

Friedel-Crafts acylations reactions produce ketones

FRIEDEL-CRAFTS

$\text{CH}_3\text{CH}_2\text{COCl} + \text{C}_6\text{H}_6 \xrightarrow{\text{AlCl}_3} \text{C}_6\text{H}_5\text{CH}_2\text{COCH}_3 + \text{HCl}$
 $\text{C}_6\text{H}_6 + \text{CH}_3\text{COCl} \xrightarrow{\text{AlCl}_3} \text{C}_6\text{H}_5\text{COCH}_3 + \text{HCl}$
 $\text{C}_6\text{H}_6 + \text{HNO}_3 \xrightarrow{\text{H}_2\text{SO}_4} \text{C}_6\text{H}_5\text{NO}_2 + \text{H}_2\text{O}$
 $\text{C}_6\text{H}_6 + \text{CO} \xrightarrow{\text{Ni}, \text{H}_2} \text{C}_6\text{H}_5\text{CHO} + \text{H}_2$

Ketones acylium ion Lewis acid

Answer all the questions below as fully as you can then check your answers

1. What is an electrophile?
2. What is a Lewis acid?
3. Draw the structure of the following molecules:
 - i. ethanoyl chloride ii. Butanoyl chloride iii. ethanoic anhydride
- b. What is the useful product of a Friedel-Crafts acylation reaction?
4. What is the reactive electrophile in a Friedel-Crafts acylation reaction?
 - a. The acylium ion is a resonance stabilised ion. Draw the two resonance forms of the acylium ion.
 - b. What is resonance?
 - c. How is the acylium ion produced?
 - d. Write an equation to show how an acylium ion is formed when ethanoyl chloride reacts with the Lewis acid aluminium chloride (AlCl_3).

- e. Draw the mechanism to show how this acylium ion then reacts with benzene. Name the products of this reaction.
- f. How can phenylethanone be converted into ethylbenzene?
- g. Write an equation to show how the Lewis acid catalyst, aluminium chloride is regenerated in a Friedel-Crafts acylation reaction.
5. Write an equation to show how Butanoyl chloride reacts with benzene when heated to 80°C in the presence of anhydrous aluminium chloride.
6. Name one way in which a Friedel-Crafts acylation reaction is generally more useful than a Friedel-Crafts alkylation reaction.

Answers

1. What is an electrophile?

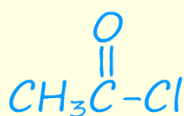
An electron deficient species.

2. What is a Lewis acid?

An electron pair acceptor. Lewis acids have vacant or empty orbitals that are able to accept a pair of electrons. Lewis acids are normally molecules which do not have an octet of electrons, such as AlCl_3 . Here for example the aluminium atom only has 6 electrons in its outer valency shell.

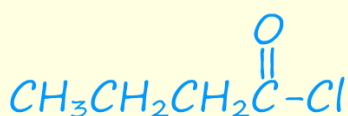
3. Draw the structure of the following molecules:

i. ethanoyl chloride



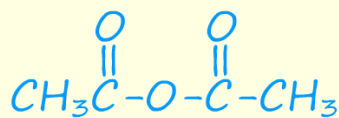
ethanoyl
chloride

ii. Butanoyl chloride



butanoyl
chloride

iii. ethanoic anhydride



ethanoic anhydride

b. What is the useful product of a Friedel-Crafts acylation reaction?

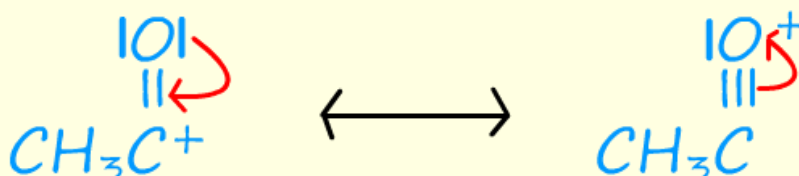
Aryl ketones

4. What is the reactive electrophile in a Friedel-Crafts acylation reaction?

An acylium ion

a. The acylium ion is a resonance stabilised ion.

Draw the two resonance forms of the acylium ion.



