# *KÉMIA IDEGEN NYELVEN*

## Kémia angolul

***Szerkesztő: MacLean Ildikó***

**Kedves Diákok!**

A 2012/5. számban az előző lapszámban ismertetett tematikának megfelelően szerves kémiához kapcsolódó fordítási feladatot kaptok a téli szünetre. Az itt megjelenő szöveget *ebben a formában fordítsátok le*, ne az eredeti forrásokból dolgozzatok, azoknak csak bizonyos részei kerültek be a fordítandó szövegbe.

**Beküldési határidő: 2013. január 7.**

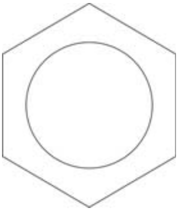
A fordítást továbbra is kizárólag a következő e-mail címre küldjétek:
kokelangol@gmail.com.

### 1./ Aromatic hydrocarbons

An aromatic hydrocarbon or arene is a hydrocarbon with alternating double and single bonds between carbon atoms forming rings. The term ‘aromatic’ was assigned before the physical mechanism determining aromaticity was discovered, and was derived from the fact that many of the compounds have a sweet scent. The configuration of six carbon atoms in aromatic compounds is known as a benzene ring, after the simplest possible such hydrocarbon benzene. Aromatic hydrocarbons can be **monocyclic** or **polycyclic**.

Some non-benzene-based compounds called **heteroarenes**, which follow Hückel's rule, are also aromatic compounds. In these compounds, at least one carbon atom is replaced by one of the heteroatoms, oxygen, nitrogen, or sulfur. Examples of non-benzene compounds with aromatic properties are furan, a **heterocyclic** compound with a five-membered ring that includes an oxygen atom, and pyridine, a heterocyclic compound with a six-membered ring containing one nitrogen atom.

## Benzene ring model



Benzene, $C_6H_6$, is the simplest aromatic hydrocarbon and was recognized as the first aromatic hydrocarbon, with the nature of its bonding first being recognized by Friedrich August Kekulé von Stradonitz in the 19th century. Each carbon atom in the hexagonal cycle has four electrons to share. One goes to the hydrogen atom, and one of each to the two neighboring carbons. This leaves one to share with one of its two neighboring carbon atoms, which is why the benzene molecule is drawn with alternating single and double bonds around the hexagon.

The structure is also illustrated as a circle around the inside of the ring to show six electrons floating around in delocalized molecular orbitals the size of the ring itself. This also represents the equivalent nature of the six carbon-carbon bonds all of bond order ~1.5. This equivalency is well explained by resonance forms. The electrons are visualized as floating above and below the ring with the electromagnetic fields they generate acting to keep the ring flat.

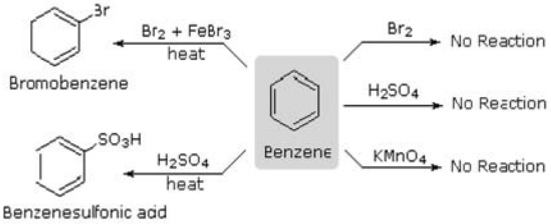
General properties:

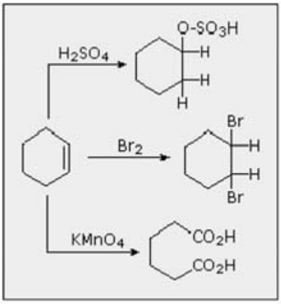
1. They display **aromaticity**.
2. The carbon-hydrogen ratio is high.
3. They burn with a sooty yellow flame because of the high carbon-hydrogen ratio.
4. They undergo **electrophilic substitution** reactions and **nucleophilic aromatic substitutions**.

The circle symbol for aromaticity was introduced by Sir Robert Robinson and his student James Armit in 1925 and popularized starting in 1959 by the Morrison & Boyd textbook on organic chemistry. The proper use of the symbol is debated; it is used to describe any cyclic pi system in some publications, or only those pi systems that obey e in others.

## Substitution Reactions of Benzene

The chemical reactivity of benzene contrasts with that of the alkenes in that substitution reactions occur in preference to addition reactions, as illustrated in the following diagram (some comparable reactions of cyclohexene are shown in the gray box).





Many other substitution reactions of benzene have been observed, the five most useful are listed below (chlorination and bromination are the most common halogenation reactions). Since the reagents and conditions employed in these reactions are electrophilic, these reactions are commonly referred to as **Electrophilic Aromatic Substitution**. The catalysts and co-reagents serve to generate the strong electrophilic species needed to effect the initial step of the substitution. The specific electrophile believed to function in each type of reaction is listed in the right hand column.

