CHM2123 Exp 2 Problem Set

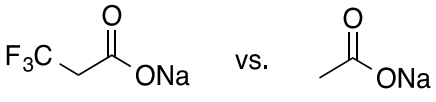
1. Amongst the following pairs, predict which one would be the best nucleophile in a solution of ethanol. Justify your answer.

a) CH_3CH_2OH vs. CH_3CH_2ONa

Bases are better nucleophiles than their corresponding conjugate acid.

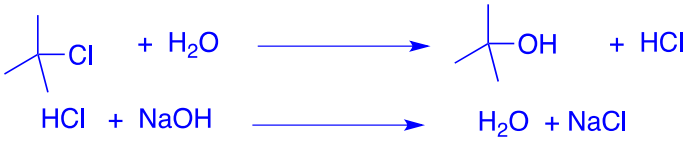
b) Br^- vs. I^-

Nucleophilicity increases down the periodic table. An increase in atom size means the valence electrons are held less tightly to the nucleus. Since I is a larger atom than Br, it is a better nucleophile.

c) 

The $-CF_3$ group on the acetate on the left renders its conjugate acid a stronger acid owing to inductive effects, thus implying that the acetate on the right is the weaker acid or stronger base and thus better nucleophile of the two.

2. What is the role of NaOH in part B of the experiment?



NaOH has three key roles:

1) *It acts as a nucleophile over the course of the reaction.*
2) *It neutralizes the HCl produced in the reaction*
3) *It provides a method to monitor the reaction in partnership with the methyl blue indicator.*

3. a) Following the procedure as described in Part A, determine the initial concentration of KOH in the reaction.

$C_1V_1 = C_2V_2$

$$C_2 = \frac{(2.0\ M)(0.01\ L)}{0.05\ L}$$

$[KOH]_i = 0.4\ M$

b) As you begin your second titration point after 30 minutes, you quickly pipette a 5.2 mL aliquot from your reaction system into a flask, add indicator, and titrate the sample with 0.1 M HCl. When the burette volume drops from 20.7 mL to 14.0 mL, your sample has reached the equivalence point. Determine the concentration of KOH remaining in your reaction mixture after 30 minutes.

20.7 - 14.0 = 6.7 mL HCl

$0.0067\ L \times 0.1\ M = 6.7 \times 10^{-4}$ mol HCl 1 mol of HCl neutralizes 1 mol of KOH

ie. 6.7×10^{-4} mol KOH remaining in the aliquot

$$\frac{6.7 \times 10^{-4}\ mol}{0.0052\ L} = 0.129\ M\ KOH\ remaining$$

After 30 minutes of the reaction, there is 0.129 M KOH remaining in the reaction mixture. The aliquot is a representative sample of the reaction mixture with the same concentration of KOH prior to addition of HCl.

4. 1-bromo-3-methylcyclopentane can undergo a substitution reaction in the presence of ammonia. Predict the product(s) and construct a potential energy diagram (reaction profile) for the reaction. Show the transition state species, intermediate, rate-determining step, and activation energy. Indicate the proper stereochemistry throughout the reaction.