

Multistep synthesis essay



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Results: Limiting Reactant: Eq 1 Limiting reactant = Benzoin Theoretical yield of Benzil: Eq 2 Theoretical Yield Benzil| 0. 296 g| Mass of Crude Benzil| 0. 188 g| Mass of Final Benzil| 0. 127 g| % Yield| 43%| % Recovery| 66%|

Table 1: Mass of crude/final Benzil, % yield, and % recovery Percent Yield: % Yield = (Final product/Theoretical product) x 100 Eq 3 = (0. 127 g/0. 296 g) x 100 = 43% yield Percent Recovery % Recovery = (Final product/Crude product) x 100 Eq 4 = (0. 127 g/0. 188 g) x 100 = 66% recovery Theoretical Yield Benzilic Acid:

Eq 5 Theoretical Yield Benzilic Acid| 0. 109 g| Final Benzilic Acid| 0. 060g| Percent Yield| 55%| Table 2: Final weight and percent yield of benzilic acid | Degrees Celsius | Crude Benzil| 82. 5 – 85. 6| Final Benzil| 94. 2| Final Benzilic Acid| 148. 3| Table 3: Melting Points Wavenumbers (cm-1)| Functional groups| 1593| Aromatic| 3065| Sp² C-H bond| 1659| C= O bond/carbonyl group| Table 4: IR wavenumbers and functional groups of Benzil Wavenumbers (cm-1)| Functional groups| 1600| Aromatic| 3100-3000| Sp² C-H bond| 3100-2900| Carboxylic Acid| 300| O-H alcohol| 1650| C= O bond/carbonyl group| Table 5: IR wavenumbers and functional groups of Benzilic Acid Discussion: In this experiment, benzoin was oxidized by nitric acid to benzil, which in turn was rearranged to benzilic acid. Prior to beginning the experiment, the theoretical yield of benzil was discovered. The limiting reactant in the reaction, benzoin + nitric acid benzil, was benzoin at 0. 00141 moles. This value was discovered by the initial amount of the reactants used: 0. 30 grams benzoin and 1. 5 ml Nitric Acid (see Eq 1).

Using the moles of the limiting reagent benzoin, the theoretical yield of benzil was calculated to be 0. 296 grams (see Eq 2). Before crystallization,

the weight of the crude benzil was 0.188 grams and the final weight after crystallization was 0.127 grams (Table 1). The percent yield, calculated using the theoretical and final amount of benzil, was 43% (see Eq 3). The percent recovery, calculated using the crude and final amount of benzil, was 66% (Eq 4). The melting points of crude and final benzil were 82.5 – 85.6°C and 94.2°C respectively (Table 3). The literature value for pure benzil is 95°C and the final crystallized benzil temperature value is very close to the literature value. This testifies the purity of the experimental benzil. The melting point value of the crude was much lower and the range was much wider due to the impurities. For further confirmation of the purity of experimental benzil, the infrared spectroscopy was observed. The following functional groups were determined on the infrared spectroscopy according to their corresponding wavenumbers: aromatic, sp² C-H bonds, and C=O/carbonyl group (Table 4). Benzil incorporates all of the above functional groups.

The melting and infrared spectroscopy confirmed that the final product created was Benzil. In the following reaction, benzil was rearranged to from benzilic acid by reacting it with potassium hydroxide in ethanol. 0.100 benzil was utilized and the theoretical yield of benzilic acid was 0.109 grams (see Eq 5). The final yield and weight of benzilic acid was 0.60 grams. The final yield and theoretical yield were used to calculate the percent yield, 55% (similar to Eq 3). The melting point of benzilic acid was 148.3°C and the literature value for benzilic acid is 150°C.

The melting points of experimental benzilic acid and the literature value are in close proximity to each other emphasizing the purity of experimental

benzilic acid. The following functional groups were seen on the infrared spectroscopy of benzilic acid according to their corresponding wavenumbers: aromatic, sp^2 C-H bonds, carboxylic acid, alcohol, and carbonyl group (Table 5). Benzilic acid incorporates all of the above functional groups. The melting and infrared spectroscopy confirmed that the final product created was indeed benzilic acid. The objective of this experiment was accomplished and benzilic acid was created.