

Chemistry 416, Fall Semester 1997, Dr. Glaser

Quiz II: "Mass Spectroscopy", Monday, December 8, 1997, 20 minutes, sort of announced

Your Name: Rainer Glaser's Answer Key

Question 1. Terminology.

Fill in the blanks as required (or chose from the selection given in parentheses). (15 points)

Mass spectroscopy has progressed in a most exciting fashion over the past decade. A significant role for these advances have played the developments of new methods to generate cations in the gas phase. The oldest method, the EI method, has the disadvantage to require the samples to be in the gas phase. With the development of _____ **CI** _____ and _____ **DI** _____ it is now possible to generate ions directly from solid or dissolved samples. Another method has recently been described that allows for the analysis of molecules with more than a million mass units, that method is called electrospray ionization. After the ions are in the gas phase, we can use **E** and **B** fields to select according to the mass/charge ratio. In the time-of-flight method, for example, we accelerate the ions in an electric field and measure the time they need to hit the detector. The TOF experiment requires a pulsed ion source. In an ion cyclotron resonance mass analyzer a magnetic field is used to accelerate the ions. Double focusing devices provide the highest resolution; these devices contain a _____ **sector** _____ and a _____ **sector** _____ in series. The effect of double-focusing is that ions with the same m/z but with different velocity and with different direction hit the detector at the same time. The detector consists in an electron multiplier placed after a conv. dynode.

To complete this question, give the full names of the following abbreviations.

SIMS: Secondary Ion Mass Spectroscopy

FAB: Fast Atom Bombardment

FD: Field Desorption

EI: Electron Ionization

LD: Laser Desorption

OVER

Points for Question 1:	/15		
Points for Question 2:	/7		
Points for Question 3:	/8		
Points for Question 4:	/10	Total Points:	/40

Question 2. Electrospray Ionization.

Describe the principle of ESI with as many appropriate technical terms as possible. (7 pts)

Technical term for reaction type:

Generate aerosol in the presence of a strong electric field: highly charged drops.
The highly charged drops lose solvent and undergo "Coulomb Explosion"
The droplets lose solvent or undergo DI.

Question 3. Negative Ions.

In the lecture, we discussed several ways to generate negative ions. Among the examples were two ways for the generation of 2,4,6-trichlorophenoxide from the corresponding phenol. Show the ionizing reaction for one of these cases and write down the technical term used to describe the type of reaction for that case. (8 points)

Technical term for reaction type:

Give any of the answers provided by Lambert's book.

Question 4. Isotopic Substitution Patterns. (10 points)

Predict the rel. intensities of the (M), (M+1), & (M+2) peaks for $C_{10}H_{22}$ based on the natural abundances of the heavy isotopes.

$(M) : (M+1) : (M+2) = 100 : 11 (10 \times 1.1\%) : 0.12 (10 \times [1.1\%]^2)$

The (M+2) peak reflects the occurrence of _____.

Predict the rel. intensities of the (M), (M+1), (M+2), (M+3), & (M+4) peaks for $C_2H_4Br_2$ based on the natural abundances of the heavy isotopes.

$(M) : (M+1) : (M+2) : (M+3) : (M+4) = 100 : 2.2 : 200 : 4.4 : 100$

M: light iso.; M+1: C^{13} ; M+2: Br^{81} ; M+3: $^{13}C + Br^{81}$; M+4: $2Br^{81}$ (first approx. to answer)

