Hello everyone,welcome to

this course in chemistry

for FY

BSc. I'm Dr. Rajesh Parvatkar assistant professor

of organic chemistry from Government College, Sankhali, and

I'm going to discuss module no. 17 that is Huckel's rule.

This is what I'm going to present in my presentation.

That is, Huckel's rule and Aromaticity, under which I'm

going to discuss the Aromaticity in General, Huckle’s rule

and then annulenes.

OK, at the end of the session students will know and

understand Huckel's rule and aromaticity. They are also

going to understand relation between aromaticity and

stability and will be able to apply Huckel's rule in determining and classifying the compounds, as aromatic or anti-aromatic or non-aromatic.

Well, this is a brief introduction of aromaticity.

Aromaticity refers to special stability of certain

completely conjugated cyclic molecules.

The word aromaticity of aromatic have been derived from

Greek word aromatikos meanings with spice. Now

stability an aeromoticity has no connection in English.

But most of the benzene compounds which were initially

found had very pleasant smell and therefore they were called aromatic. But now that Aromaticity is related to the stability, Aromaticity is not restricted to benzene containing compounds only. OK.

You can classify organic molecule on the basis of aromaticity into three classes that is aromatic, non aromatic, and antiaromatic. Now why are we studying this aromaticity? The the reason is very simple. If we know the aromatic character of a molecule, we can know its stability and reactivity.

If the compound is aromatic,it is going to attain stability and therefore less reactive, whereas anti-aromatic compounds are going to be highly reactive and non aromatic compounds are going to be of intermediate stability and reactivity.

OK, let's understand the Huckel's rule of aromaticity.

It states that a planar monocyclic, completely conjugated hydrocarbons will be aromatic when the ring contains 4n + 2π electrons. And if it has 4π electrons in it, then the compound is anti-aromatic.

We need to understand this rule in more detail and simplified way. For finding out the aromatic nature or

antiaromatic nature, you need to consider three

things.

You should see for a planar ring system in a molecule.

You should also see a close conjugation in molecule in a

ring and also you should see number of Pi electron involve

In closed conjugation. So if there are four N + 2π electrons

in a ring, then compound is aromatic. If you don't find four

N + 2π electrons then you should check for four n π electrons.

If compound has four N π electrons in the ring, then it

is antiaromatic. Here n is a whole number which can be 0, 1, 2, 3

and so on.

Now earlier I had mentioned aromaticity means stability.

We're going to now discuss the compounds which belongs to

aromatic class of compound.It's not only the benzene

compounds which are aromatic.One of the class is Annulenes

where benzene also belongs to.Then cyclic cations and anions

can be aromatic. Heterocyclic Compounds can be aromatic.

Polycyclic compounds can be aromatic. Will take each of

these classes, and in this module will consider only annulenes, whereas the other three

Classes we're going to discuss our next module module, #18.

OK, let us take an example of annulene which is benzene. Benzene

is known as six annual because it has got 3 double

bonds in its ring. 3 pi bond means 6 electron and therefore

it is called us and annulene [6].

Now we need to find out whether it obeys Huckel's rule. We

know that benzene is aromatic compound, but whether it obeys

Huckel'sl rule? Whether it satisfies all the criteria to

be called to qualify it as aromatic compound will see that.

the first thing that you should be looking in benzene that

weather benzene has a planar ring or not, and to know whether

benzene has a planar ring or not, you should try and find out

the hybridization of each carbon atoms in a ring. Now if you look

at the hybridization in the figure to the right, you will

find that all the carbons are SP2 hybridized. So if all the

carbons are SP2 hybridized they need to be coplanar.

And therefore the ring is planar.

The second criteria is you should see whether benzene have

a close conjugation or not, and to know that you must delocalize

the Pi bonds inside the benzene ring. On delocalising, you

generate a Canonical form which is different from the first one.

Further, you delocalize it in the same direction. That is

clockwise direction and you find that the original structure that

is started with will be obtained. Therefore we can say that

benzene has a close conjugation,the lasti.e. 4th structure

is a hybrid of all the three structures. Therefore we can say

that benzene also has a close

conjugation. 3rd criteria that it must satisfy is number of π

electrons. So how many π electrons does the benzene ring have?

