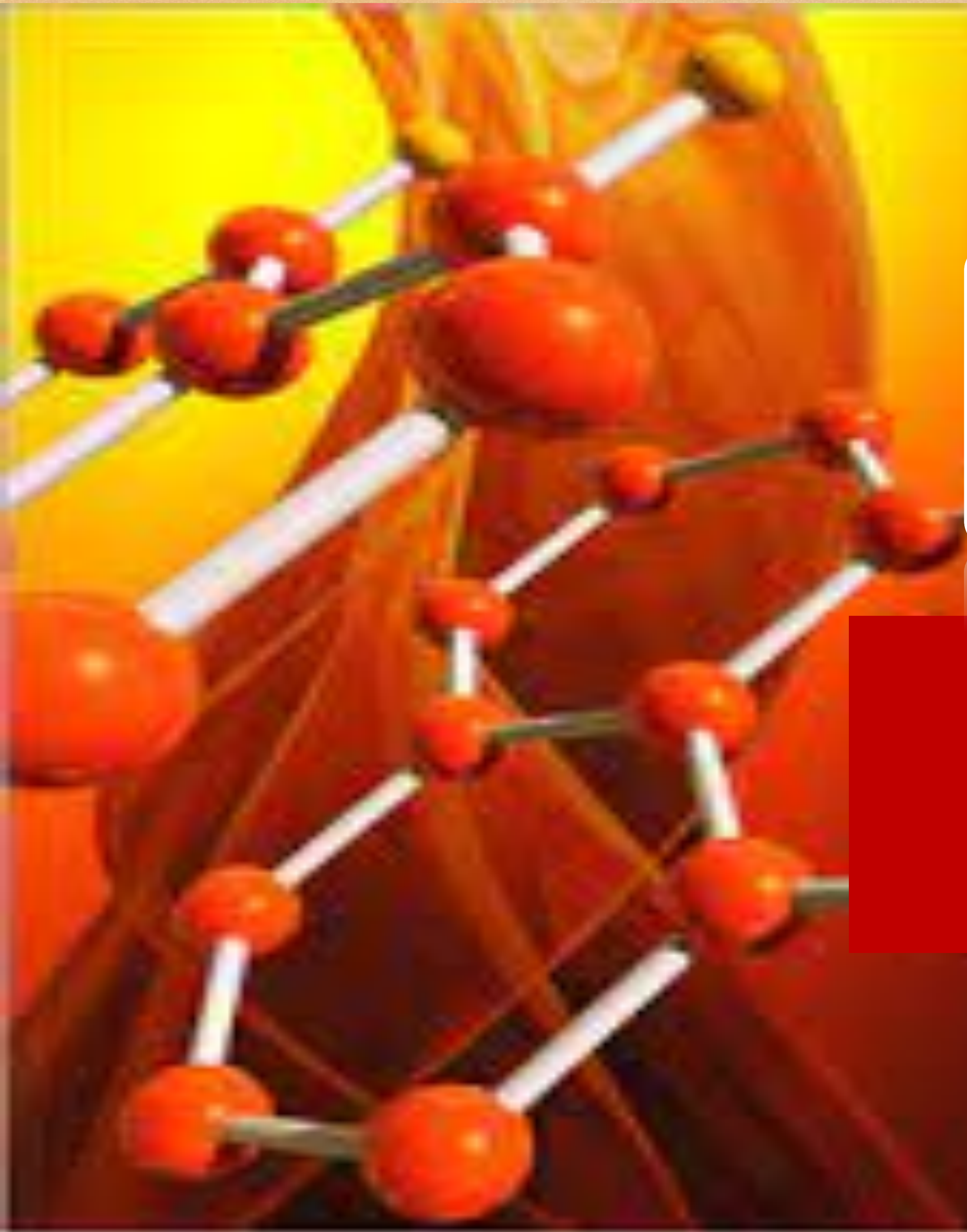


Aromatic Hydrocarbons

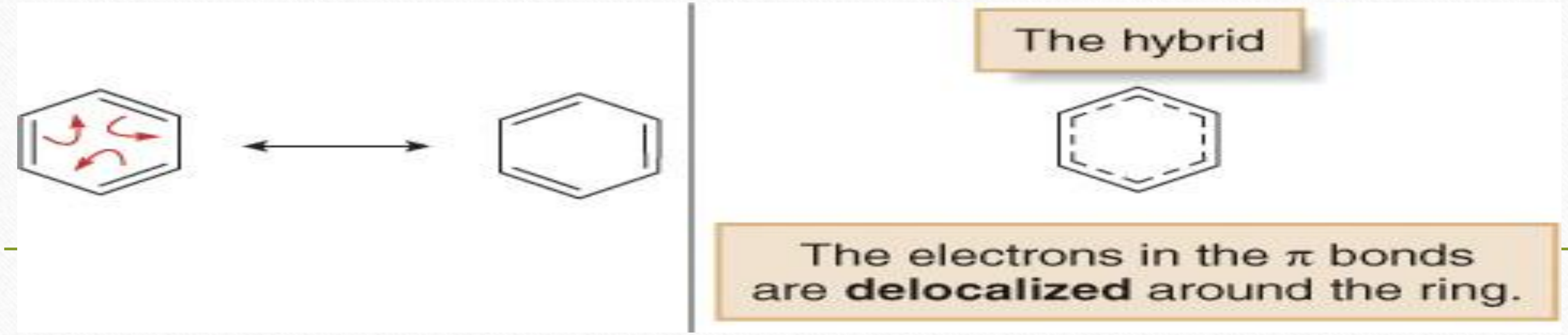
Prof. Dr. May Jaleel

Aromatic Compounds

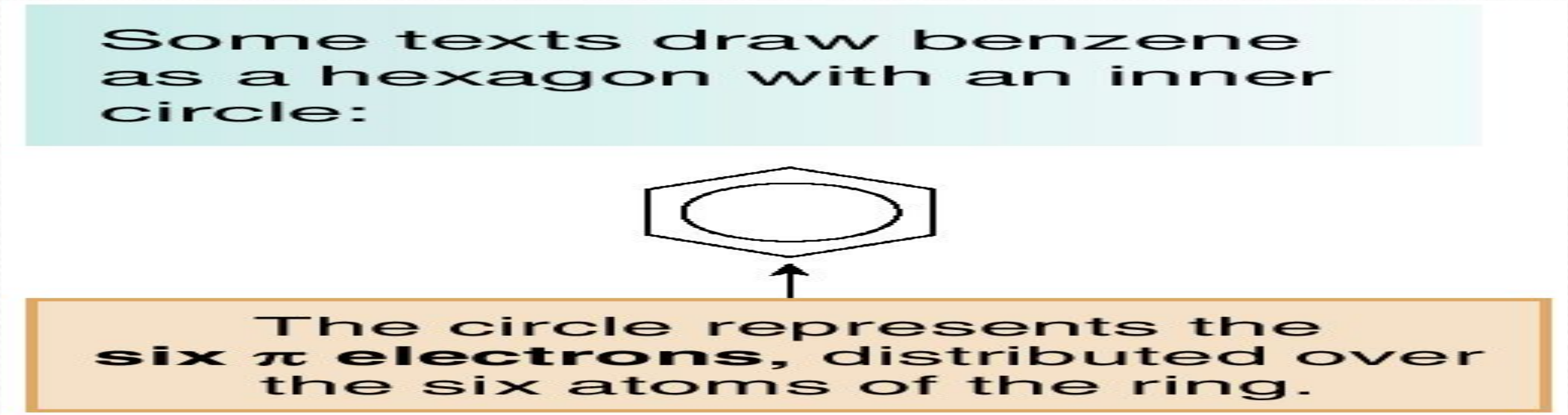
- **The Term Aromatic used to be used to describe a fragrant substance. Today the word aromatic refers to benzene and its structural relatives.**
- **Benzaldehyde, toluene, and benzene are all aromatic compounds. The steroidal hormone estrone, the analgesic morphine, and the tranquilizer diazepam (Valium) are all examples of aromatic compounds.**

Benzene and Aromatic Compounds

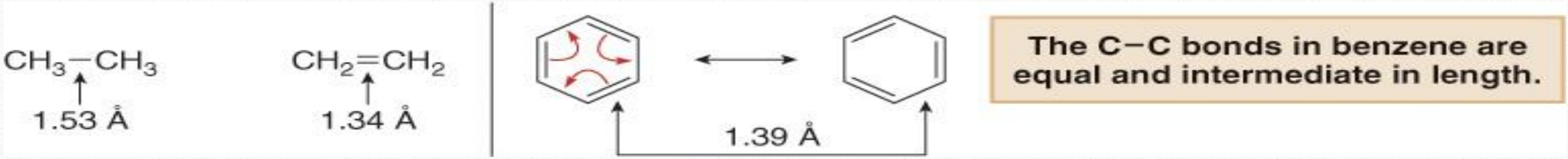
- **Benzene (C6H6) is the simplest aromatic hydrocarbon (or arene).**
