Chemistry 260 Summer 2024

E11 The Aldol Reaction

**<<This report will be completed as an “in-lab assignment” that you will work on and hand in at the end of the period. You can do some of the work (e.g., the 13C NMR) in advance and bring your own copy of this template if you wish, but copies will be provided in the lab.>>**

Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Section:\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Date: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**Observations**

**Reagents and Products Tables**

Table 1. Reagents for the Aldol reaction

| Compound | MW (g/mol) | Used | mmol | Physical and Safety Data |
| --- | --- | --- | --- | --- |
| benzil | 210.23 |  |  | Irritant, combustible solid. Mp 94-95oC |
| 1,3-diphenylacetone | 210.28 | 0.5 g | 2.378 | Irritant. Mp 30-34oC |
| ethanol | 46.08 | ~50 mL total | N/A | Flammable liquid; irritant. Bp 78 oC; density 0.789 g/mL. |
| Potassium hydroxide | 56.11 | ~0.5 g | ~9  | Toxic, corrosive |

Table 2. Product of the Aldol reaction

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Physical Description | MW (g/mol) | Amount Isolated | mmol | % yield |
| tetraphenylcyclopentadieneone |  | 384.47 |  |  |  |

**Results**

**Percent Yield Calculation:**

**Melting Range:**

UV-Visible Spectroscopy Data:

Table 4. UV-vis data for tetraphenylcyclopentadienone

|  |  |  |
| --- | --- | --- |
| Compound  | Maximum wavelength (max) | Colour of solution |
| Tetraphenylcyclopentadienone |  |  |

Draw a rough sketch of and briefly describe the UV-Visible spectrum in your own words:

**Carbon NMR Data:**

Table 6. 13C NMR data for tetraphenylcyclopentadienone

|  |  |  |  |
| --- | --- | --- | --- |
|  | Assignment |  | Assignment |
| 200.3 |  | 128.5 |  |
| 154.5 |  | 128.0 (higher) |  |
| 133.0 |  | 128.0 (lower) |  |
| 130.7 |  | 127.4 |  |
| 130.1 |  | 125.3 |  |
| 129.3 |  |  |

Labelled structure:

IR Data:

Table 5. **KEY** signals in the IR of tetraphenylcyclopentadieneone (only list key peaks used for identification)

|  |  |  |
| --- | --- | --- |
| Wavenumber (cm-1)  | Strength (s/m/w) | Assignment and/or Comment |
|  |  |  |
|  |  |  |
|  |  |  |

**In-lab Assignment Questions:**

 UV-Visible Spectroscopy:

What was the max for your UV-vis measurement? What colour does this mean is absorbed by the solution? Is this consistent with the colour of the compound that you observed with your eyes? (**3 marks**)

Most of the organic compounds you have made thus far have been white or colourless. What is different about this compound? (i.e., what feature of the molecule produces the visible colour?) (**2 marks**)

**13C NMR**

How many carbon atoms are in the product? How many signals are in the 13C NMR? Why are these numbers different? (**2 marks**)

Provide a *brief* justification of how you assigned the peaks in the 13C NMR spectrum. (**3 marks**).