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| --- | --- | --- | --- | --- |
| **CHEM 202 LABORATORY REPORT** | | **Name:** | | Harry Stanley |
| **Experiment 1** | **Lab Day:** | **Thursday** | **Date:** | 27/2/2025 |

***Nitration of aromatic hydrocarbons: Measurement of reactivities by the competition technique***

**Abstract**

A large excess of an equimolar mixture of benzene (**1**) and toluene (**2**) was treated with a nitrating mixture (HNO3 / Ac2O) to produce a mixture containing nitrobenzene (**3**), *o*-nitrotoluene (**4**), *m*-nitrotoluene (**5**) and *p*-nitrotoluene (**6**). The relative concentrations of **3**-**6** in the reaction mixture were measured by GLC and the relative reactivities of **1** and **2** towards nitration were calculated from this data after taking the number of equivalent reaction sites into consideration. Comparison of the relative concentrations of **4-6** allowed the determination of the relative reactivities of the different sites in **2**.

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|  |

**Experimental**

The experiment was performed as detailed in the CHEM 202 laboratory manual (p 17), without modification.

Aqueous waste generated by washing the crude reaction mixture was disposed of down the fumehood sink. Magnesium sulfate used to dry the organic extracts was also disposed of down the fumehood sink with the aid of copious amounts of cold water. Ether removed from the product under reduced pressure was disposed of in the Organic Residues bottle. The final product mixture was disposed of in the Organic Residues bottle provided after GLC analysis.

**Results and calculations**

*Table 1: GLC analysis of the reaction mixture after work-up*

|  |  |  |
| --- | --- | --- |
| **Retention time/min** | **Assignment** | **Peak area** |
| 1.250 | Nitrobenzene | 8.832 |
| 1.604 | o-nitrotoluene | 150.283 |
| 1.789 | m- nitrotoluene | 5.994 |
| 1.929 | p- nitrotoluene | 102.810 |

*Table 2: A comparison of the relative reactivities of aromatic carbon atoms in benzene and toluene towards nitration*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Substrate** | **Combined peak areas of nitration products** | **Number of equivalent reaction sites** | **Reactivity per equivalent site** | **Relative reactivity per equivalent site** |
| benzene | 8.832 | 6 | 1.472 | 1.0 |
| toluene | 259.087 | 5 | 51.817 | 35.202 |

*Table 3: A comparison of the relative reactivities of the different substitution sites in toluene towards nitration*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Site** | **Peak area of derived product** | **Number of equivalent reaction sites** | **Reactivity per equivalent site** | **Relative reactivity per equivalent site** |
| *ortho* | 150.283 | 2 | 75.142 | 25.072 |
| *meta* | 5.994 | 2 | 2.997 | 1 |
| *para* | 102.810 | 1 | 102.810 | 34.304 |

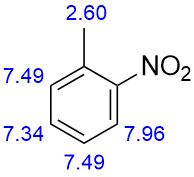
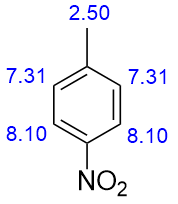
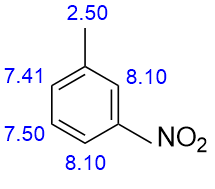
**Discussion of experimental results**

*ADD YOUR DISCUSSION SECTION HERE.*

**Discussion of procedures involved in the experiment**

During the extraction step it was better to rinse the reaction flask twice with small portion of diethyl ether instead of one larger volume, this allows for increased efficiency allowing for more product to be removed from the flask, increasing overall yield of the reaction products.

**Discussion of 1H NMR data for nitrotoluene isomers**

*Isomer A: Isomer B: Isomer C:*

*o-nitrotoluene p-nitrotoluene m-nitrotoluene*

### Table 4: 1H-NMR (400 MHz, CDCl3)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **/ppm** | **Relative # of hydrogens** | **multiplicity** | **J/Hz** | **Assignment** |
| **Isomer A** |  | 3 | s | - | CH3 |
|  |  | 2 | m | - | CH |
|  |  | 1 | t | 7.6 | CH |
|  |  | 1 | d | 8.5 | CH |
| **Isomer B** | 2.50 | 3 | s | - | CH3 |
|  | 7.31 | 2 | d | 8.3 | CH |
|  | 8.10 | 2 | d | 8.7 | CH, |
| **Isomer C** | 2.50 | 3 | s | - | CH3 |
|  | 7.41 | 1 | T | 7.9 | CH |
|  | 7.50 | 1 | d | 7.7 | CH |
|  | 8.02 | 2 | d | 9.4 | CH |

*NOTE: Add table rows as required. For convenience* ***(and for this lab only!!)*** *you can ignore any observed small splittings (J<2 Hz). See Appendix 12 (p86) for estimating δ-values to guide your assignments.*

**Discussion**

*ADD YOUR NMR DISCUSSION HERE*