**CHE2060: Does a structure have resonance?**

So, you’re given a structure and asked whether it has resonance. How can you tell? There are two methods that work well.

**FIRST METHOD:**

The first method has the advantage of actually moving (or ‘pushing’) electrons to create all possible resonance structures. Ask yourself whether you could use a curved arrow to push a pair of electrons to make one of these three resonance changes to the structure:

1. Change : to π
2. Change π to :
3. Change π to π

And, you can only make these changes if they don’t violate these two commandments:

1. Do not break any single bonds (because that would break the molecule)
2. Do not overload an atom with too many bonds

So, if you can make one of the three changes *without* breaking either commandment, you are dealing with a resonance structure.

Now, when you push a pair of electrons, sometimes you change the charges of the atoms losing and gaining that pair of electrons, and sometimes you do not. How do you know? Learn to recognize this set of patterns:

1. Negative charge 🡪 lose : pair 🡪 becomes neutral
2. Neutral (no charge) 🡪 loses : pair 🡪 becomes positively charged
3. Positive charge 🡪 gains : pair 🡪 becomes neutral
4. Neutral (no charge) 🡪 gains : pair 🡪 becomes negatively charged

**SECOND METHOD:**

This method looks for specific patterns of bonding within the molecule, so it’s *pattern recognition* rather than whether you can make a change. The following patterns of bonding indicate resonance when they are separated by a single bond:

1. Pair : next to π
2. Pair : next to positive charge (+)
3. π next to positive charge (+)
4. Electronegative atom, next to π, next to electronegative atom
5. π all the way around a ring (alternating with single bonds; conjugated)

**EXAMPLES of first method of pushing electrons:**

O

**:**

**:**

**:**

**-**

**+**

O

**:**

**:**

This move of the double bond to the electronegative oxygen atom doesn’t break either commandment. Since the carbon of the double bond started without a charge, it becomes positive after losing the electrons. The neutral oxygen becomes negative after gaining the electrons. So this IS a resonance structure.

N

+

H

H

Moving this double bond breaks the second commandment since the nitrogen already has four bonds, and cannot have 5 without exceeding an octet (four pairs of electrons, not five). So this is NOT a resonance structure.

Moving the single bond violates the first commandment, since it breaks that single bond and the molecule’s ring structure. So this is NOT a resonance structure either.

**EXAMPLES of second pattern recognition method:**

O

**:**

**:**

O

**:**

**:**

1. Lone : pair next to a π bond:

O

**:**

**:**

**+**

2. Lone pair next to positive charge:

**+**

3. Pi bond next to positive charge:

N

4. Pi bond next to an electronegative atom:

5. Pi bonds all the way around a ring: