Chem 220a

Problem Set 10

Chapters 12 and 14

Due: Monday, December 9, 2002

Material in this Problem Set will be covered in the final exam.

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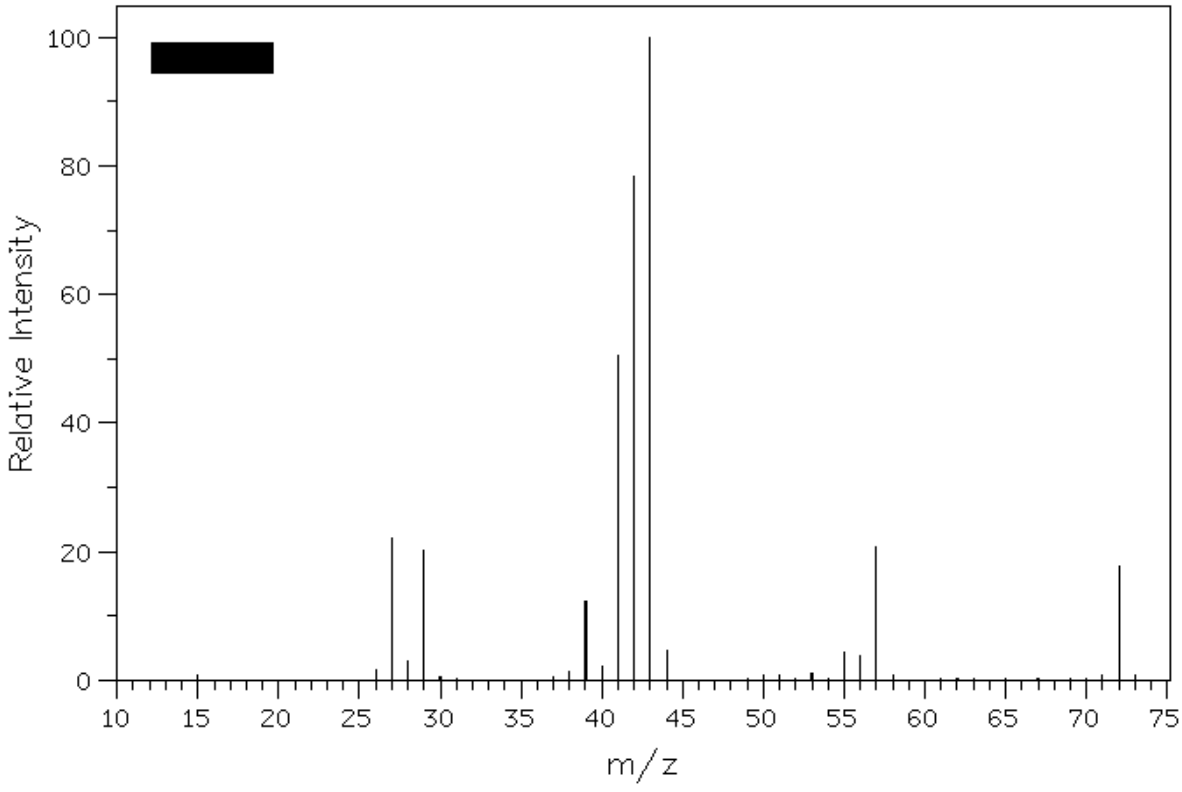
