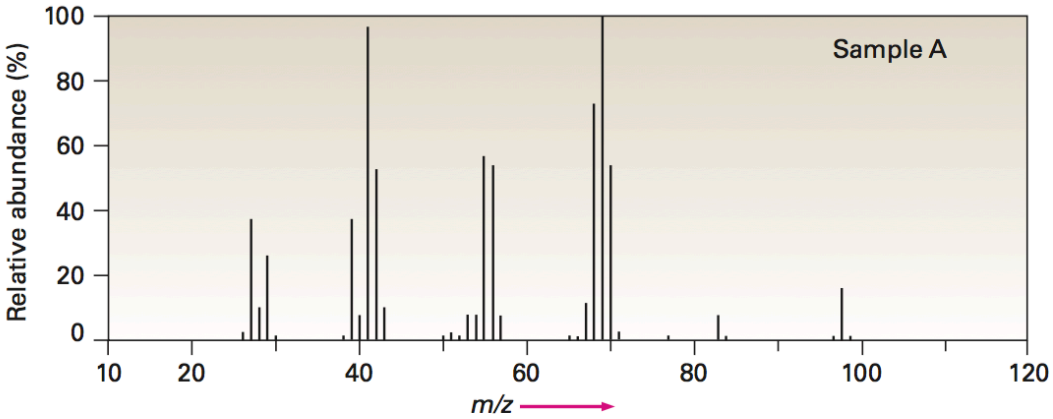
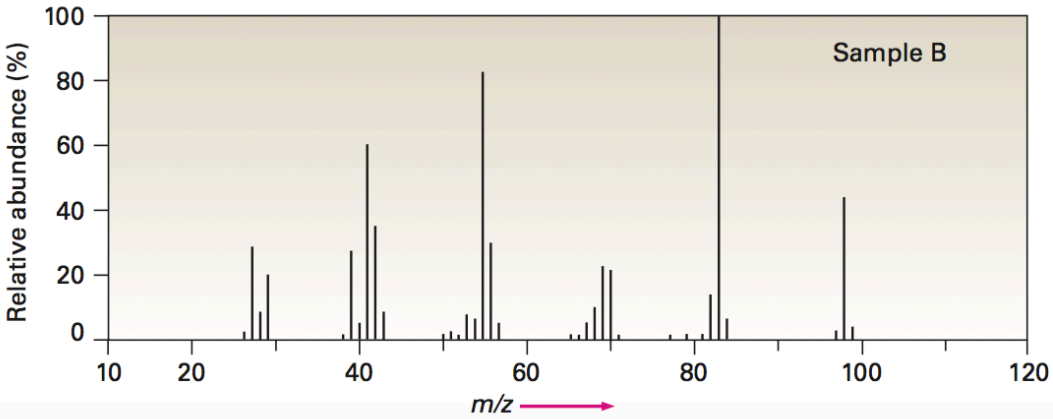
Chemistry 201: Mass Spectroscopy

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?

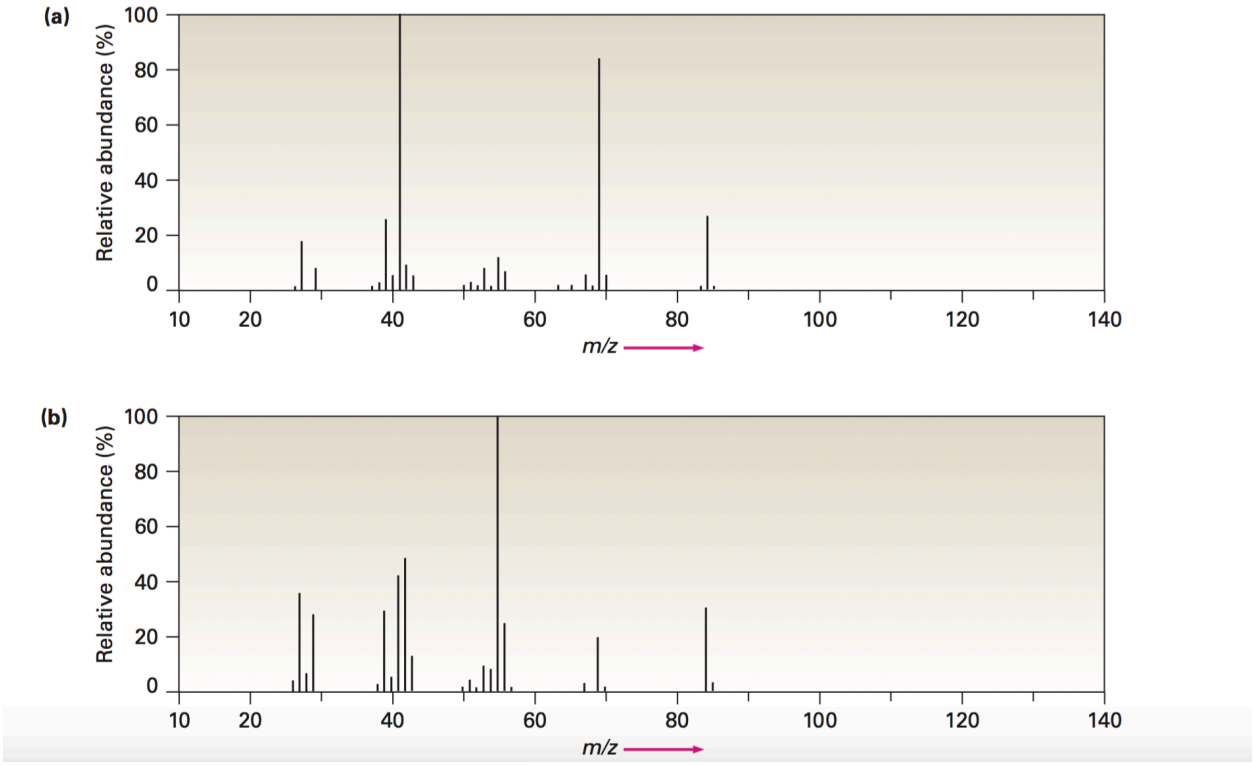




3) The male sex hormone testosterone contains only C, H, and O and has a mass of 288.2089 amu as determined via mass spectrometry. What is the likely molecular formula of testosterone?

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 is 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