 ( $M^+$  seen on the mass spectrum as  $m/z = 94$ ). If the mass is 95, a nitrogen must be present. Although the IR absorbance for an N-H bond shows in a similar region as does an OH, an OH absorbance is broad while an N-H absorbance is more defined (sharp) - see textbook page 444. If a nitrogen atom was included by mistake, there is no structure that exists that matches the carbon NMR.
  - b. other than C and H, what other atoms are in our molecule?
    - i.  $M^+$  is even, so even number of nitrogens (probably zero)
    - ii. IR shows an OH stretch at  $3300\text{ cm}^{-1}$  and no  $\text{C}=\text{O}$  near  $1700\text{ cm}^{-1}$
    - iii. Halogens not seen in mass spectrum
  - c. to find molecular formula, assuming only C, H and O
    - i. Subtract one oxygen from 94 ( $94 - 16 = 78$ ) and add C and H into 78.

$\text{C}_5\text{H}_{18}\text{O}$  - not possible (try working through the degree of unsaturation, and prove it to yourself)

$\text{C}_6\text{H}_6\text{O}$  - looks like a winner

$\text{C}_7\text{O}$  - mass  $> 94$  - can't work

2. Degree of unsaturation = 4

3. If degree of unsaturation is equal to or greater than 4, a benzene ring is likely

4. Carbon NMR shows 4 signals in the  $\text{C}=\text{C}$  region - this could be a benzene ring that has an element of symmetry so that it has 4 electronically unique carbons.