Now benzene ring has three double bond means it has got six

Pi electron. So you have to put.

4n + 2 equal to six and find out the value of n. So we

get it equal to 1 and therefore it is a whole

number. Therefore benzene satisfiers 4n + 2 criteria

and hence it can be called as aromatic as per Huckle's

theory.

OK, now we'll move on to another annulene and that is 4 annulene

 which is cyclobutadiene..So again, we need to find out

whether it is planar or not planar. We have to look for

the hybridization of each carbon Atom and what we find that each

carbon Atom is doubly bonded.Therefore, SP2, hybridized and

Planar. conjugation? Yes, it has got close conjugation. You can

see that I have now moved in anticlockwise direction. I will maintain anticlockwise in second

structure also. Where I will get my the first structure back so

therefore there is a close conjugation present in this particular molecule. so now the number of π electrons. So there are two double bonds. That Means there are four Pi electrons. Now put or equate 4n + 2 equal to four. In doing so, we find the value of n =2.5, which is not an whole number and therefore this molecule does not satisfy the rule for n + 2, so cannot be called aromatic. now what we have to do is put 4 n equal to four. In doing so, we find that n is equal to 1, which is a whole number and therefore this particular compound satisfies 4n rule and therefore this compound is antiaromatic. So Cyclobutadiene is antiaromatic.

OK, let's take an example of another annulenel in that is 8 annulenel which is Octatetraene. look at the molecule writtent at the top with Octagon and 4 double bonds in it. All the carbons are SP2 hybridized and therefore it has to be planar. But let me tell you it is not planar in reality but for a minute will assume that it is planar. And will move further, OK will see the second condition if it is satisfying. Does this molecule have a close conjugation? Yes, it has close conjugation. You can

just verify that by delocalizing electrons the way we did for benzene and cyclobutadiene and we will find that there is a closed conjugation. OK, let's find out how many electrons it has. 4 double bond that means eight π electrons. So it will satisfy the four n π rule and therefore this molecule has to be antiaromatic. But Experimentally this has been found to be a non-aromatic, not anti-aromatic. Now why it is non-aromatic it is because itdoes not remain in Planar form the reason behind is that it loses planarity because of strain Planar form it has got a high bond angle strain and therefore it changes its shape to a tub shape which is shown below. This is basically to overcome the strain that is there in the planar form, and therefore it loses its planarity and therefore it does not satisfy one of the conditions of Huckel's rule and this is a nonaromatic compound. OK, we take another example that is 10annulene. 5 double bond and 10 electrons in it. Now look at the structure. How it is written and compare it with the previous three. What we will find is there Here you have hydrogen projected inside the ring. And there is a trans double bond. There are two trans double bonds and it's trans double bonds are possible as the ring

becomes bigger and bigger bigger

than 9. OK, let's analyze this with Huckel's rule. All the

carbons are SP2 hybridized.Therefore it has to be planar,

but again I'll mention that it is not planar. but why it is not

planar? I will Mention it later, let's assume that it is planar and try

to verify the other condition. molecule has closed conjugation.

We can write that closed conjugation just as we wrote for

benzene and cyclobutadiene.Now it has got five double

bonds. That means 10electrons. This belongs to 4n + 2 pi type.

n Equal to two, and therefore this should be called aromatic

compound, but in reality it is not showing Aromaticity. It

is non aromatic compound.

The reason is it is not planar. Now why it is not planar? The

reason is that two hydrogens which are inside the ring, they

are too close to each other as there is a steric repulsion

which causes the disturbance in the planarity and structure gets

twisted and therefore this does not meet the criteria of

planarity and hence this molecule is not aromatic and it

has to be non aromatic.

OK, larger annulenes and then 10annulene's. Faces lesser or

no such strain. Hence observe Huckel’s rule to qualify as aromatic or

antiaromatic. We're not going to discuss this here now. Further, in our next module, we are going to discuss the other types of aromatic compounds. Meanwhile,you can read these books to understand a aromaticity in detail that is advanced organic chemistry, 5th edition, by Carey and Sundberg Chapter 9 and also organic chemistry, 10th edition by Solomons and Fryle Chapter 14. Thank you.