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Substitution vs. Elimination

Instructions:
Read the instructions carefully and answer the following questions in the space provided. Then attach the PDF file on Discussion Board for peer discussion and peer review.

1. Compare and contrast SN1, SN2, E1 and E2 reactions. What are some obvious similarities and differences between each reaction pathway? What are the requirements for each reaction to work? Discuss why SN2 is in direct competition with E2 while SN1 is in direct competition with the E1 reaction pathway. What is the rate expression for each? Which reactions are concerted? Which reactions are step-wise? Which reactions are stereospecific and what is the stereospecificity of each that are? How do the variables below help influence which reaction pathway will lead to the major product formed?

    a. Substrate (substitution pattern and leaving group ability)
    b. Nucleophile/base strength (weak or strong) and size (unhindered or hindered)
    c. Solvent (polar-aprotic or polar-protic)
    d. Temperature (low/ambient temps vs. higher temps)

SN2 and E2 reactions are bimolecular. The substrate (alkyl halide) and base/nucleophile both participate in the rate determining step. The rate = k [alkyl halide] [nucleophile] These reactions are concerted which mean that the attack of the nucleophile and the loss of the leaving group occur simultaneously.

SN1 and E1 reactions are unimolecular. These reactions are stepwise reactions. There is the loss of the leaving group which leaves an intermediate carbocation. The nucleophile then attacks the intermediate carbocation. There is also the proton transfer. Depending on leaving group this can occur as the first step if the leaving group is weak. Since these do not occur at the same time the rate limiting step is the substrate. k = [substrate].

SN2 is in direct competition with E2 because they are both bimolecular. Which reaction takes place depends on the strength of the nucleophile or base, whether the base is bulky or non-bulky, and if the alpha carbon is methyl, primary, secondary, or tertiary.

SN1 and E1 are in competition because both are unimolecular. If the reaction contains heat then E1 will be favored.

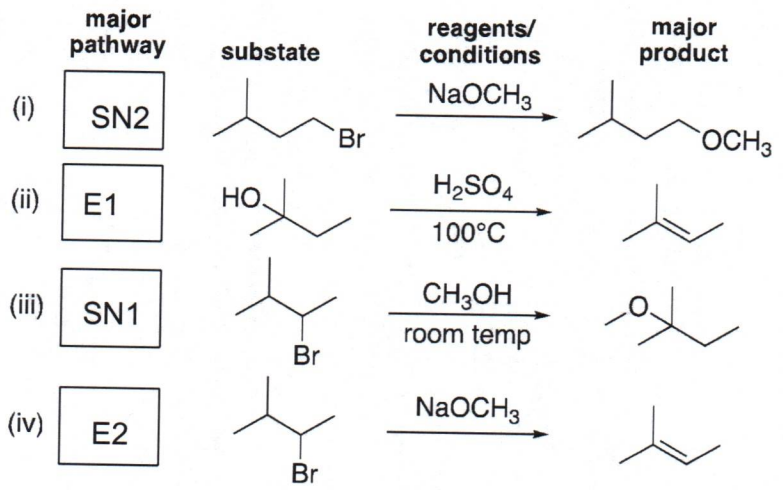
a. The substrate is the starting material that turns into the organic product. In a substitution pattern the nucleophile attacks the carbon attached to the leaving group and the group leaves. The leaving group is replaced by the nucleophile.

b. If the nucleophile/base is strong then a SN2 or E2 reaction. If the nucleophile is weak the reaction will be Sn1 or E1. If the base is bulky (hindered) E2 reactions are favor and non-bulky (unhindered) SN2 reactions favored.

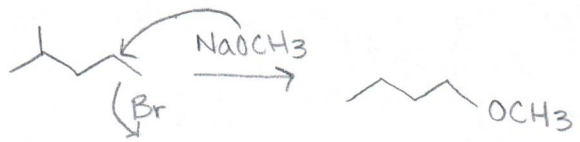
c. Polar-aprotic solvents favor SN2 and E2 reactions. Polar protic solvents favor Sn1 and E1 reactions.

d. Low temperature favor SN1 reactions while high temperatures favor E1 reactions.

2. Below (on the next page) are 4 reactions. For each, indicate what reaction pathway lead to each major product shown. Discuss the factors that led you to each decision. Use each pathway (SN1, SN2, E1, and E2) only one time. Where there any reactions where you had a more difficult time deciding versus others? Draw an arrow-pushing mechanism for each reaction to clearly show the electron movement which led to each major product shown.