- **The resonance description of benzene consists of two equivalent Lewis structures, each with three double bonds that alternate with three single bonds.**
- **The true structure of benzene is a resonance hybrid of the two Lewis structures, with the dashed lines of the hybrid indicating the position of the π bonds.**

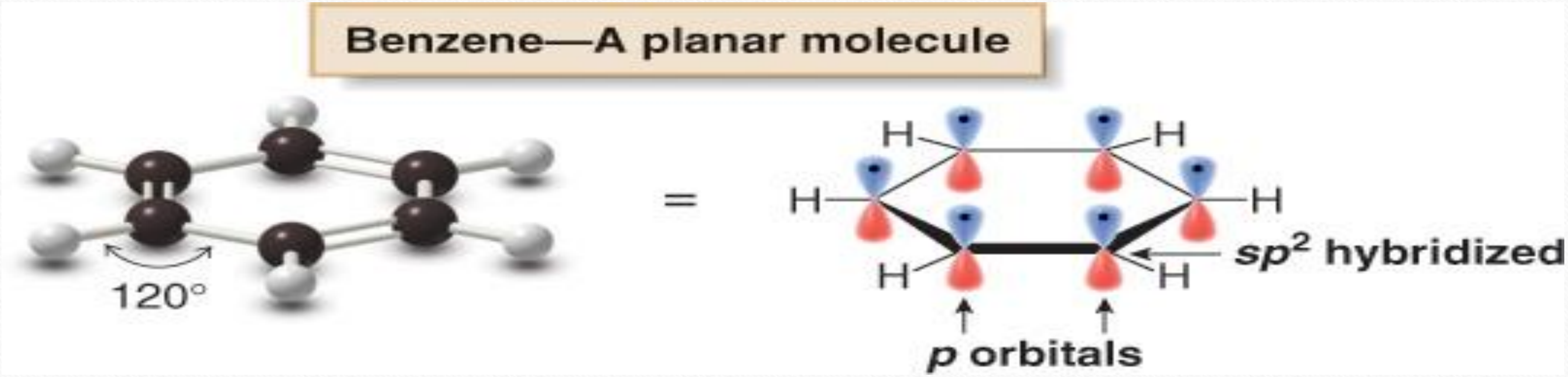


Because each π bond has two electrons, benzene has six π .electrons



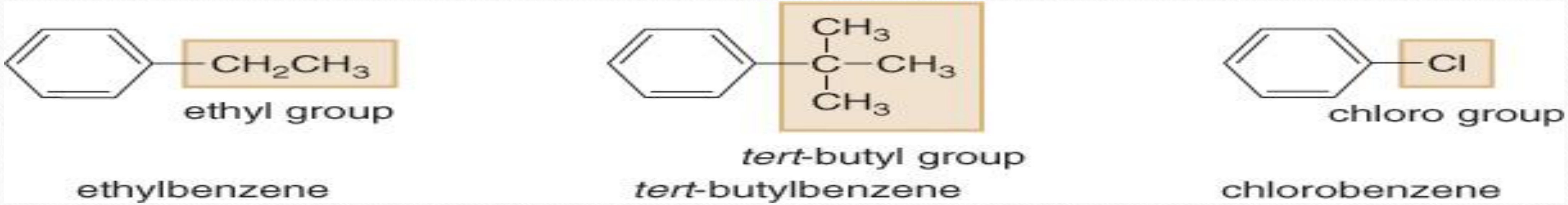
- In benzene, the actual bond length (1.39 Å) is intermediate between the carbon—carbon single bond (1.53 Å) and the carbon—carbon double bond (1.34 Å).



