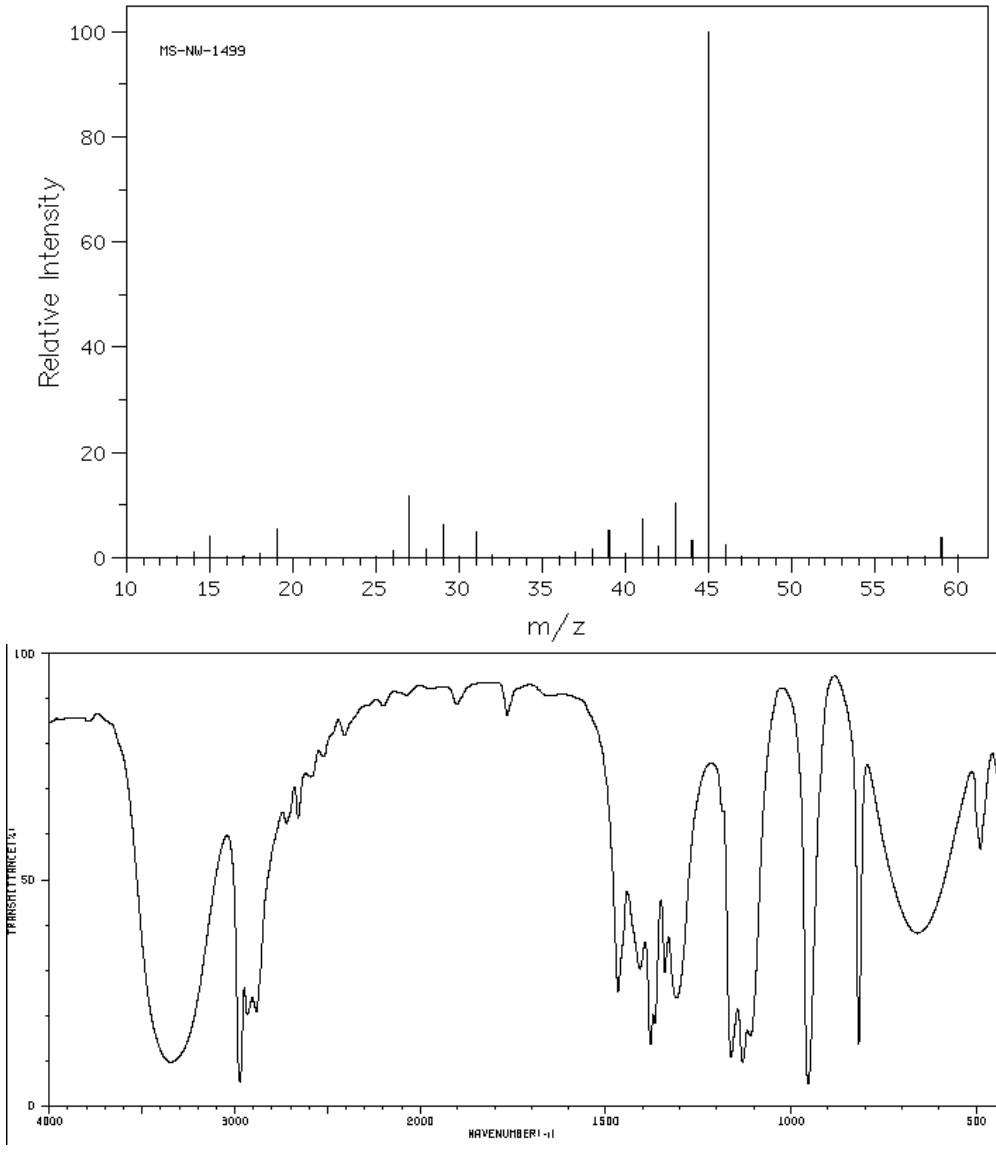
Organic Chemistry II

CHM 224

Take Home Problem Set

This compound contains C, H, and O atoms. Based on the spectral data, 1) Determine the most likely molecular formula for this compound, 2) Identify and label the IR absorption that indicates the presence of an oxygen-containing functionality, 3) Propose a structure for this compound, and 4) Assign a chemical structure to the MS fragment at 45.



DON'T LOOK ON THE OTHER SIDE UNLESS YOU WANT TO SEE THE ANSWER!

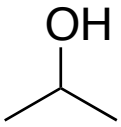
Solution Strategy

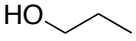
1. Try to get a molecular formula
   a. Mass spectrum shows signal at 59, however this is an odd number - and we were told this contains only C, H and O (no nitrogens). Since there are no nitrogens, this should lead you to think that 59 is not the mass of the molecular ion. Do you see the small peak at 60? We've seen loss of 1 unit (M - 1) from a particular functional group, before.
   b. Since we're told we have oxygen (let's assume just one), subtract oxygen (16) from 60 to get 44. This is the mass you must now fit C and H into.
   c. $C_2H_{20}O$ (too many H's)
   d. C_3H_8O - this is it! Molecular mass of 60.
   e. Can't be C_4 because this exceeds 44.

2. IR shows a clear O-H at 3300 cm^{-1} (which is what can give us a fragment ion of M - 1) and no C=O near 1700 $^{cm-1}$. Furthermore, since the degree of unsaturation is 0, we couldn't have a C=0.

3. Degree of unsaturation = 0, therefore this must be an acyclic linear molecule that contains no double bonds.

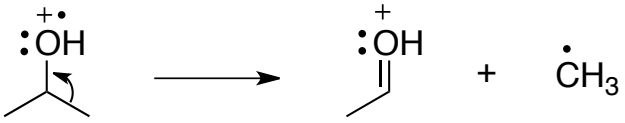
   Mass fragment of 45 must result from loss of 15 (60-45) = likely a methyl group due to alpha fragmentation. A good guess for the structure of the molecule would be:



If you were to suggest 

, alpha fragmentation would give a strong signal at 31 due to loss of an ethyl group and NOT a mass fragment of 45.

5. The molecular structure of the mass fragment at 45 results from loss of a methyl group after alpha fragmentation:



m/z = 45