

Names of all students (please print) _____

CHEM 243 Organic Chemistry I

Points _____ (10 max)

Worksheet #17: October 25, 2021. Complete the following worksheet by collaborating with a group of 3-4 students. You can use a text book or your lecture video notes. You must work together, with the names of all students included on **ONE** sheet and turned in for a group grade.

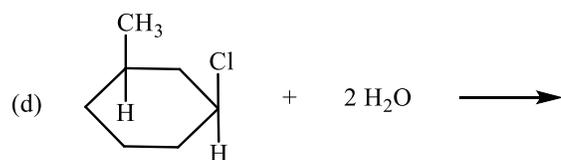
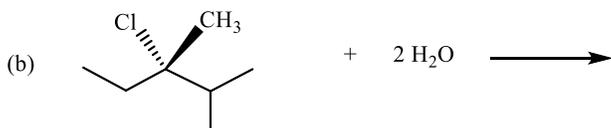
(1) SN1 Reactions – Predicting Reaction Products. Complete the reactions shown below by drawing the structure of the substitution product. It is not necessary to balance these equations. Draw the proper product **stereochemistry**, if relevant. NOTE: I am no longer giving any “no reaction” problems!



EXPLAIN why the substitution reaction shown in (a) is classified as an SN1 reaction and not an SN2.

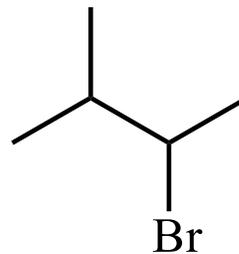
Background info for SN1 reactions b, c, d:

- These are solvolysis SN1 reactions, where the nucleophile is also the solvent.
- Note that:
 - if the solvent is water (H₂O), the substitution product is an alcohol (R-OH)
 - if the solvent is an alcohol (R'-OH), the product is an ether (R-O-R').
- Note that water and alcohols are both poor nucleophiles (weak bases), which are ideal SN1 nucleophiles.
- With these poor nucleophiles (H₂O or R-OH), the oxygen forms the new bond to the positive carbon of the substrate. The oxygen always loses ONE H, and everything else bonded to the oxygen remains bonded in the product. Note that the correct stoichiometry is **TWO** molecules of H₂O or R-OH. The 2nd molecule is used as a base to remove the H₂O or R-OH proton (see mechanism in question 4).
- Stereochemistry: Remember, SN1 reactions are **NOT** stereospecific, so you get a Racemic Mixture of products (both the R and S enantiomers).



(2) Inefficient Chemical Reactions: Substitution + Elimination Reactions. Many chemical reactions are not very efficient. The yield may be low (<75%), and you can have two or more reactions occurring at the same time, in the same beaker. Many substitution reactions are also accompanied by Elimination reactions. In an elimination reaction, the leaving group and an H are “eliminated” from the substrate to form alkenes as products. The C=C double bond of alkenes is formed between the carbon containing the Lg (α -carbon) and the adjacent carbons that have H’s (β -carbons).

(a) In the alkyl bromide at the right, label the α and β carbons.



(b) If you have more than one β -carbons, you can get more than one alkene products. Based on your α - and β -carbons, draw all possible elimination products.

(3) SN2 Two-Step Mechanism. The following, balanced SN2 net reaction requires TWO steps. In Step #1 the nucleophile substitutes for the Lg forming a positively charged intermediate. In Step #2 you need to do an acid-base neutralization of the intermediate from Step #1. Note the stoichiometry has two moles of NH_3 . One mole is the nucleophile in Step #1, and the second is the base in Step #2.



(NOTE: This is an SN2 reaction because we have a 1 $^\circ$ alkyl halide substrate, and a good nucleophile.)

Write a complete mechanism that explains the formation of all products in the balanced net reaction shown above. Your mechanism must consist of balanced chemical equations, and curved arrows to show electron pair movement.

Step #1: Nucleophile substitutes for the Lg forming a positively charged intermediate.

Step #2: You need to do an acid-base neutralization of the intermediate from Step #1. The organic product (intermediate) from Step #1 becomes the reactant for Step #2, plus the second mole of nucleophile which now acts as a base.

(4) SN1 Three-Step Mechanism. The following, balanced SN1 net reaction requires THREE steps in the mechanism. In Step #1 the Lg leaves forming a carbocation. In Step #2 the nucleophile adds. In Step #3 you need to do an acid-base neutralization of the intermediate from Step #2. Note the stoichiometry has two moles of alcohol. One mole is the nucleophile in Step #2, and the second is the base in Step #3.

(a) Write a complete mechanism that explains the formation of all products in the balanced net SN1 reaction shown below (3 steps). Your mechanism must consist of a series of balanced chemical equations, and curved arrows to show electron pair movement.



Step #1: The Lg leaves forming a carbocation.

Step #2: The nucleophile (HOCH₃) adds to the carbocation intermediate from Step #1.

Step #3: You need to do an acid-base neutralization of the intermediate from Step #2 using the 2nd molecule of HOCH₃.

(b) Draw and label the **Energy Diagram** for this 3-step, exothermic reaction (R, P, ts-1, ts-2, ts-3, intermediates, and activation energy for the RLS).

Potential
Energy

Reaction Progress