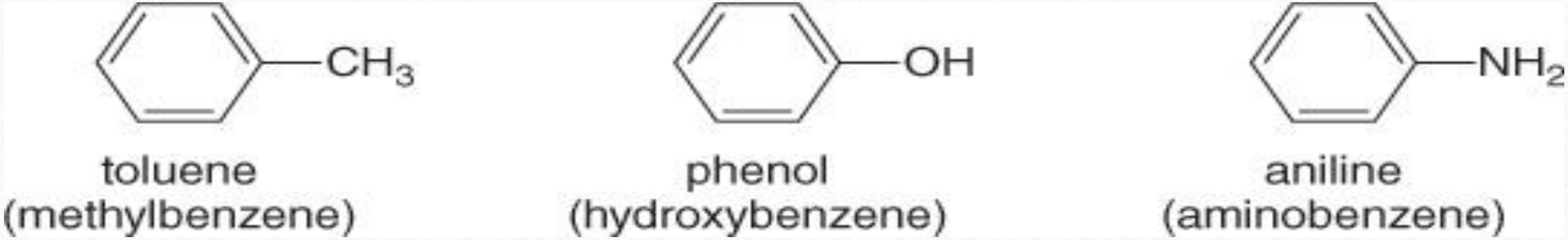


Nomenclature of Benzene Derivatives

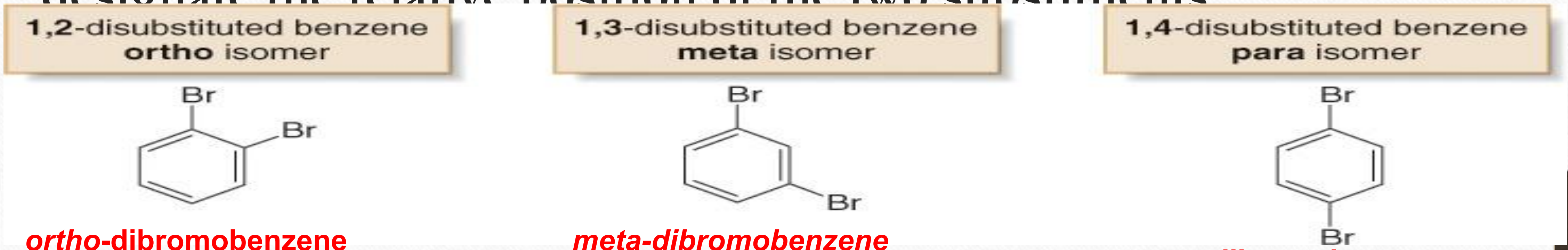
- To name a benzene ring with one substituent, name the substituent and add the word benzene.



- Many monosubstituted benzenes have common names which you must also learn.



- There are three different ways that two groups can be attached to a benzene ring, so a prefix—ortho, meta, or para—can be used to designate the relative position of the two substituents

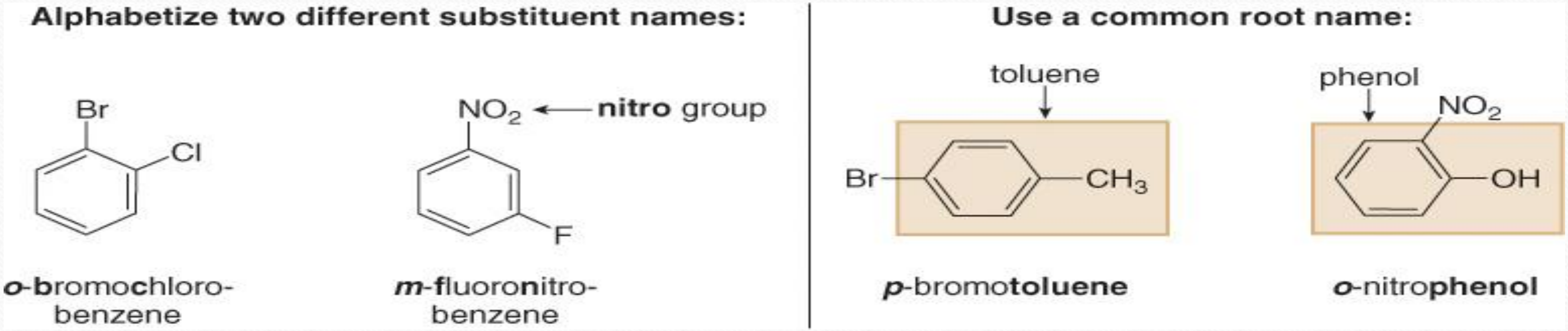


ortho-dibromobenzene
or
o-dibromobenzene
or 1,2-dibromobenzene

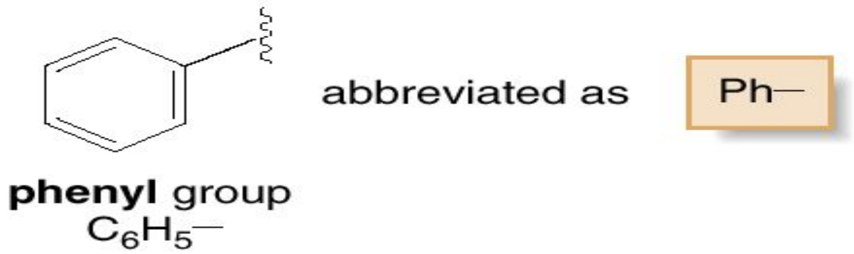
meta-dibromobenzene
or
m-dibromobenzene
or 1,3-dibromobenzene

para-dibromobenzene
or
p-dibromobenzene
or 1,4-dibromobenzene

- If the two groups on the benzene ring are different, alphabetize the names of the substituent preceding the word benzene. If one substituent is part of a common root, name the molecule as a derivative of that monosubstituted benzene.



A benzene substituent is called a phenyl group, and it can be abbreviated in a structure as "Ph-".



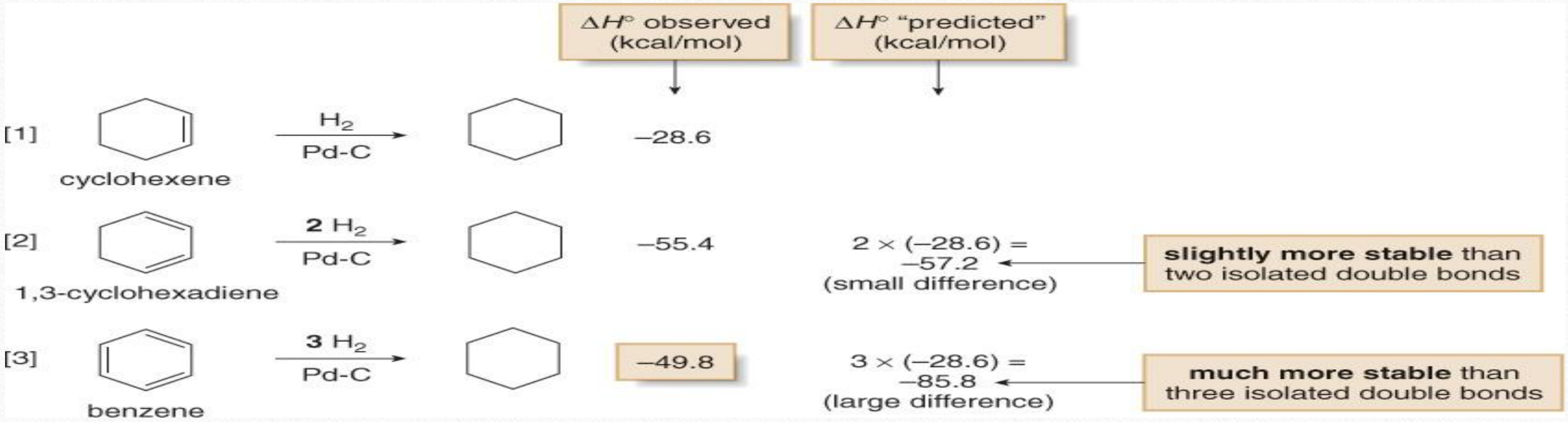
- A phenyl group (C_6H_5-) is formed by removing one hydrogen from benzene (C_6H_6).