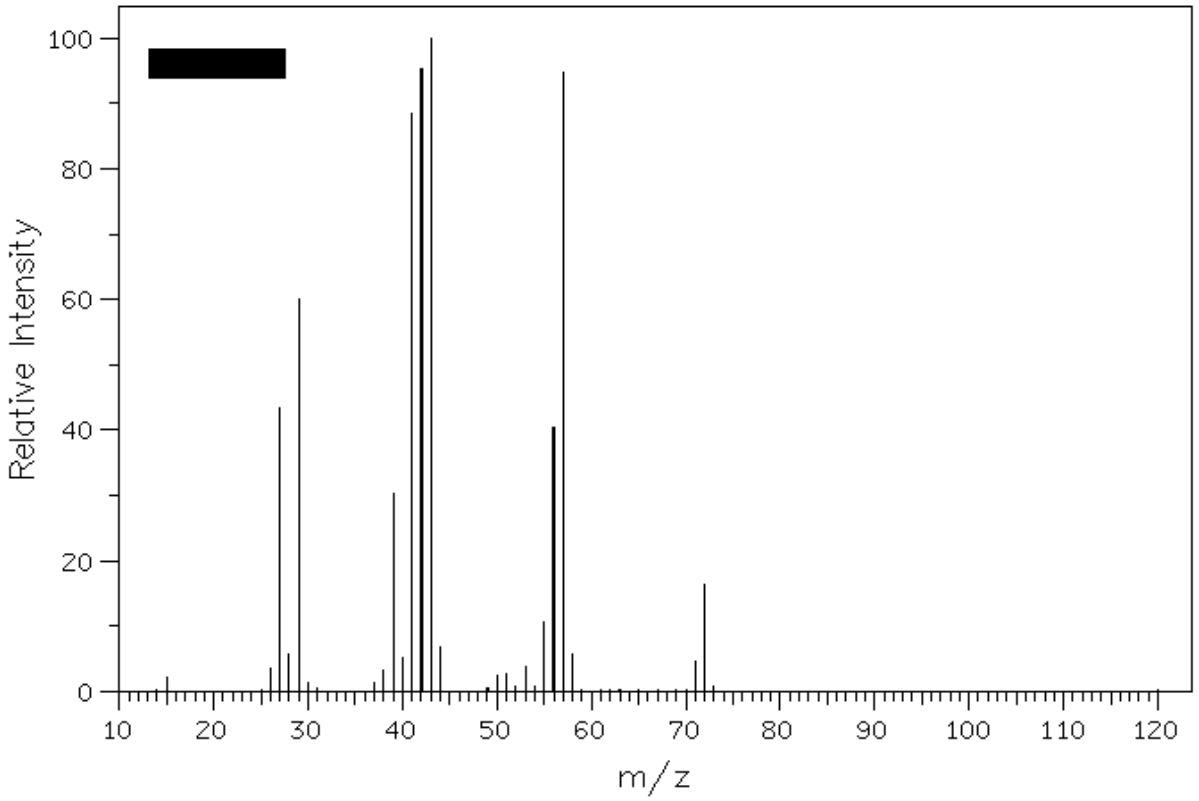
1. The two mass spectra shown below represent constitutional isomers of C_5H_{12}. Which two isomers fit these spectra? Explain. Predict the molecular ion and the base peak in the isomer whose spectrum is not shown.

