

GC-MS Laboratory - Prelaboratory Exercises

Read the handouts listed below and answer the following questions prior to beginning the GC-MS laboratory on odor:

1. M. M. Campbell, O. Runquist, Fragmentation Mechanisms in Mass Spectroscopy, *J. Chem. Ed.*, **49**, 104-108, 1972.
2. E. L. Saul, *J. Chem. Ed.*, **23**, 296-297, 1949.
3. D. A. Skoog et al., *Principles of Instrumental Analysis*, Fifth Edition; Saunders College Publishing: Philadelphia; 1998, pp 258-260. Quadrupole Mass Analyzers, (section 11B-2).

Answer the following:

- 1a. Within the context of mass spectrometry, what is meant by a low pass filter?
- b. Explain in two or three sentences how the quadrupole mass analyzer simultaneously acts as a low- and high-pass filter using four poles and AC and DC voltages.
2. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow 2 \text{CH}_3\text{CH}_2\cdot$ is an example of a homolytic bond cleavage. What would the products be for heterolytic cleavage of the same bond?
3. Mass spectra showing the fragmentation pattern of two ketones, acetone and cyclopentanone, are shown in figures 1a and 1b on the next page.
 - a. Draw these two molecules.
 - b. Which spectrum is associated with which ketone?
 - c. The molecule associated with spectrum A, undergoes a three step fissioning process resulting in a total of three fragments, including the fragments at m/z 28 and 55. Draw the details of the three step bond fissioning process, and identify the fragments at m/z 28 and 55.
 - d. Identify the fragments at m/z 15 and 43 in spectrum B.