- Therefore, benzene can be represented as PhH, and phenol would be PhOH.

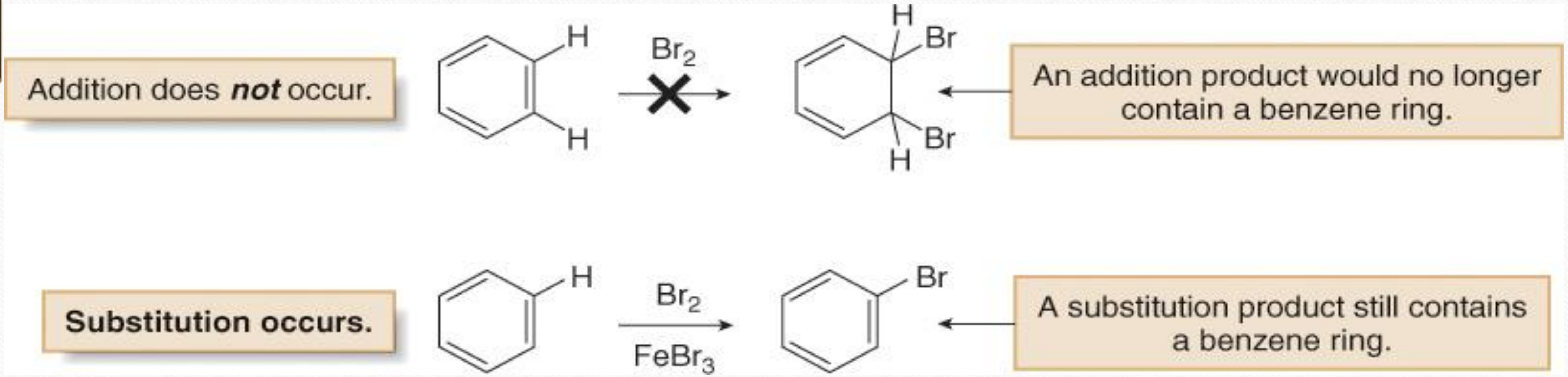
- The benzyl group, another common substituent that contains a benzene ring, differs from a phenyl group.

Stability of Benzene

- **Consider the heats of hydrogenation of cyclohexene, 1,3-cyclohexadiene and benzene, all of which give cyclohexane when treated with excess hydrogen in the presence of a metal catalyst.**



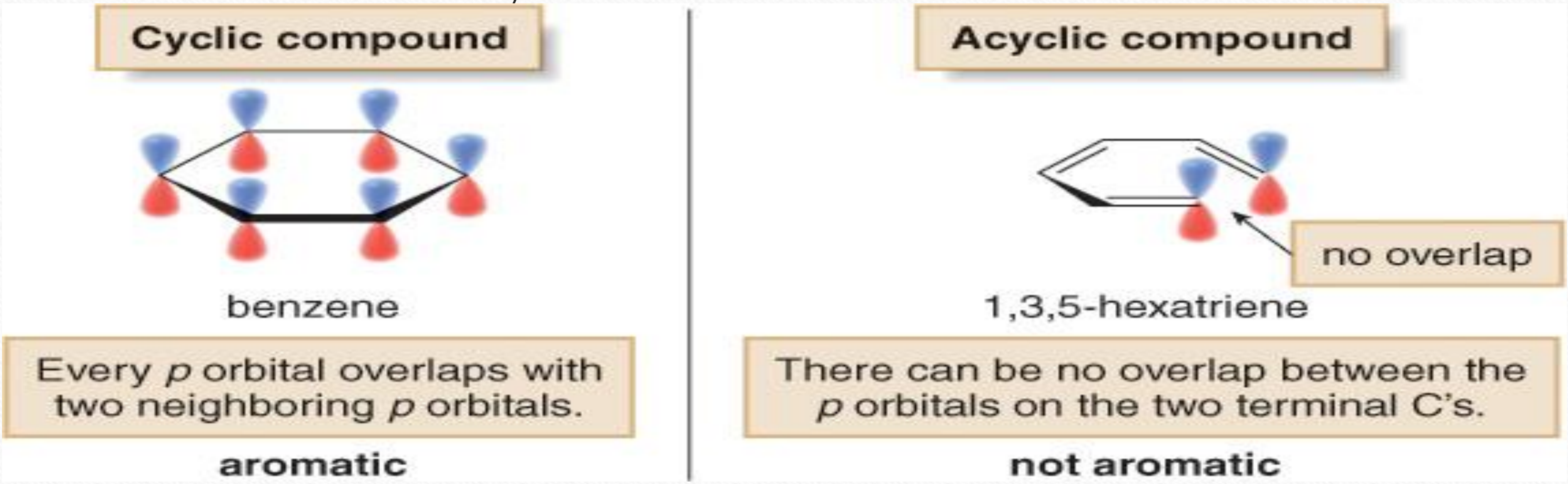
- The low heat of hydrogenation of benzene means that benzene is especially stable. This unusual stability is characteristic of aromatic compounds. Benzene's unusual behavior is not limited to hydrogenation. Benzene does not undergo addition reactions.
- Benzene does not react with Br2 to yield an addition product.



The Criteria for Aromaticity—Hückel's Rule

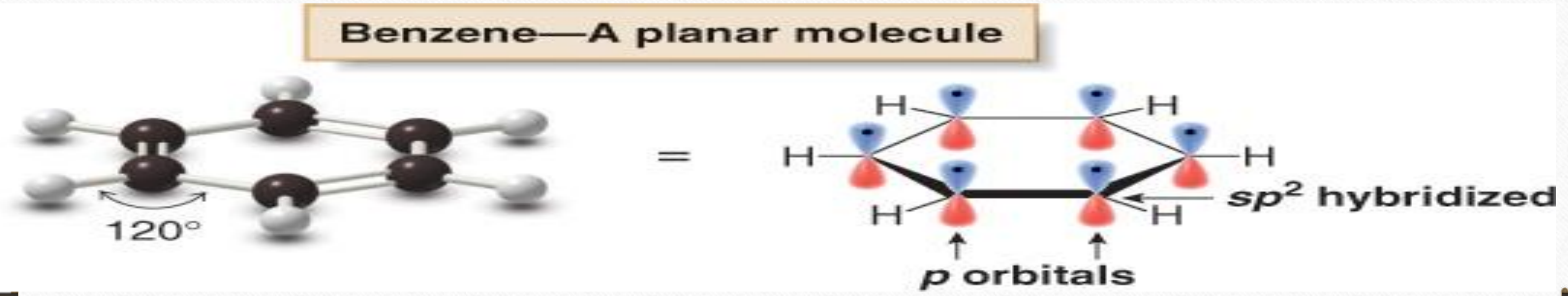
- Four structural criteria must be satisfied for a compound to be aromatic.

[1] A molecule must be cyclic.



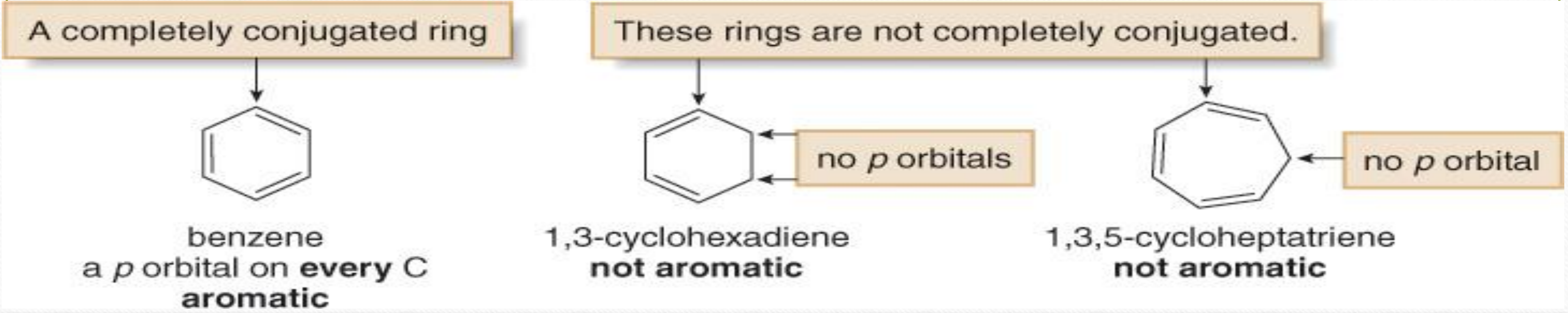
To be aromatic, each p orbital must overlap with p orbitals on adjacent .atoms

[2] A molecule must be planar.



[3] A molecule must be completely conjugated.

- Aromatic compounds must have a p orbital on every atom.



A molecule must satisfy Hückel's rule, and contain [4] a particular number of π electrons •

:Hückel's rule

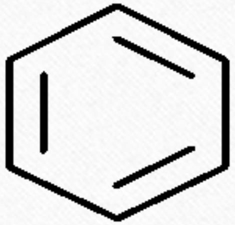
- An aromatic compound must contain 4n+2π electrons [n (integer no.) = 0, 1, 2, and so…]
- Benzene is aromatic and especially stable because it contains 6 π electrons. Cyclobutadiene is nonaromatic and especially unstable because it contains 4 π electrons.

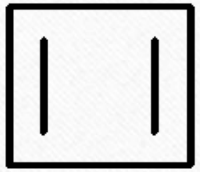
Benzene

An aromatic compound

Cyclobutadiene

non-aromatic compound





4n+2= 6π e

4n=6 - 2=4

n=4/4=1

aromatic

4n+2=4π e

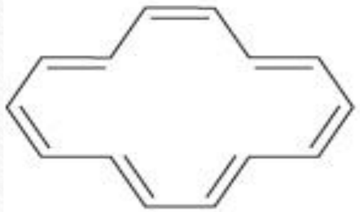
4n= 4 - 2 =2

n=2/4 = 1.5

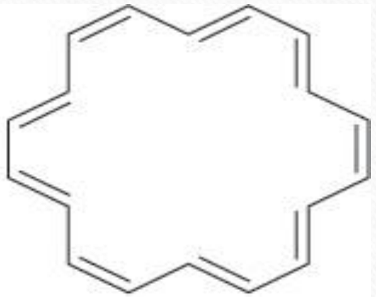
non-aromatic

Examples of Aromatic Rings

- Completely conjugated rings larger than benzene are also aromatic if they are planar and have $4n + 2$ π electrons.
- Hydrocarbons containing a single ring with alternating double and single bonds are called annulenes.
- To name an annulene, indicate the number of atoms in the ring in brackets and add the word annulene.

