**Structure and Reactivity Relationships - Nucleophillic Substitution Reactions**

Together, you and your TA are comparing the reactivity of an assortment of alkyl halides under SN1 and SN2 reaction conditions. Watch the required videos of the experiment when noted. These will help you to determine what you will see when performing the reaction. Experimental details will be provided where necessary. Please use ChemDraw for all of your figures and schemes.

Answer the following questions:

1. Complete the following table:

|  |  |  |
| --- | --- | --- |
| **Compound** | **Structure** | **Reaction Site: Sp3 (3°, 2°, 1°) or sp2** |
| *n*-Butyl chloride |  |  |
| *n*-Butyl bromide |  |  |
| *Sec*-Butyl chloride |  |  |
| *Sec*-Butyl bromide |  |  |
| *Tert*-Butyl chloride |  |  |
| *Tert*-Butyl bromide |  |  |
| Chlorobenzene |  |  |
| Benzyl Chloride |  |  |

1. Define leaving group. What makes a good leaving group?
2. Draw the general mechanisms for a SN1 and SN2 reaction.
3. Explain the naming for SN1 and SN2 (eg. What does the acronym mean)?
4. What is the rate limiting step for an SN1 reaction? What is the rate limiting step for an SN2 reaction? What affects the rate in each case?
5. How can you assess whether a reagent will promote SN1 or SN2 chemistry? Consider nucleophilicity in your answer.

Time for the lab to commence! You have 8 unknown sample vials. You know that the contents of each of the vials corresponds to one of alkyl halides you outlined above. Assess the following reactions to help you determine which unknown number belongs to which alkyl halide!

1. To a 0.1 mL sample of each unknown you add 1 mL of NaI in an acetone solution in a single dose. The test tubes are shaken, and the time recorded for each reaction. Watch the following video and assess your in-lab data in the table below to help you determine which alkyl halide belongs to which unknown number.

<https://www.youtube.com/watch?v=o-Cl88fLixs>

|  |  |  |
| --- | --- | --- |
| **Unknown Number** | **Observations** | **Reaction Time (minutes)** |
| 1 | The solution became cloudy | 26.00 |
| 2 | A white precipitate formed | 1.30 |
| 3 | The solution became cloudy and slowly precipitated | 15.20 |
| 4 | A white precipitate formed instantly | 0.02 |
| 5 | Reaction solution remained clear | 60.00 |
| 6 | A white precipitate formed | 1.00 |
| 7 | A white precipitate formed slowly | 12.00 |
| 8 | The solution become cloudy | 24.02 |

1. What are the two general products formed during the reaction of NaI with an alkyl halide? Which product is the precipitate?
2. Is the reaction of NaI with an alkly halide an SN1 or an SN2 reaction? Explain.
3. To a 0.1 mL sample of each unknown you add 1 mL of AgNO3 in an ethanol/water solution in a single dose. The test tubes are shaken, and the time recorded for each reaction. Re-watch the following video and assess your in-lab data in the table below to help you determine which alkyl halide belongs to which unknown number.

<https://www.youtube.com/watch?v=o-Cl88fLixs>

|  |  |  |
| --- | --- | --- |
| **Unknown Number** | **Observations** | **Reaction Time (minutes)** |
| 1 | A white precipitate formed quickly | 0.75 |
| 2 | The solution became cloudy | 24.60 |
| 3 | A white precipitate formed | 6.50 |
| 4 | A white precipitate formed instantly | 0.50 |
| 5 | No change to the solution | 60.00 |
| 6 | The solution became cloudy and a yellow precipitate slowly formed | 16.00 |
| 7 | A bright yellow precipitate formed | 5.00 |
| 8 | A yellow precipitate formed instantly | 0.50 |

1. What are the three general products formed during the reaction of AgNO3 with an alkyl halide? Which product is the precipitate?
2. Is the reaction of an alkyl halide with AgNO3 an SN1 or an SN2 reaction? Explain.
3. Complete the following table assigning each alkyl halide to an unknown number

|  |  |
| --- | --- |
| **Unknown Number** | **Hydrocarbon** |
| 1 |  |
| 2 |  |
| 3 |  |
| 4 |  |
| 5 |  |
| 6 |  |
| 7 |  |
| 8 |  |

1. Describe how you assigned each alkyl halide to an unknown number. Take into consideration the reaction type, the reaction intermediates, what controls the rate of each reaction, factors that affect the stability of various intermediates, and the colour of products. A well-rounded discussion will make it clear *chemically* why a reaction order or type is expected for each of the alkyl halides.

**BONUS QUESTIONS:**

2-bromobutane is reacted with NaI in an acetone solution. Draw the product(s) showing stereochemistry. Explain your choice.



2-bromobutane is reacted with AgNO3 in an ethanol/water solution. Draw the product(s) showing stereochemistry. Explain your choice.

