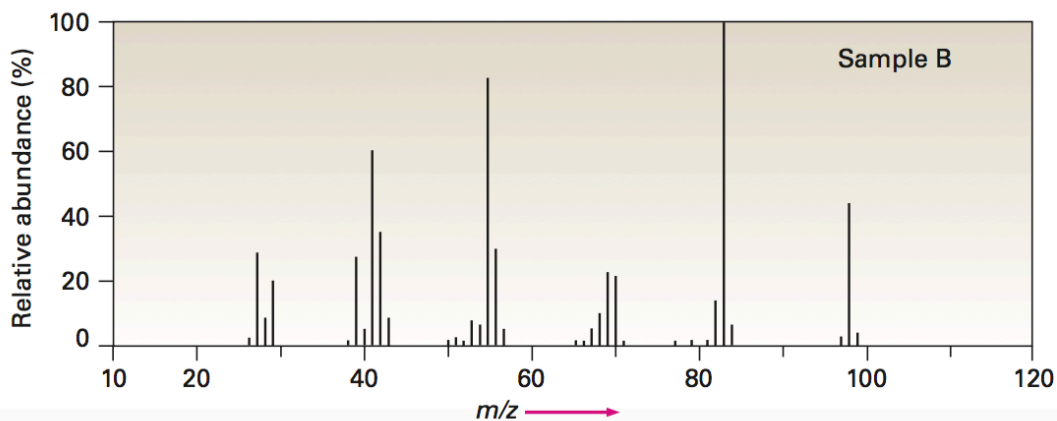
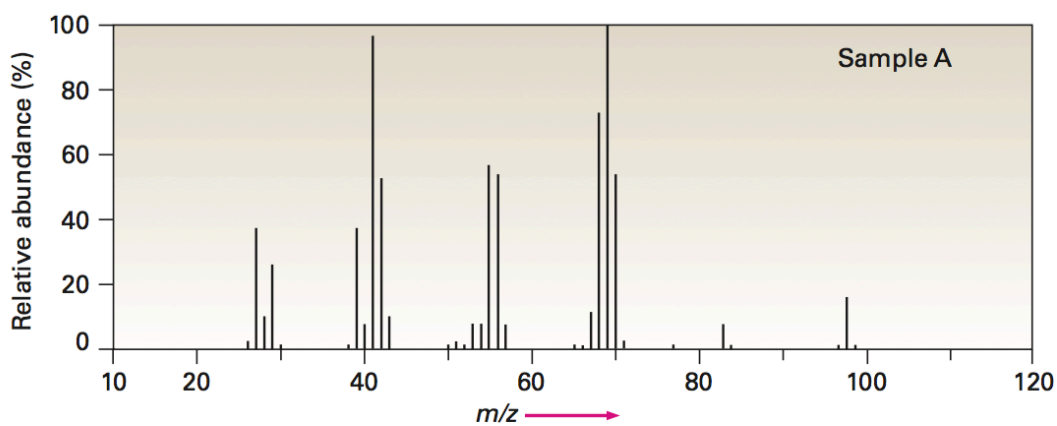


Chemistry 201: Mass Spectroscopy

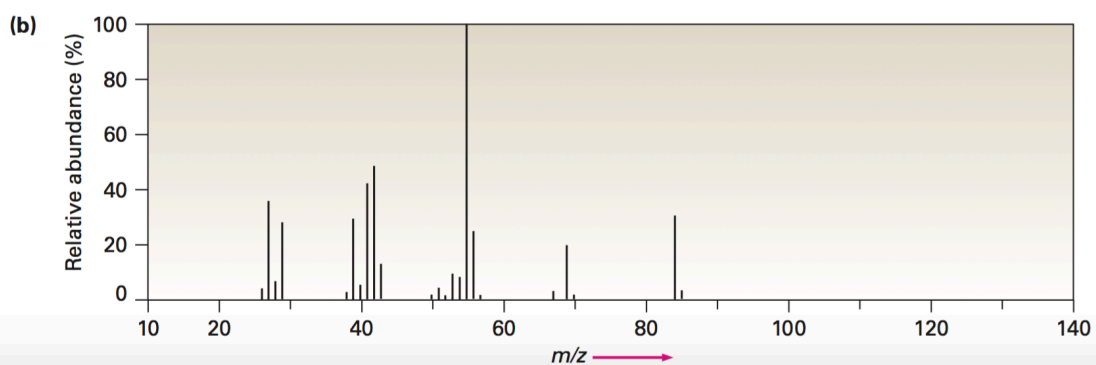
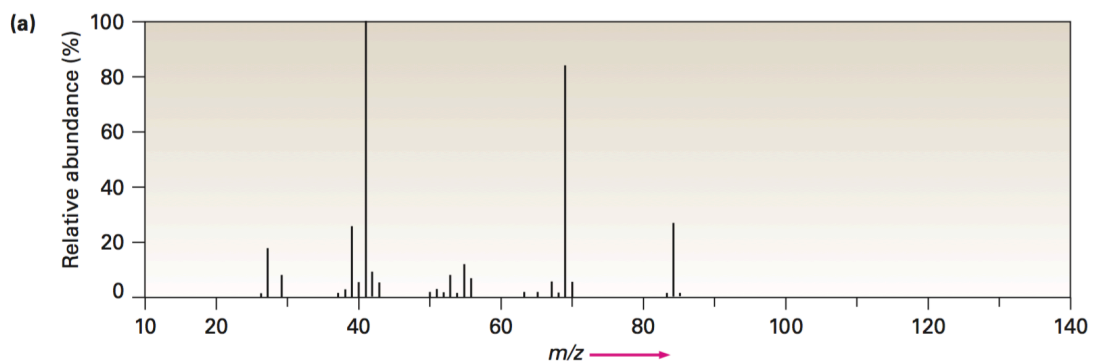
Mass Spectroscopy

