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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)

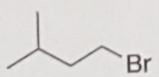
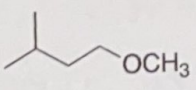
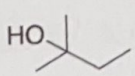
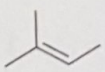
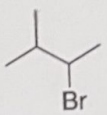
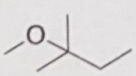
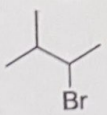
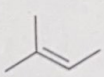
E1
- competes w/ SN1 because both have carbocation intermediates
- elimination reaction
- favor poor nucleophile/weak base, higher temp, polar protic

SN1
- rate is unimolecular
- tertiary is fastest
- loss of leaving group, attack of nucleophile
- substitution reaction
- favor poor nucleophile/weak base, polar protic

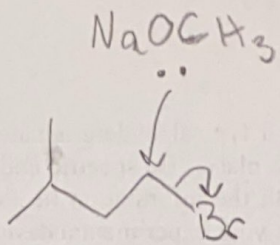
E2
- stereospecific
- elimination reaction
- favor strong base
- polar protic

SN2
- second order
- methyl fastest
- stereospecific
- substitution reaction
- favors strong nucleophile, polar aprotic

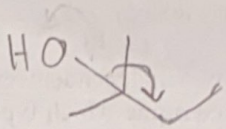
**2.** Below (on the next page) are 4 reactions. For each, indicate what reaction pathway lead to each major product shown. Discuss the factors that led you to each decision. Use each pathway (SN1, SN2, E1, and E2) only one time. Where there any reactions where you had a more difficult time deciding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

| | major pathway | substate | reagents/ conditions | major product |
|---|---|---|---|---|
| (i) | SN2 |  | $NaOCH_3$ |  |
| (ii) | E1 |  | $H_2SO_4$, 100°C |  |
| (iii) | SN1 |  | $CH_3OH$, room temp |  |
| (iv) | E2 |  | $NaOCH_3$ |  |

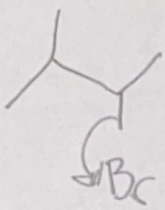
i)



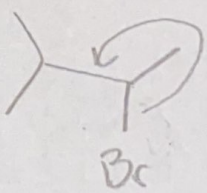

ii)



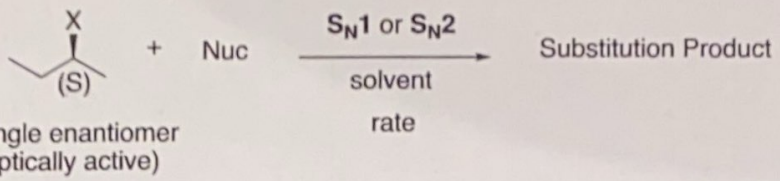

iii)




iv)



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.

For one experiment, SN1 and SN2 are set up the same. A polar aprotic solution is used. The equation that reacts is SN2.

For a second experiment, methyl groups are used. The faster reaction is SN2.

Additionally, a strong nucleophile could be tested. The favored reaction would be SN2.