Problem Set 3Out: December 3, 1999 Due Back: December 10, 1999 Chemistry 221, 1999

Answers to the following problems should be written, in order and labeled, on $8\ 1/2\ x\ 11$ inch paper. Answers written on the problem set itself will not be graded.

A. For each of the following 2 reactions, provide the mechanism type which best fits the situation and evidence as you see it. Clearly but briefly justify your choice by interpreting the facts given about these reactions. The explanation of the mechanism will be more important than your choice, so try to be clear and complete. Don't forget to read the structures and include the relevant information into your answers.

Questions to Answer for Each Reaction:

- a. Reaction type $(S_N1, S_N2, E1, E2)$.
- b. Draw the structure of the **major product**. Be sure to specify stereochemistry, if appropriate.
- c. Show the **stepwise mechanism** of the reaction.
- d. Draw a reaction energy diagram (energy vs. reaction progress).
- e. Describe the **stereochemical outcome** of the reaction, using words or structures as needed.
- f. Describe **one experiment** you could do to prove your idea about the mechanism type. Be sure to include both the description of the experiment **and** what results you expect to get. Explain how that experiment excludes the alternate mechanisms (the ones you didn't choose).
- **B.** Consider the stereoisomers of 2-bromo-1,3-dimethylcyclohexane.
 - 1. Draw all of the stereoisomers of this molecule. [Note the symmetry, and don't draw more than you need to.]
 - 2. Draw the product of an E2 elimination of HBr from one of your isomers (conditions might be 1M NaOCH₂CH₃). Are all the products exactly the same?
 - 3. Rank all of your isomers in order of reactivity in this E2 elimination.
 - 4. Comment on your ranking for each compound. Explain why the fastest shouldbe fastest, etc.
 - 5. Would you expect the isomers to have the same order of reactivity for an S_N2 reaction (say, with NaCN)?

C. The following reaction occurs when the diol shown is treated with sulfuric acid.

$$HO \underbrace{C}_{H_{2}} \underbrace{C}_{H_{2}} \underbrace{C}_{OH} \underbrace{CH_{3}}_{OH} \underbrace{H_{2}SO_{4}}_{H_{2}SO_{4}} \underbrace{H_{2}C}_{C} \underbrace{CH_{3}}_{C+C} \underbrace{CH_{3}}_{H_{2}} + H_{2}O$$

- 1. Propose a plausible stepwise mechanism for this reaction. It will be helpful to use reaction arrows.
- 2. Which oxygen remains after the reaction, and which is likely to be lost as water? Explain briefly.
- 3. Another product, compound **2**, did **not** form in significant amounts. Why did compound **1** form, rather than compound **2**?