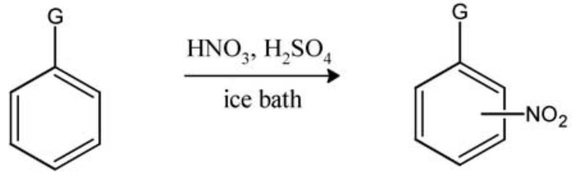
| Reaction Type | Typical Equation | Electrophile E(+) | Product |
|---|---|---|---|
| Halogenation: | $C_6H_6 + Cl_2 +$ heat → $C_6H_5Cl + HCl$<br>$FeCl_3$ catalyst | Cl(+) or Br(+) | Chlorobenzene |
| Nitration: | $C_6H_6 + HNO_3 +$ heat → $C_6H_5NO_2 + H_2O$<br>$H_2SO_4$ catalyst | $NO_2(+)$ | Nitrobenzene |
| Sulfonation: | $C_6H_6 + H_2SO_4 + SO_3 +$ heat → $C_6H_5SO_3H + H_2O$ | $SO_3H(+)$ | Benzenesulfonic acid |
| Alkylation:<br>Friedel-Crafts | $C_6H_6 + R\text{-}Cl +$ heat → $C_6H_5\text{-}R + HCl$<br>$AlCl_3$ catalyst | R(+) | An Arene |
| Acylation:<br>Friedel-Crafts | $C_6H_6 + RCOCl +$ heat → $C_6H_5COR + HCl$<br>$AlCl_3$ catalyst | RCO(+) | An Aryl Ketone |

## 2./ Nitration of an Aromatic Compound and Recrystallization

### Introduction:

In this **experiment**, you will do an aromatic nitration experiment. You will use one of the starting materials below. These only have one group on the benzene ring, so you have the possibility of three products: ortho-, meta-, and para-. You will use melting point as the primary method to determine the identity of your product.

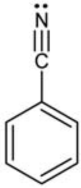
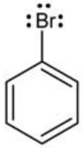
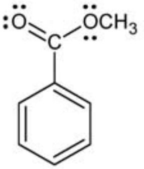
## Reaction Scheme:



Substituted benzene Nitrated product

The $-NO_2$ off the side of the benzene ring means the $NO_2$ group could be ortho, meta, or para to the G-group.

## Possible starting materials:

| Structure |  |  |  |
|---|---|---|---|
| Name | Benzonitrile | Bromobenzene | Methyl Benzoate |
| Melting Points of Possible Products | | | |
| ortho-nitro isomer | 111 | 43 | -13 |
| meta-nitro isomer | 118 | 56 | 78 |
| para-nitro isomer | 149 | 127 | 96 |
| Most likely dinitro isomer | 129 | 75 | 112 |

## Precautions:

Nitric acid is a strong acid and a powerful oxidizing agent. Sulfuric acid is a strong acid. Wear gloves. If you spill any of these, wipe them up with wet paper towels. If you spill these on you, wash the affected areas with lots and lots of soap and water. Some of the organic starting materials and solvents are **irritants**, so wear gloves when handling these as well.

**Reaction**:

Place a small **stir bar** and 10 mL of concentrated sulfuric acid in a 125 mL **Erlenmeyer flask**, and cool the flask in an ice-water bath while stirring for about 10 minutes. Prepare a mixture of 3 mL of concentrated nitric acid and 3 mL of concentrated sulfuric acid in a large **test-tube**, and cool it in your ice-**water bath**. Measure out 40 mmoles of your starting material (record exactly how much you use): weigh out liquids into another test tube. Add the starting material over a period of a minute to the Erlenmeyer flask. Keeping the Erlenmeyer flask in the ice-bath, add the cold mixture of nitric and sulfuric acids dropwise over about 10 minutes to the Erlenmeyer flask, while stirring the flask. After you have added the nitric and sulfuric acids, continue to stir the flask in the ice bath over the next 30 minutes.

**Product Isolation and Purification:**

Pour the reaction mixture, with stirring, into about 20 grams of ice in a small **beaker**. The product should **precipitate** as you stir the mixture. Collect the product by **suction filtration**, and wash it thoroughly with three small portions of ice-cold water. Remember to release the suction, add the wash solution and gently stir the wash liquid with the solid, and reapply the suction.

**Recrystallize** the product from methanol (benzonitrile or methyl benzoate products) or 95% ethanol (bromobenzene product). Start with about 10 mL of solvent, and only use more if the solid does not dissolve when boiling. Once it has all dissolved in the boiling solvent, allow the flask to cool to room temperature, then cool it further in an ice-bath. Collect the product by suction filtration, and wash the product with a **few** mL of ice-cold solvent. Allow air to pull through the crystals for a few minutes. Transfer a small amount of crystals to a watch glass, and then recrystallize the rest of your product again. Transfer the twice-recrystallized product to another watch glass. Allow the products to dry for a few days further. When the crystals are thoroughly dry, measure their mass and melting point range. Place the twice-recrystallized crystals in a **vial** labeled as follows:

Name of product

Mass

Your Name(s)

**TLC Analysis:**

You will analyze your product for purity by thin layer chromatography (TLC). Dissolve a tiny amount of your starting material and your recrystallized products in acetone in separate test-tubes. Spot these on a TLC plate, and look at the spots under the UV light to make sure they are visible. Develop the plate using dichloromethane as the TLC solvent. When the solvent is 1-2 cm from the top, remove the plate, wave the plate around in the air to evaporate the solvent, and look at it under the UV light, circling the spots. Include your plate with your report.

http://en.wikipedia.org/wiki/Aromatic_hydrocarbon

http://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/benzrx1.htm

http://cstl-csm.semo.edu/hathaway/CH344/2010%20Spring/CH344%20
Nitration%20ofan%20aromatic%20compound%20version%202.doc