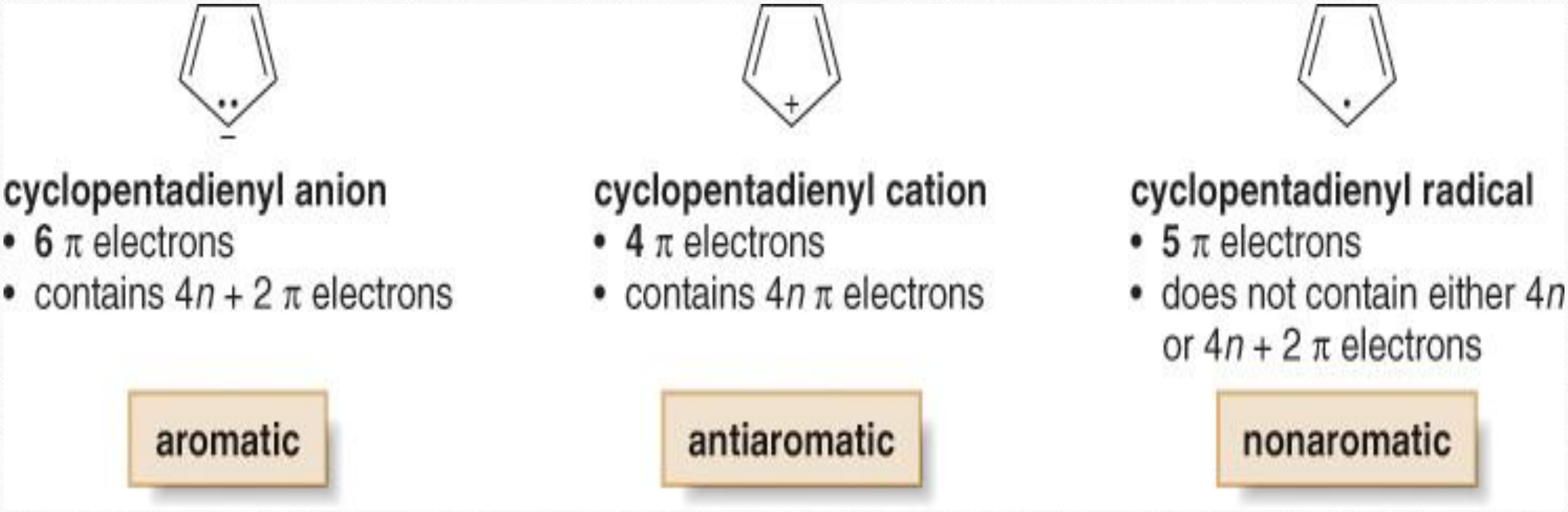


[14]-annulene
$4n + 2 = 4(3) + 2 =$
14 π electrons
aromatic



[18]-annulene
$4n + 2 = 4(4) + 2 =$
18 π electrons
aromatic

- Thus, although five resonance structures can also be drawn for the cyclopentadienyl cation and radical, only the cyclopentadienyl anion has 6 π electrons, a number that satisfies Hückel's rule.



Benzene Risks

- **Benzene is harmful especially to the tissues that form blood cells. How benzene affects human health depend on how much and how long a person is exposed to it.**

- **Benzene has been recognized as a toxic substance that causes acute and chronic health problems. The inhalation of benzene vapours causes irritation to the eyes and upper respiratory tract.**

- **Skin contact with solvents containing benzene causes dry, itching, cracked and fissured skin.**

- Long term inhalation of high levels of benzene results in headaches, dizziness, nausea, convulsions, coma and eventually death.

Scientific evidence has established that employee exposure to low levels

of benzene can cause leukemia and other diseases of the blood-forming organs, such as multiple myeloma: a cancer of the plasma cells as well as anemia which is low blood count which can result in tiredness, lung infections and bruising of the skin.

Reaction Of Aromatic Compounds

- **Aromatic compounds or arenes undergo substitution reactions, in which the aromatic hydrogen is replaced with an electrophile,**
- **hence their reactions proceed via electrophilic substitution.**
- **Arenes contain double bonds just like alkenes but they do not undergo electrophilic addition because these would result to their loss of ring aromaticity.**
- **The order of substitution on aromatic compounds is governed by the nature of substituents present in the aromatic ring.**

- **In electrophilic aromatic substitution reactions, a carbocation is generated while in nucleophilic aromatic substitutions, a carboanion is generated.**

- **Hydrogenation reactions convert aromatic compounds into saturated compounds.**
- **Metal cross-coupling such as Suzuki reaction allows formation of carbon-carbon bonds between two or more aromatic compounds.**

Hetroaromatic Copounds in Medicine

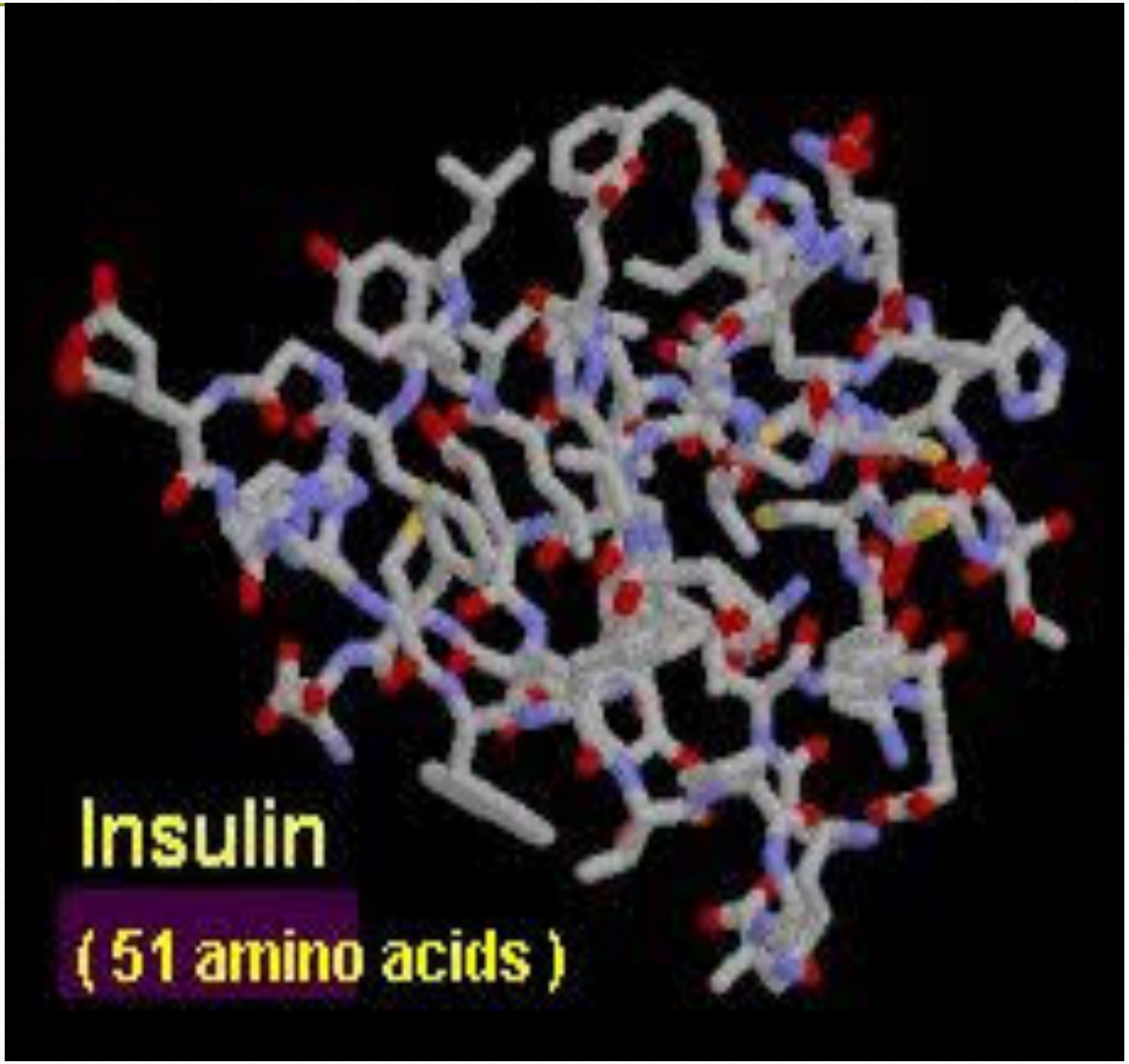
- **synthetic organic chemistry, and pharmacology and various other biological specialties, leading to the design, chemical synthesis and development of bio-active molecules, for being approved as prescribed and market purchasable pharmaceutical agents. Heterocyclic compounds, as the most important organic compounds, are frequently present in molecules of interest in medicinal chemistry. Among them, nitrogen containing heterocycles are of great importance to life science, since they are abundant in nature, existing as subunits in several natural products, for example vitamins, hormones and antibiotics.**

