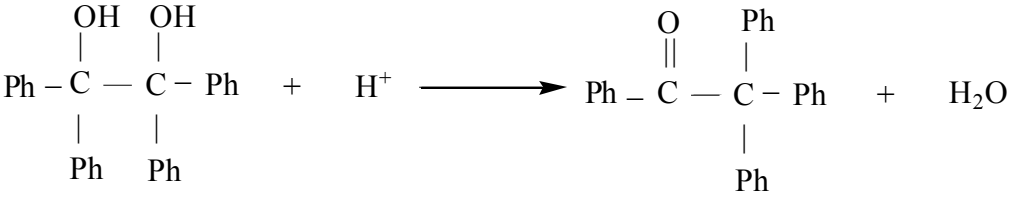
CARBOCATION REARRANGEMENTS:

Rearrangement of Benzopinacol

***Required Readings*, Ege, p. 289-291**.
Previously studied technique you will perform: Recrystallization.

The differing stabilities of carbocations can lead to rearrangement of a cation to one that is more stable, *e.g.,* secondary to tertiary. In this experiment, we will observe the rearrangement of one cation which we would expect to be quite stable to another cation which is even more stable. This demonstrates that cation stabilities are entirely relative and that rearrangement can readily occur when a more stable species can be formed.

The reaction we will perform is the conversion of benzopinacol to benzopinacolone via an acid-catalyzed dehydration reaction.



Benzopinacol Benzopinacolone

Procedure

In a 25-mL Erlenmeyer flask, mix 0.1 g iodine and 5.0 mL of glacial acetic acid. Add 1.0 g benzopinacol and a boiling chip and heat and manually stir the mixture on a hot plate in the hood (avoid boiling so vigorously that the acetic acid is boiled away; add a little more gl. acetic acid if necessary to maintain the volume). A dark red solution should result after boiling for *ca.* 5 minutes. Cool the flask in an ice bath; you should observe precipitation of the product. Add *ca.* 20 mL water and stir to break up any large crystals. Collect the product by suction filtration and wash it with a little cold water followed by a little cold ethanol. The product should be recrystallized from ethanol. Air dry the product and record the weight and melting point. Calculate the percent yield for the reaction.

The melting points for starting material and product are very close (look them up), so your instructor may have you compare infrared or nmr spectra of the starting material and product. You will receive instructions on those procedures.

CARBOCATION REARRANGEMENTS:

Rearrangement of Benzopinacol

NAME: _____

Section Number: _____

Reaction:

Mass of benzopinacol: _____

Moles of benzopinacol: _____

Theo moles product: _____

Theo mass product: _____

Mass recovered product: _____

Moles recovered product: _____

% yield of product: _____

Calculations: (you may include these on a separate attached sheet)

Questions

1. Write the electron-pushing mechanism for the reaction.

2. Explain the driving force for the rearrangement. Use a reaction coordinate-energy diagram in your explanation.

3. Besides IR and NMR spectroscopy, what other technique have you studied this semester which might help you determine that a reaction has taken place? Describe the results you would expect to see if you used this technique and explain your reasoning at the molecular level.

4. Turn in the ^{13}C NMR spectrum if the starting material and product. Draw the structure of the starting material and product on the appropriate spectrum and assign the non-equivalent carbons (a, b, c, etc.) Correlate the non-equivalent carbons to the appropriate peaks in the spectrum.

For example: