CHM2123 Problem Set #3 - Competition Between Substitution and Elimination Reactions of Alkyl Halides

1. Substitution and elimination reactions can often compete to yield a range of products. Rank the nucleophiles/bases in descending order (best to worst) in favour of the following reactions, and briefly justify your choice.

    a. A substitution reaction

Small molecules with a weak hold on their electrons make better nucleophiles

$NaI > NaOH > CH_3CH_2ONa > CH_3COONa > (CH_3)_3OK$

    b. An elimination reaction

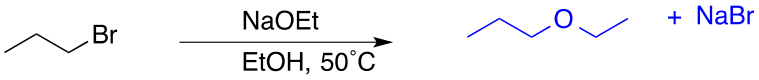
Strong or bulky bases favour elimination reactions

$(CH_3)_3OK > CH_3CH_2ONa > NaOH > CH_3COONa > NaI$

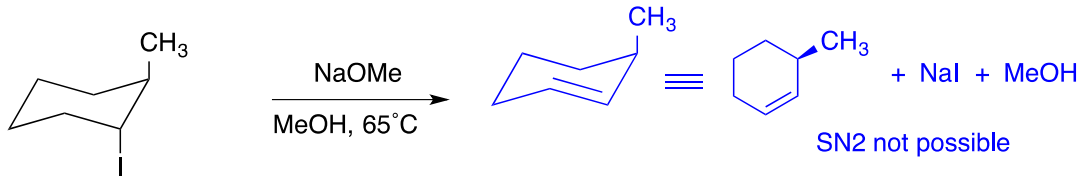
2. Predict the major product for each of the following reactions.

a)

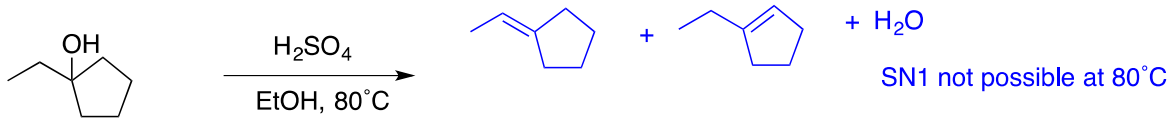
b)



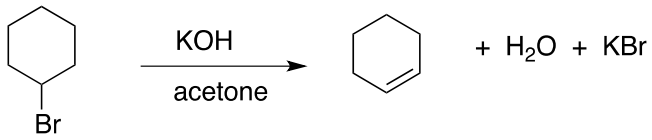
c)



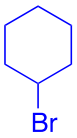
d)



3. You perform the following E2 reaction starting with 9.0 g KOH and 3.8 mL 1-bromocyclohexane (1.32 g/cm^3), and produce 2.7 mL of cyclohexene (0.81 g/cm^3).



a) Determine the number of equivalents of each reagent.

compound	MW	Amount	density	mol	eq.
KOH	56.11 g/mol	9.0 g	--	0.160	5.2
	163.06 g/mol	3.8 mL	1.32 g/cm^3	0.031	1.0
	82.14 g/mol	2.7 mL	0.81 g/cm^3	0.027	

ie. There are 5.2 mol KOH for every mol of 1-bromocyclohexane.

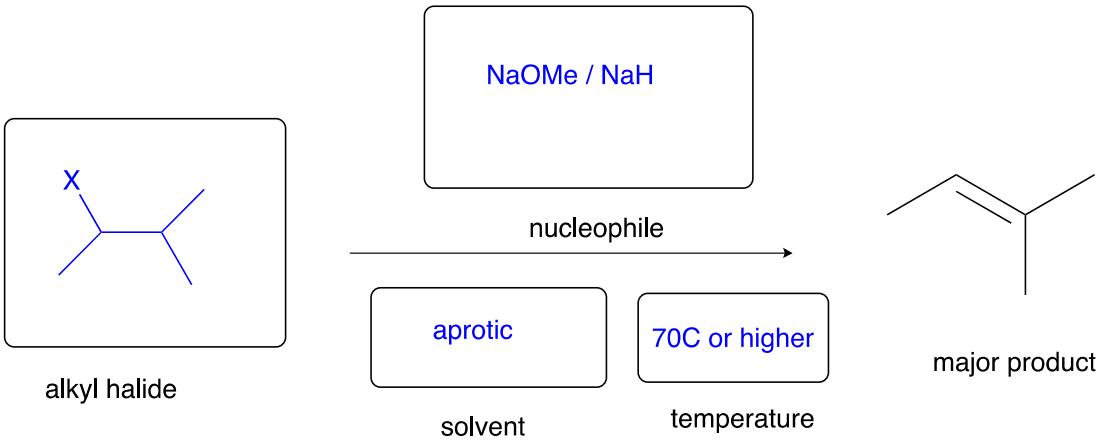
b) Calculate the yield of your product.

$$\text{Yield} = \frac{\text{moles of product}}{\text{moles limit. reagent}} \times 100$$

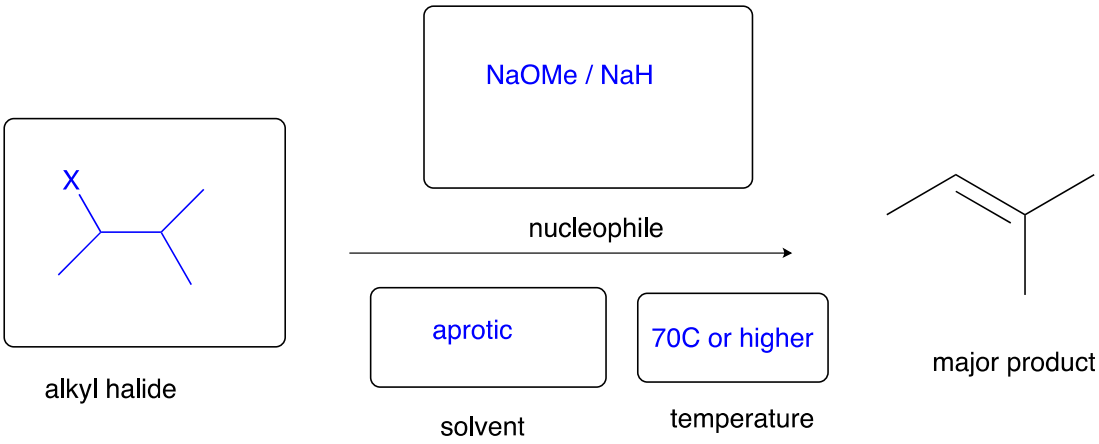
$$= \frac{0.027}{0.031}$$

$$= 87\%$$

4. Based on your knowledge of elimination reactions, propose a synthetic method for the synthesis of 2-methyl-2-butene, and indicate your choice of alkyl halide, nucleophile, solvent, and temperature.



OR



Substrate and nucleophile must be soluble in solvent. (ie. NaOH, KOH not soluble in acetone)