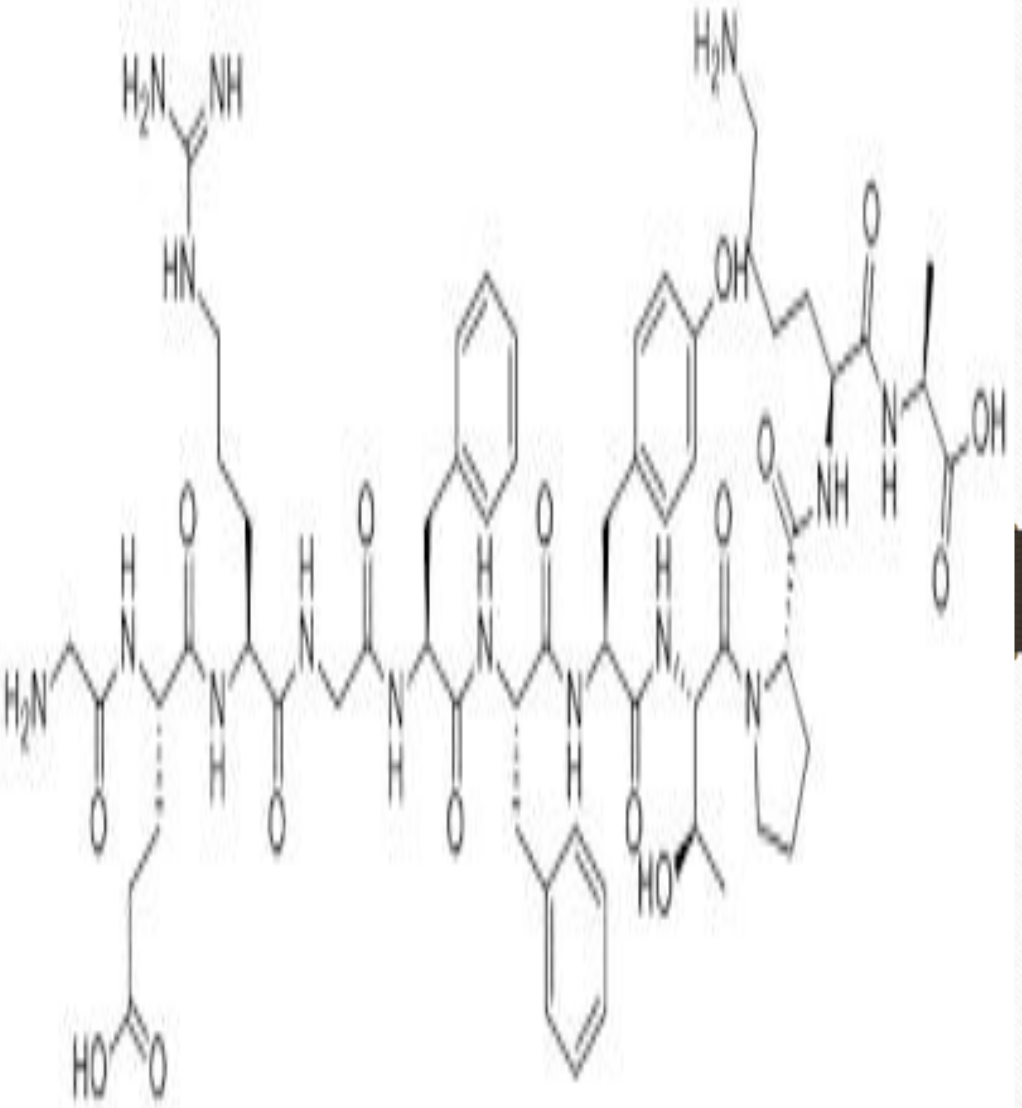
- **Some representative alkaloids and other nitrogen containing natural products, showing diverse biological activities, and several of them are even prescribed drugs such as serotonin, thiamine, which is also called vitamin B1, atropine, notorious morphine, codeine, (greater benefit may be gained when it is combined with acetaminophen or a nonsteroidal anti-inflammatory drug such as aspirin or ibuprofen), papaverine, coniine, caffeine and nicotine. Furthermore, N-based heterocycles are indispensable diet components such as thiamin (vitamin B1), riboflavin (vitamin B2), pyridoxol (vitamin B6), nicotinamide (vitamin B3).**

Hormones

- Hormones are your body's chemical messengers. They travel in your bloodstream to tissues or organs. They work slowly, over time, and affect many different processes, including:
- Growth and development
- Metabolism - how your body gets energy from the foods you eat
- Sexual function
- Reproduction
- Mood

- **Endocrine glands, which are special groups of cells, make hormones. The major endocrine glands are the pituitary, pineal, thymus, thyroid, adrenal glands, and pancreas. In addition, men ~~produce hormones in their testes and women produce them in their~~ ovaries.**
- **Hormones are powerful. It takes only a tiny amount to cause big changes in cells or even your whole body. That is why too much or too little of a certain hormone can be serious. Laboratory tests can measure the hormone levels in your blood, urine, or saliva.**


Insulin
(51 amino acids)



enzymes

- enzymes are proteins that help speed up chemical reactions in our bodies. Enzymes are essential for digestion, liver function and much more. Too much or too little of a certain enzyme can cause health problems. Enzymes in our blood can also help healthcare providers check for injuries and diseases.
- Enzymes are proteins that help speed up metabolism, or the chemical reactions in our bodies. They build some substances and break others down. All living things have enzymes.
- Our bodies naturally produce enzymes. But enzymes are also in manufactured products and food.

