Nitration of methyl benzoate

Part 1 - Purpose

The purpose of the lab is to better understand electrophilic aromatic substitution by carrying out the nitration of methyl benzoate

Part II - Results

Substances Used:

Formulas Used

Grams to Milliliters for Methyl Benzoate:

Theoretical Yield of Methyl 3-Nitrobenzoate:

Percent Yield:

Percent Error:

Calculations:

- Recovered Methyl 3-Nitrobenzoate: 0. 125 g
- Grams to Milliliters for Methyl Benzoate: 0. 3 mL
- Theoretical Yield of Methyl 3-Nitrobenzoate: 0. 40 g
- Percent Yield: 30%
- Percent Error: 233%

Part III - Discussion/Conclusion:

Discussion

Aromatic ester is dissolved in sulfuric acid and reacted with nitric acid: the nitration of methyl benzoate is an example of electrophilic aromatic

substitution where the nitronium ion acts as the electrophile in attacking the aromatic ring. The nitronium ion is generated due to a reaction that takes place between the concentrated nitric acid and sulfuric acid. After the sulfuric acid protonates the methyl benzoate, the nitronium ion reacts with the intermediate at the meta position thus forming an intermediate arenium ion. The intermediate arenium ion would have a sigma complex containing four resonance structures. Because the sigma complex is made up of several resonance structures, the positive charge is more delocalized creating for a more stable complex. Furthermore, the more stable the sigma complex, the more likely it is to form in the mechanism for electrophilic substitution. The reaction then continues with the arenium ion intermediate transferring a proton to the basic bisulfate ion, yielding a methyl 3-nitrobenzoate.

The reaction is highly exothermic, thus must be kept cool during the addition process. After filtration, the product is recrystallized from methanol.

Conclusion

With the completion of the experiment, the very low yield was calculated providing a high percent error. Several possible sources of error include:

- (1) Not providing enough time on the vacuum
- (2) allowing the methanol to get too warm
- (3) loss of product while transferring

1. If the crystals aren't allowed enough time to dry during suction filtration, the product would appear heavier. Although this may cause a

higher calculated recovery, the value would not be accurate to the experiment.

2. It is important that the methanol is ice cold prior to washing the product. As the temperature increases, the product would become more soluble within the methanol. Thus if the methanol is not ice cold, a substantial amount of the product could be lost decreasing the yield and increasing the percent error.
3. It is important to be as efficient as possible when transferring material, for it is likely to lose product with each time the substance changes containers. Rather than using a new tray to weight the product, the weight of the container used for the reaction should have been observed and subtracted from the final weight.