Lecture 20B • 03/08/12

What is different between non-aromatic, anti-aromatic, and aromatic? The only reason anything happens special, aromatic or antiaromatic, is when you make a ring. You have to have a cyclic compound to have either aromatic or antiaromatic. Antiaromatic only happens the same reason aromatic does: because you have full conjugation. That means that the same two Hückel rules apply to antiaromatic systems like they do to aromatic systems. That also means they both have to be planar. The only difference between aromatic and antiaromatic is how many electrons. What is that difference? If you draw a Frost circle, you look at the molecular orbitals, no matter what molecule you're dealing with, aromatic systems only have their bonding electrons filled. That's where this odd pairs of electrons rule comes from, because if you only have one bonding orbital, that's one pair of electrons. In any cyclic system, if you have more than one bonding orbital, you have one plus two or another two – in other words, it goes up in pairs after that. You start with one bonding pair, which would then become three, and then five, and then seven, and that's why it's odd numbers that determine whether it's aromatic. Antiaromatic is if you've got too many electrons. Since electrons tend to come in pairs, the most common case is to have one extra pair; so, if you're supposed to have one, you've got two, if you're supposed to have three, instead you have four. That's why it's even pairs of electrons that make something antiaromatic. I still don't like that way of phrasing it, because what if you had fifteen bonding orbitals, but only had two electrons? Yeah, you have one pair of electrons, which is an odd number of pairs, but you have all of these other empty bonding orbitals, which means the molecule would have to have however many plus charges to be lacking in that number of bonding electrons. The best way to express it is if you only have exactly the bonding orbitals filled. If you have more than that, it's antiaromatic.

When is it anti versus non-aromatic? Non-aromatic means it's like any molecule that's not cyclic – either because physically the molecule's not cyclic, or you have lack of conjugation: if you had an sp3 center that blocked conjugation, for example. The same things that make something not aromatic are the same things that make something not anti-aromatic; the only difference is the number of electrons. In the cyclobutadiene case, is it antiaromatic? It's a bad question, because yes, in the idealized, perfect molecule – which doesn't want to exist – if it were a symmetric shape, a square, it'd be perfectly antiaromatic. But we know in real life that it distorts, so it's got still some of that antiaromatic character, because while it exists those bonds are close enough that those p orbitals interact, but it is distorted so it's not a perfect system. What about cyclooctatetraene? Is it antiaromatic or non-aromatic? It depends – are you forcing it to be planar or not? That's the point. What you're not learning is how to take the molecule and say it's this; what you've learned in that example is how does the molecule's true shape get affected by what would happen. When you make that molecule planar, that's when you make it cyclic, planar, fully conjugated, and antiaromatic. WHen that molecule distorts and it's no longer planar, it can't be aromatic or antiaromatic, cause it has to have the whole ring involved. Once it distorts, it's neither.

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Structures

No structures for this lecture.