- 1) The mass spectrum of 2-methyl-3-pentanol has a molecular ion $M^+=102$. What are the possible fragments you might expect of to come from this molecule?
- 2) Assume that you have two unlabeled samples: methylcyclohexane and ethylcyclopentane. How would you use mass spectrometry to tell the two compounds apart from each other?



- 3) The male sex hormone testosterone contains only C, H, and O and has a mass of 288.2089 amu as determined via mass spectrometry. What is the likely molecular formula of testosterone?
- 4) The two mass spectra are shown in the figure below. One of the spectra is for the chemical compound 2-methyl-2-pentene; the other spectra is for the chemical compound 2-hexene.

Which compound belongs to which spectra?



- 5) Given a mass spectrum, what are the fragmentation ions you would expect from an alpha cleavage of 2-pentanone?
- 6) What is the mass of the fragmentation ion produced from the dehydration of cyclohexanol?
- 7) What is the mass of the fragmentation ion produced from the alpha cleavage of triethylamine?

Solutions

Mass Spectroscopy

- 1) The molecule undergoes alpha-cleavage and lost C_3H_7 ($M^+ - 43$) and C_2H_5 ($M^+ - 29$). The loss of C_3H_7 gives a peak mass of 59 and the loss of C_2H_5 gives a peak mass of 73.
- 2) Both of the samples have an $M^+ = 98$, but the spectra shown has different fragmentation patterns. Methylcyclohexane has a methyl $-CH_3$ group while ethylcyclopentane has an ethyl $-CH_2CH_3$ group. The spectra for Sample A show a base peak at $m/z = 69$. The spectra for sample B show a base peak at $m/z = 83$. The loss of a $-CH_2CH_3$ group is approximately 29 amu which correlates to a base peak at $m/z = 69$. The loss of a $-CH_3$ group is approximately 15 amu which correlates to a base peak at $m/z = 83$. Given these fragmentation patterns, that would mean that Sample A is ethylcyclohexane and Sample B is methylcyclopentane.
- 3) Divide the molecular formula of testosterone by 13. The quotient of $288/13 = 22.15$. The quotient represents the number of carbons while the quotient plus the remainder represents the number of hydrogens. The number of carbons = 22 and the number of hydrogens = 24. Testosterone also contains an O atom. Given the known formula thus far you have **$C_{22}H_{24}O_x$** . Calculate the mass of the predicted formula. The molecular formula of testosterone is **$C_{19}H_{28}O_2$** .
- 4) The two compounds have the same molecular formula of C_6H_{12} . They will both show $M^+ = 84$. They are isomers therefore they will have different fragmentation patterns. You have to determine the possible fragmentation patterns of free-radicals and ions that are generated for each spectrum. For spectra A the base peak = 41 and for spectra B the base peak = 55. The compound 2-hexene can undergo a free-radical rearrangement in which it loses a propyl group, leaving the fragmented ion with a base peak = 41. The compound 2-methyl-2-pentene undergoes a free-radical rearrangement in which it loses an ethyl group, leaving the fragmented ion with a base peak = 55. This means the 2-hexene belongs to spectra A and 2-methyl-2-pentene belongs to spectra B.
- 5) The alpha cleavage of 2-pentanone would produce two fragmentation ions at $m/z = 71$ and $m/z = 43$
- 6) The dehydration of cyclohexanol produces a fragmentation ion at $m/z = 82$
- 7) The alpha cleavage of triethylamine produces a fragmentation ion at $m/z = 86$