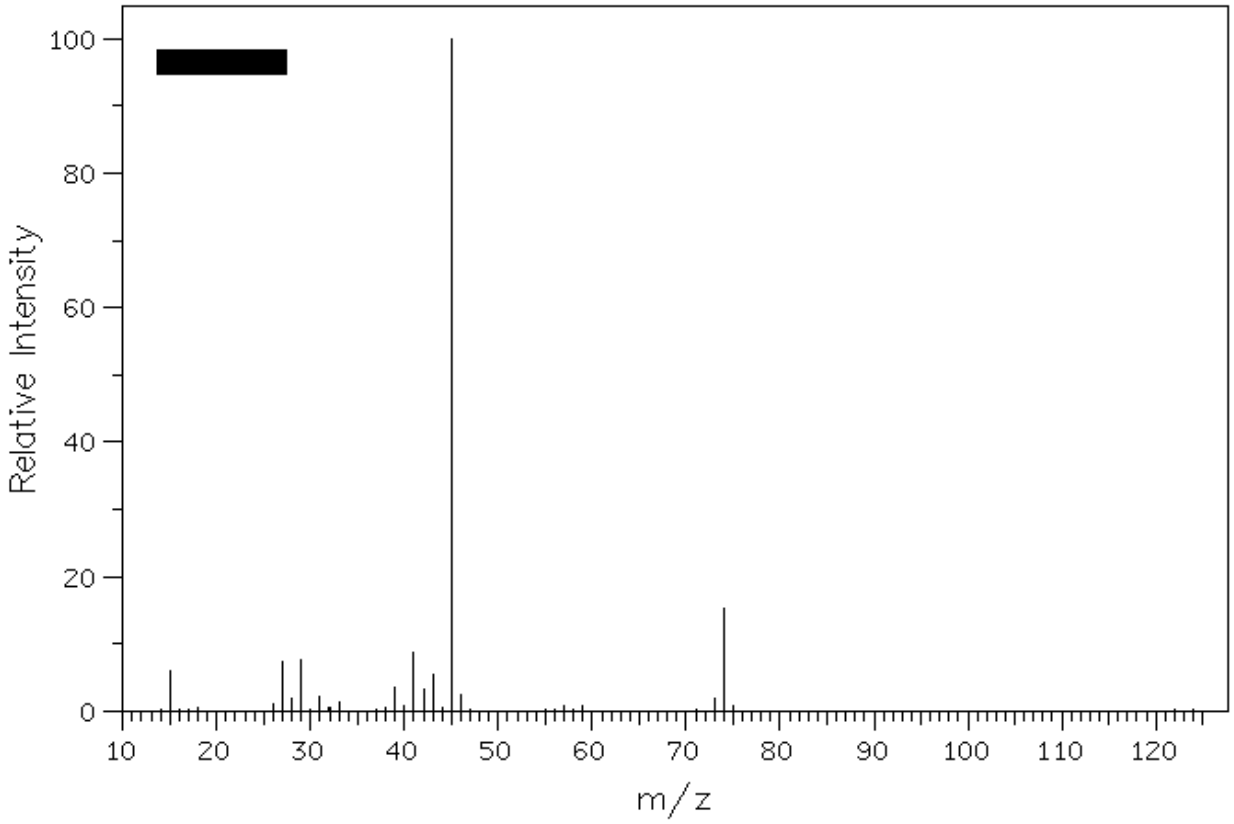
Spectrum 1a



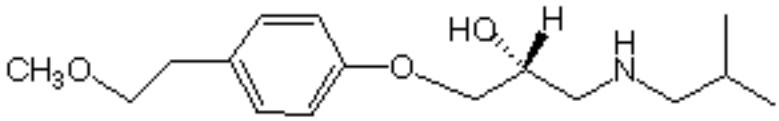
Spectrum 1b



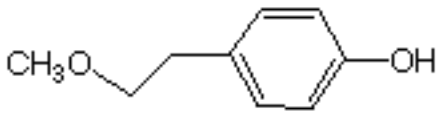
2. The mass spectrum shown on the right represents methyl n-propyl ether, contrary to what is shown and explained on page 619. What is the structure of the ion in the base peak shown in the spectrum below. The spectrum on page 619 is that of diethyl ether. The peak at m/z 59 represents what cation?



3. Lopressor (**1**), which is manufactured and sold as the racemate, is a β-adrenergic blocker. To prepare the (R)-enantiomer of Lopressor, (S)-epichlorohydrin **3** is treated successively with the phenoxide of **2** and then isobutylamine.

