Mass spec prob set 2; chem 124/224

1. [a] The low resolution mass spectrum for compound X shows a molecular ion at m/z 97. Use Appendix 11 of Pavia, Lampman, and Kriz to determine the possible molecular formula corresponding to this mass.

   - How many nitrogens are present in each formula? Is it an even or an odd number?
   - Look at the formula corresponding to 91, 93, 95, 97, and 99. How many nitrogens?
   - How many nitrogens are there in the formula corresponding to the even masses?

   Together, the observations you've made are representative of the so-called 'nitrogen rule'. Why is it so?
   Read about it in your texts.

[b] Consider, again, compound X. Suppose you received a HRMS analysis from Dr. Pavlovich that showed an exact mass of 97.0530. What molecular formula best matches this outcome?

2. [a] Provide reagents to achieve the selective conversion of 1-butene to
   - 1-butanol
   - 2-butanol

[b] Formulate a mechanism for each process. Do so!
[c] Indicate how mass spectral fragmentation patterns could be used to differentiate between the isomers.
[d] Formulate a mechanism to account for the formation of the most abundant fragment ions.

3. Someone was uncertain whether a container was full of bromine or chlorine gas. To determine which it was, he/she elected to allow the gas to react with cyclohexane.

[a] Draw the product, specifying stereochemistry, in each instance.
[b] Formulate a mechanism to account for their formation.
[c] What's the "typical" solvent used in such transformations?
[d] At what temperature does one conduct such reactions?

   How could one use isotope cluster patterns to determine
   [I] the number of halogens contained in each product?
   [ii] whether Br or Cl has been incorporated?

4. Determine the most likely fragmentation pathways for the methyl-THF isomers shown below.
   Formulate mechanisms. How could this information be used to differentiate between the isomers?

5. Formulate a mechanism to account for the formation of fragment ion at 68 and 70 that appear in the mass spectrum of the structure shown below.