EXPERIMENT 3: STUDYING S_N1 and S_N2 REACTIONS: NUCLEOPHILIC REACTIONS AT SATURATED CARBON

[In addition to your prelab information, you need to turn in quite a bit of additional information, answer some questions, get some information downloaded, show spectra, and interpret your results. Again, my comments to you will be in the [] brackets. For simplicities sake I will take the liberties of MAKING UP data and times that I will need to complete this experiment.]

OBSERVATIONS:
PART 1 Bimolecular Nucleophilic Substitution: S_N2

5.21 grams butanol
15.17 grams HBr
4.0 ml H_2SO_4
reflux started @ 1:27
reflux stopped @ 2:35
round bottm flask in water bath for 8 minutes
add 10 ml water, swirl
distillation started;
temp of first material collected: 92C cloudy
temp of last material collected: 110C clear

add 5 ml water, wash with 5 ml 5% bicarb X2
add 1 scoop $CaCl_2$, appears clear
weight of tared flask: 54.0654 g
weight of tared flask and bromobutane: 61.1572 g

IR collected and added to notebook

	gram	mol
amount of butanol used	5.21/74.1g	0.0703
amount of 1-bromobutane produced	7.0918/137g	0.0518

product theoretical yield 9.6311 = .0703 mol (137 g/mol)

product percent yield, % 73.7% = .0518/0.0703 * 100%

IR confirms that OH group present in the starting material is not present in IR from product.

OBSERVATIONS continued
Part 2 Unimolecular Nucleophulic Substitution: S_N1

PART A
Made 200 ml 1:1 2-propanol: water solution
Added 50 ml to two Erlen flasks
Added 5 drops phenolphthalein to each Erlen flask
Using pipeter, added 200 µl NaOH soln to each Erlen flask

Add 50 µl 2-bromo-2-methylpropane:
35 secs to clear soln

Add 50 µl 2-chloro-2-methylpropane:
75 secs to clear soln

PART B
Added 50 ml 1:1 2-propanol:water to two Erlen flasks
Added 5 drops phenolphthalein to each Erlen flask
Using pipeter, added 200 µl NaOH soln to each Erlen flask

Add 50 µl 2-bromo-2-methylpropane:
39 secs to clear soln

Add 50 µl 2-bromopropane:
> 900 secs to clear soln

Part C
Added 20 ml water to 30 ml 2-propanol, pour into Erlen flask and mixed.
Added 30 ml water to 20 ml 2-propanol, pour into Erlen flask and mixed.
Added 5 drops phenolphthalein to each Erlen flask
Using pipeter, added 200 µl NaOH soln to each Erlen flask
Add 50 µl 2-bromo-2-methylpropane to 40% soln
25 secs to clear soln
Add 50 µl 2-bromo-2-methylpropane to 60% soln
70 secs to clear soln

Unimolecular Nucleophulic Substitution: S_N1

Compound	Time (sec)
2-bromo-2-methylpropane	35
2-chloro-2-methylpropane	75

Leaving group

Alkyl structure

2-bromo-2-methylpropane	39
2-bromopropane	> 900

Solvent polarity

40% 2-propanol	35
60% 2-propanol	78

Saw predicted effects: Br was better LG, 3^o does a faster S_N1 than a 2^o, and more polar solvents produced faster S_N1 results.

Discussion: [This is the place where you will see if the rules that you have been learning in class will hold when actually tested in the laboratory]

PART 1:

The conditions that were used for the butanol / n-butylbromide transformation were classic S_N2 conditions. The acids used provided both the nucleophile (Br-) and the proton source that would make OH- into an acceptable leaving group (H_2O). According to the textbook, my yield for this reaction was very good as these conditions could promote a few side reactions that would slightly reduce the overall yield.

My IR was fairly clean, but there was a trace of water as shown by a small peak around 3400 wavenumbers. My spectra was generated by using the FT-IR and was very similar to the spectra I downloaded from the given website.

PART 2:

In this part of the experiment, I conducted several experiments to see a few of the factors that affect S_N1 chemistry: Leaving Group effects, Alkyl structure, and Solvent Polarity.

All of these reactions used –OH as the nucleophile and phenolphthalein as the indicator: removal of –OH from the solution would reduce the pH and the indicator would show that the solution was no longer alkaline.

According to the textbook, bromide is a better leaving group that chloride. This was verified since the 2-bromo-2-methyl propane solution went clear faster than the 2-chloro-2-methylpropane.

Also, according to the textbook, the starting materials that can most easily form 3^o cations will undergo S_N1 faster than 2^o cations. This was observed when it took far less time for the 2-

bromo-2-methyl propane solution to clear that the 2-bromopropane solution.
More polar solutions will help stabilize a cation better than less polar solutions, which supports the observations from the experiment that a 40% isopropanol solution will cause faster reaction times than a 60% isopropanol solution.

POST LAB QUESTIONS:

1. Calculate the percent yield of 1-bromobutane produced in Part I of this experiment.

amount of butanol used ___5.21/74.1g__ __0.0703____

amount of 1-bromobutane produced ___7.0918/137g__ __0.0518____

product theoretical yield ___9.6311__ = .0703 mol (137 g/mol)

product percent yield, % ____73.7% = .0518/0.0703 * 100%

2. What experimental evidence can you provide that the product isolated from your synthetic experiment is 1-bromobutane?

The IR is very similar; the product is more dense than water or the starting material, and the odor is different.

3. yada yada yada!!
[Just keep going! I've given some of the answers earlier in the discussion section, but answer that specific question without referring the grader to other parts of the lab report. Your answers should be clear and concise.]
4.
5.
6.
7.
8.

Conclusion: [This is where 2 or 3 sentences of the general ideas examined should be added to show that you understand the principles observed]
Be of good cheer!
LPS