Role of enzymes

- One of the most important roles of enzymes is to aid in digestion. Digestion is the process of turning the food we eat into energy. For example, there are enzymes in our saliva, pancreas, intestines and stomach. They break down fats, proteins and carbohydrates. Enzymes use these nutrients for growth and cell repair.
- Enzymes also help with:
- Breathing.
- Building muscle.
- Nerve function.
- Ridding our bodies of toxins.

Different types of enzymes

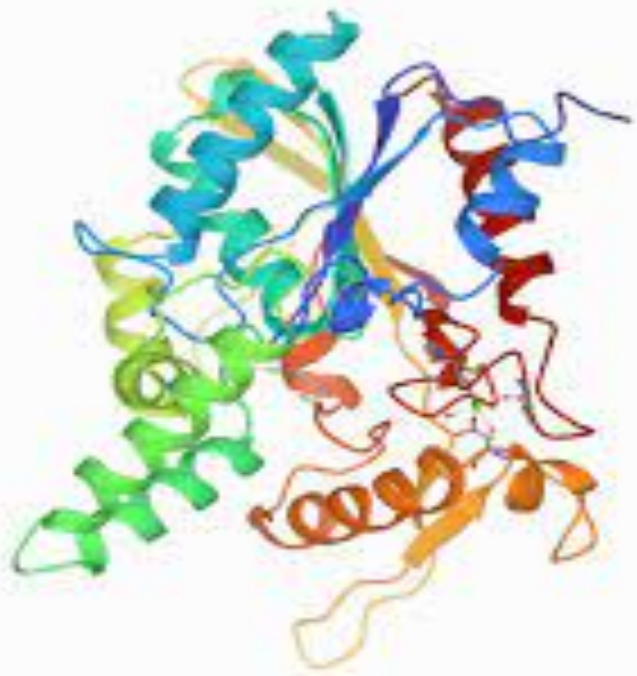
- There are thousands of individual enzymes in the body. Each type of enzyme only has one job. For example, the enzyme sucrase breaks down a sugar called sucrose. Lactase breaks down lactose, a kind of sugar found in milk products.
- Some of the most common digestive enzymes are:
- Carbohydrase breaks down carbohydrates into sugars.
- Lipase breaks down fats into fatty acids.
- Protease breaks down protein into amino acids.

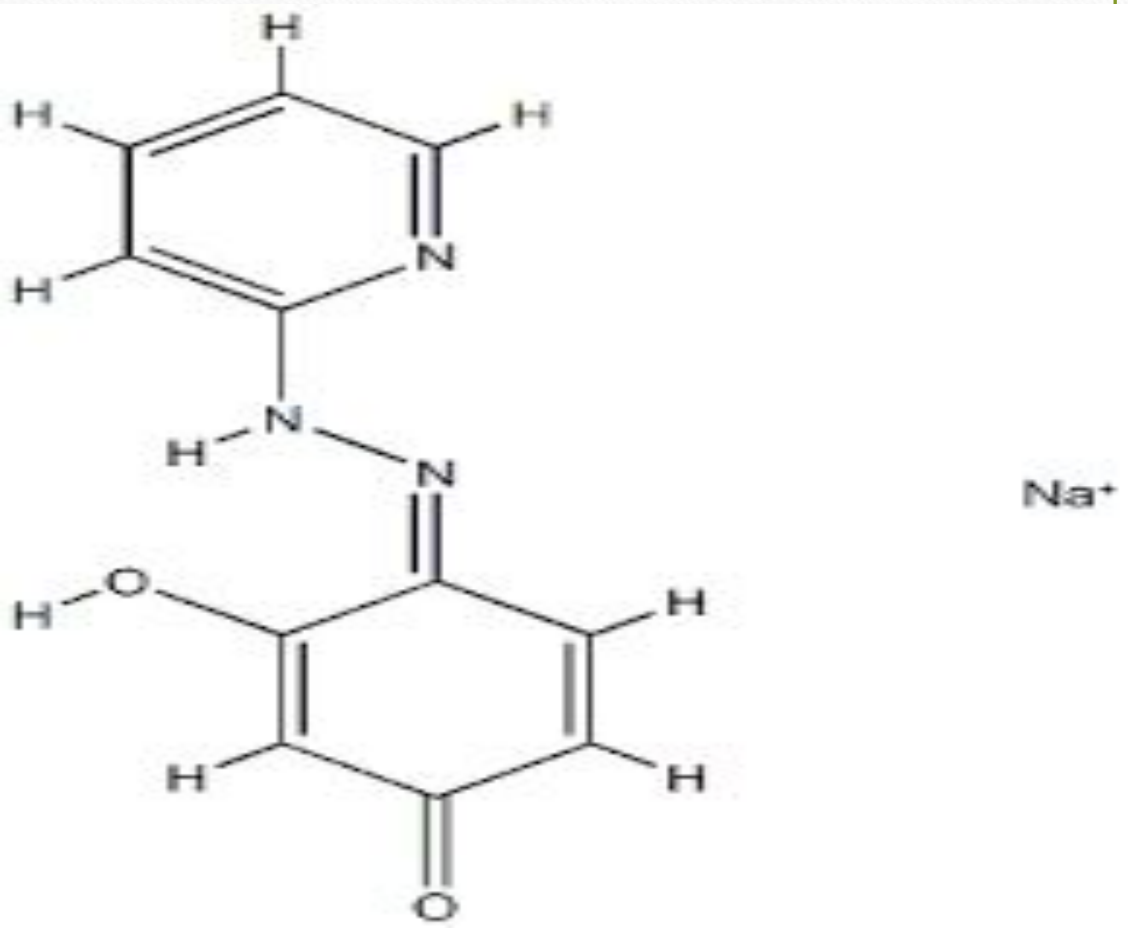
Effect of temperature and pH on enzymes

- Enzymes need the right conditions to work. If conditions aren't right, enzymes can change shape. Then, they no longer fit with substrates, so they don't work correctly.
- Each enzyme has an ideal temperature and pH:
- pH: Enzymes are sensitive to acidity and alkalinity. They don't work properly if an environment is too acidic or basic. For example, an enzyme in the stomach called pepsin breaks down proteins. If your stomach doesn't have enough acid, pepsin can't function optimally.

- **Temperature:** Enzymes work best when your body temperature is normal, about 98.6°F (37°C). As temperature increases, enzyme reactions increase. But if the temperature gets too high, the enzyme stops working. That's why a high fever can disrupt bodily functions.

Lipase Enzyme






thank you