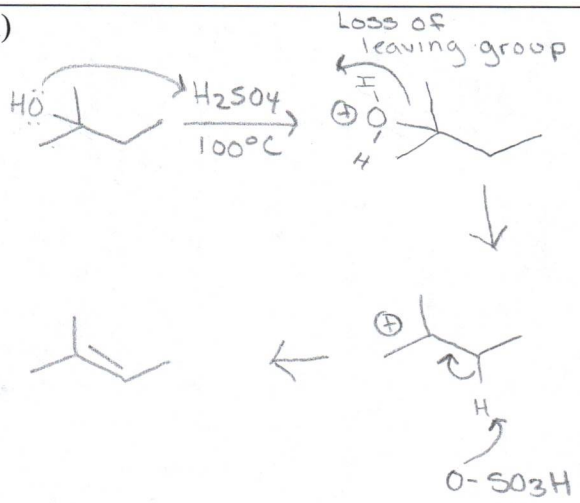


i)



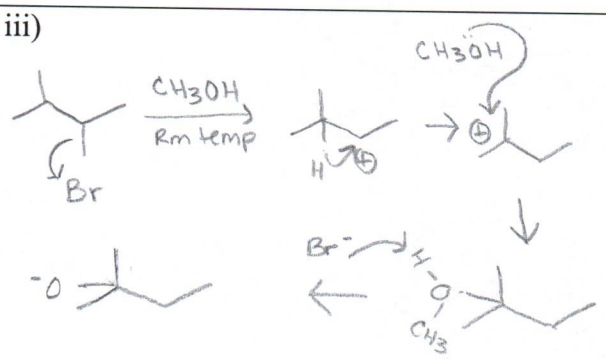
I chose SN2 becuase the reaction is a substitution where a nucleophile replaces the halogen. The alpha carbon is primary which favors a SN2 reaction.

ii)



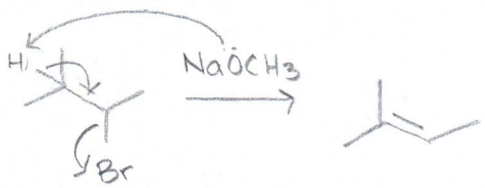
I chose E1 due to the fact the major product was an alkene and the reaction contained heat and heat favors a E1 reaction.

iii)



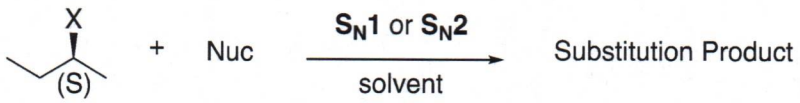
I chose SN1 becuase the major product is substitution and the nucleophile is weak. I found this one to be the most difficult becuase I don't know what happened to the methyl group. What did it drop off? Why is the major product not

iv)



I chose E2 becuase the major product is an alkene.

3. Consider the reaction scheme shown below.



single enantiomer
(optically active)

Discuss two independent experiments you could do in a typical undergraduate lab to experimentally determine which type of substitution reaction took place. Be specific and briefly explain how each experiment would be able to provide you with the information necessary to determine this. In other words, what outcomes do you expect from your experimental design. The experiments could also include an instrumental technique. Your answer should not be something along the lines of simply saying to "check (R) and (S)". Each experiment should have at least two parallel reactions that you are describing. Make sure to include any instrumentation you would need to analyze products in order to decide which substitution product is taking place and what the analysis would be expected to tell you.

Since the alpha carbon in the substrate is chiral due to the backside attack on the nucleophile in an SN2 reaction we would expect a change in configuration of the chiral center. Since the substrate is (S) if the substitution product is (R) we know that the reaction was SN2. If the reaction was SN1 the leaving group leaves which leave an intermediate carbocation. Since the carbocation is planar the nucleophile is able to attack from the top or bottom which results in a 50:50 mixture which is racemic. There would be no change in stereochemistry. If the is not an inversion of the substitution product then the reaction was SN1.

Another experiment would be to change the concentration of the nucleophile. In and SN2 reaction the rate = k [alkyl halide] [nucleophile] and in an SN1 reaction rate = k [substrate]. If you were to double the concentration of the substrate only, then we will see the rate in both reactions change. However, since changing the concentration of the nucleophile has no effect on SN1 reactions but does in an SN2 reaction if we were to increase the concentration of the nucleophile and the reaction rate increases, then we would know it was a SN2. If the reaction rate does not change then it would be SN1.