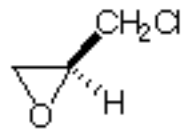


1



2

3

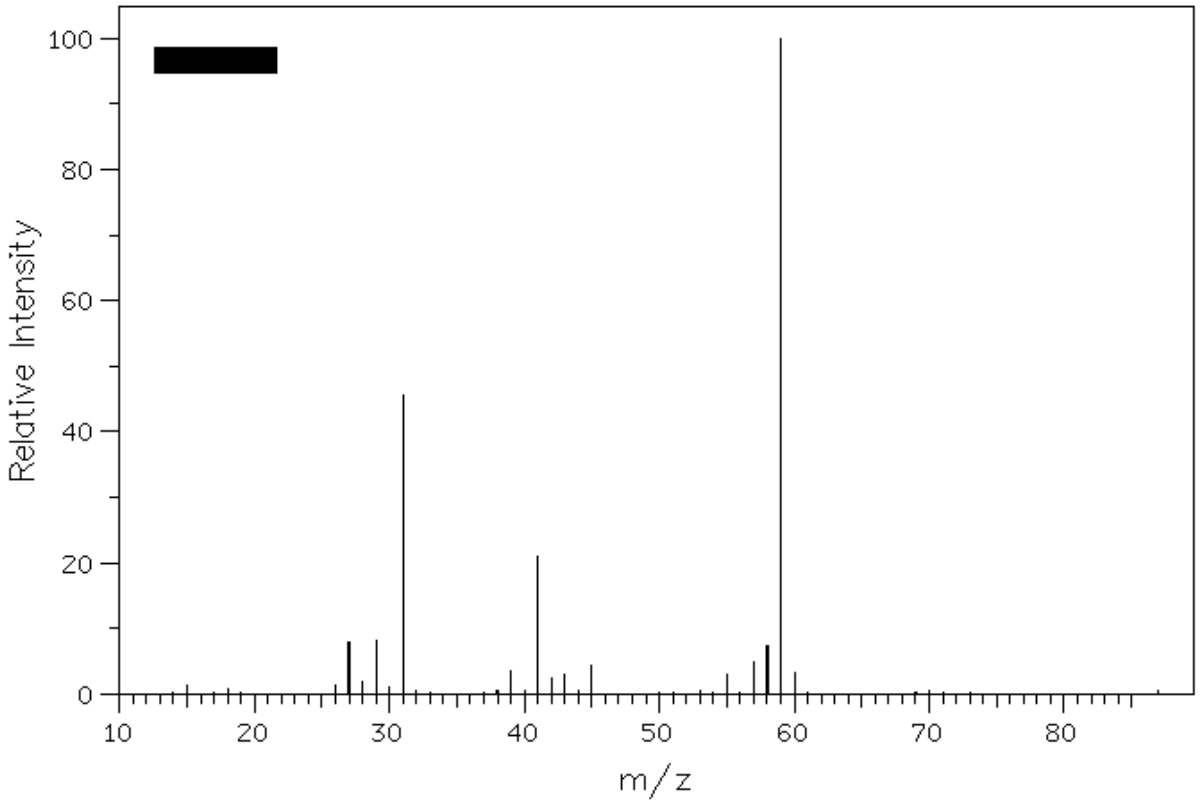


a) Would you prepare the phenoxide of **2** with aqueous $NaHCO_3$ or NaOH? Explain. [pKa (H_2O) = 15.7, pKa (phenol) = 10.2, pKa1(H_2CO_3) = 6.4]

