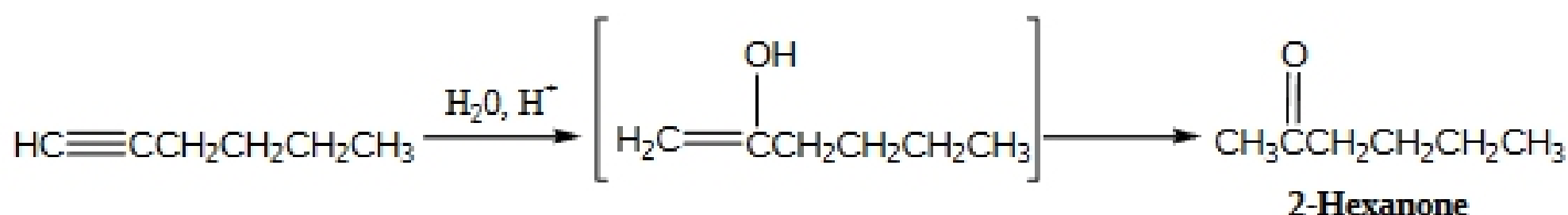


Hydration of 1-Hexyne

The hydration reaction is an addition of water across a π -bond. When hydration is carried out on an alkyne, water is added to only one π -bond to form an enol. Most enols are relatively unstable and equilibrate to a more stable carbonyl form through a process called tautomerization. Acid catalyzed hydration is a Markovnikov addition, and the carbonyl oxygen will always be placed on the internal carbon of a terminal alkyne. In this experiment, you will hydrate 1-hexyne to produce 2-hexanone using sulfuric acid as a catalyst.



Safety:

- Sulfuric acid is a strong acid and can cause serious burns and eye damage.

Procedure:

Add 1 mL of water and a stir bar to a 50 mL round bottom flask and cool in an ice bath. Add 6 mL of concentrated sulfuric acid with stirring then place the flask in a room temperature water bath. In a 50 mL Erlenmeyer flask, obtain 2.0 g of 1-hexyne. Add half of the 1-hexyne to the sulfuric acid solution with vigorous stirring. Let the reaction stir for 20 minutes and then add the remaining 1-hexyne, again with vigorous stirring. Let the reaction stir for another 20 minutes and then cool the reaction flask in an ice water bath. Add 20 mL of water and stir for 10 minutes. The flask should now contain two distinct layers: a dark upper layer and a lighter lower layer. Pour both layers into a separatory funnel and then drain off the lower aqueous layer. Wash the organic layer with 10 mL of water and drain off the lower aqueous layer. Pour the organic layer into a 50 mL Erlenmeyer flask and dry the crude product over Na_2SO_4 . Pipet the dried product into a 5 mL round bottom flask and distill using a Hickman still. Be sure to obtain a boiling point during the distillation and a final mass of distilled product.

Write Up:

Calculate the percent yield (show the calculation) and elaborate on the accuracy and significance of your product boiling point.

Questions:

1. Why would acid catalyzed hydration of an alkyne not be a good way to synthesize 3-heptanone?
2. Provide a synthesis of 3-hexanone starting from acetylene.
3. [Using Student Spartan, build a model of the 1-propenyl cation as follows: Build propene, then delete one of the valences on C1. Minimize the energy, then setup a calculation as follows: "Calculate" = "Equilibrium Geometry," "with" = "Hartree-Fock/3-21-G,"](#)

“Total Charge” = “Cation”. After the calculation is complete, select “Display-Properties,” and the calculated gas-phase energy of the cation will be the first entry in the list (labeled “Energy”). This is actually the “total energy” of the cation expressed in atomic units (au, 1 au = 2625 kJ/mol = 627.4 kcal/mol). Build a model of the 2-propenyl cation in a similar manner, except delete the remaining valence on C2 before performing the calculation. What is the difference in “total energy” (expressed in kcal/mol) between the two cations? Which cation is more stable? Is this consistent with your results from this experiment? Explain. Is this consistent with your understanding of the hydration of alkynes? Explain.