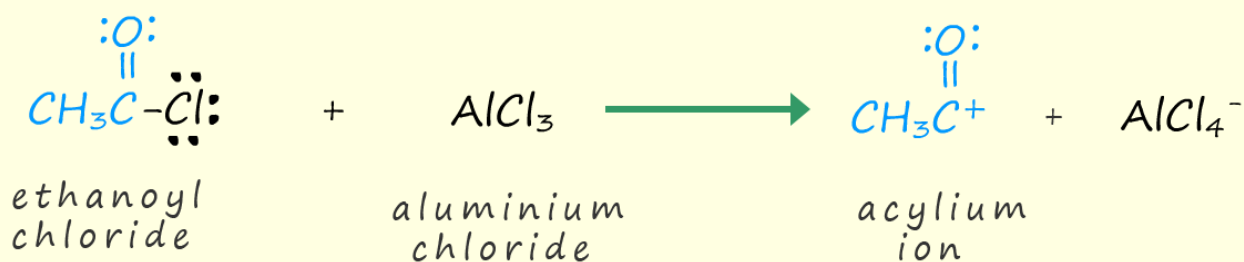
b. What is resonance?

Where delocalised electrons are spread over multiple atoms in a structure but the nuclei of the atoms remain in place.

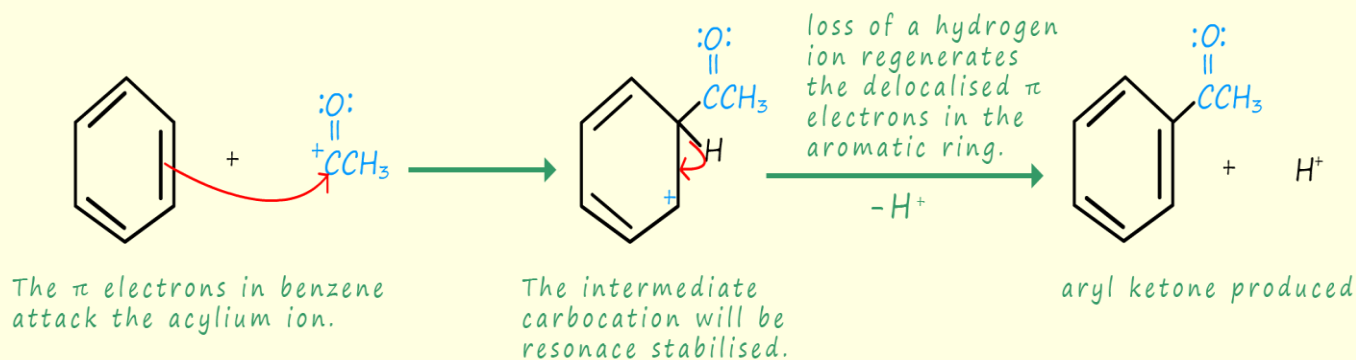
c. How is the acylium ion produced?

Reaction of an acid chloride or acid anhydride with a Lewis acid such as aluminium chloride.

d. Write an equation to show how an acylium ion is formed when ethanoyl chloride reacts with the Lewis acid aluminium chloride (AlCl_3).



e. Draw the mechanism to show how this acylium ion then reacts with benzene. Name the products of this reaction.

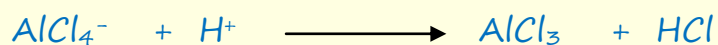


Product is phenylethanone and hydrogen ion.

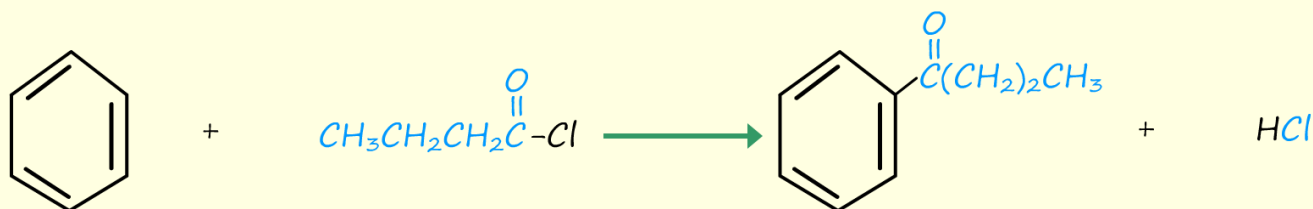
f. How can phenylethanone be converted into ethylbenzene?

Reduction using Ni/H_2

g. Write an equation to show how the Lewis acid catalyst, aluminium chloride is regenerated in a Friedel-Crafts acylation reaction.



5. Write an equation to show how Butanoyl chloride reacts with benzene when heated to 80°C in the presence of anhydrous aluminium chloride.



6. Name one way in which a Friedel-Crafts acylation reaction is generally more useful than a Friedel-Crafts alkylation reaction.

No polyalkylation with Friedel-Crafts acylation which is a major problem with Friedel Crafts alkylation, this is because the acyl group is a deactivating group while an alkyl group is an activating group.