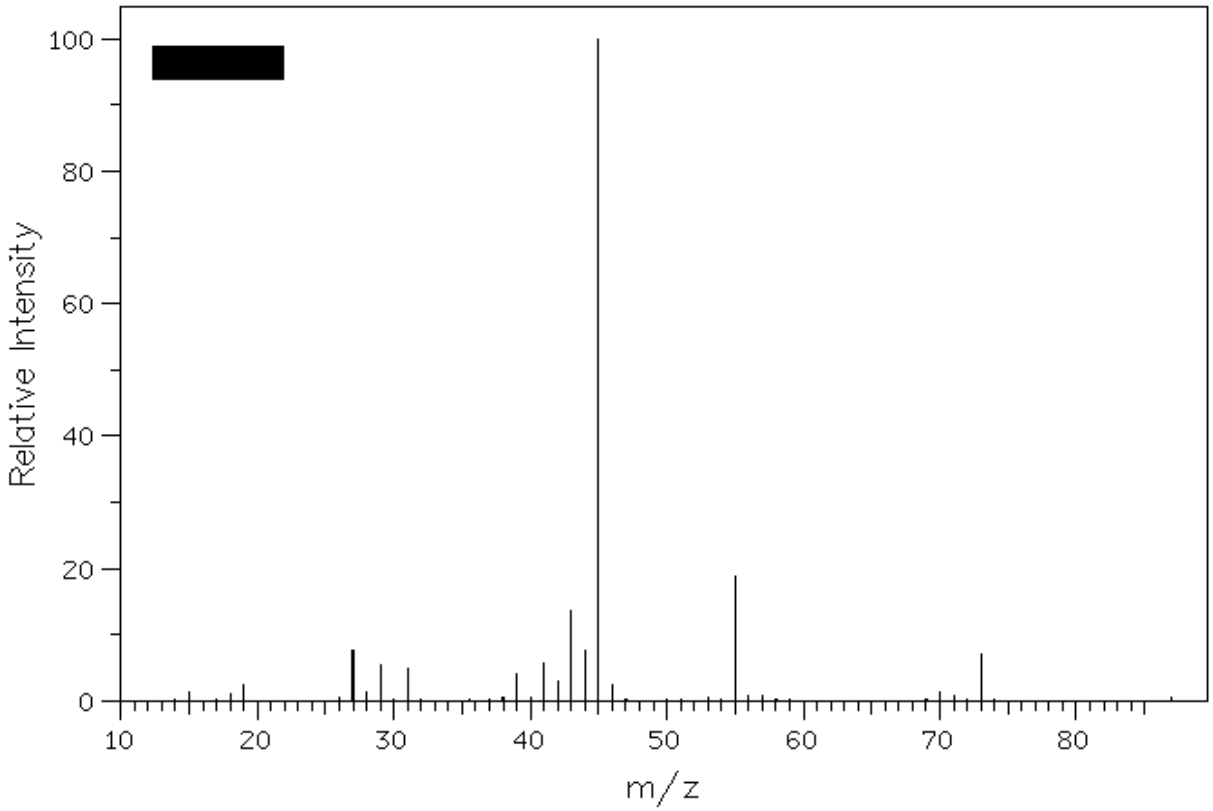
b) Provide a mechanism for the formation of (R)-Lopressor from (S)-**3**.

4. Epoxidation of (E)-2-pentene provides compound **A**. Reduction of **A** with $LiAlH_4$ gives compounds **B** and **C** ($C_5H_{12}O$), whose mass spectra are shown below. What are the structures of **A-C**? Explain. Why is m/z = 73 less intense than m/z = 45 in the spectrum of compound **C**?

Compound B

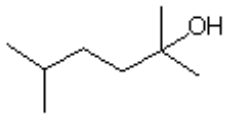


Compound C

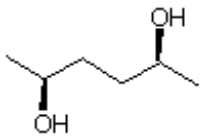


5. 1,2,3-Trichloropropane is expected to have how many molecular ions? What are their m/z value? What are their relative intensities?

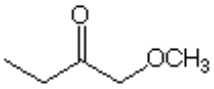
6. Provide the missing information in each of the following reactions.

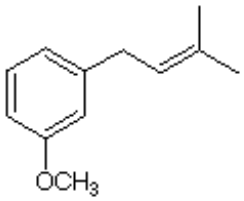
a) isobutylene → 

(only source of carbon)

b) 

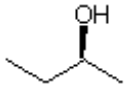
1) TsCl, pyr. (1 equiv.)
2) aq. NaOH →

c)  → 

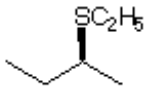
d) 

HBr
heat →

A + **B**

e) 

opt. act. →



opt.act.