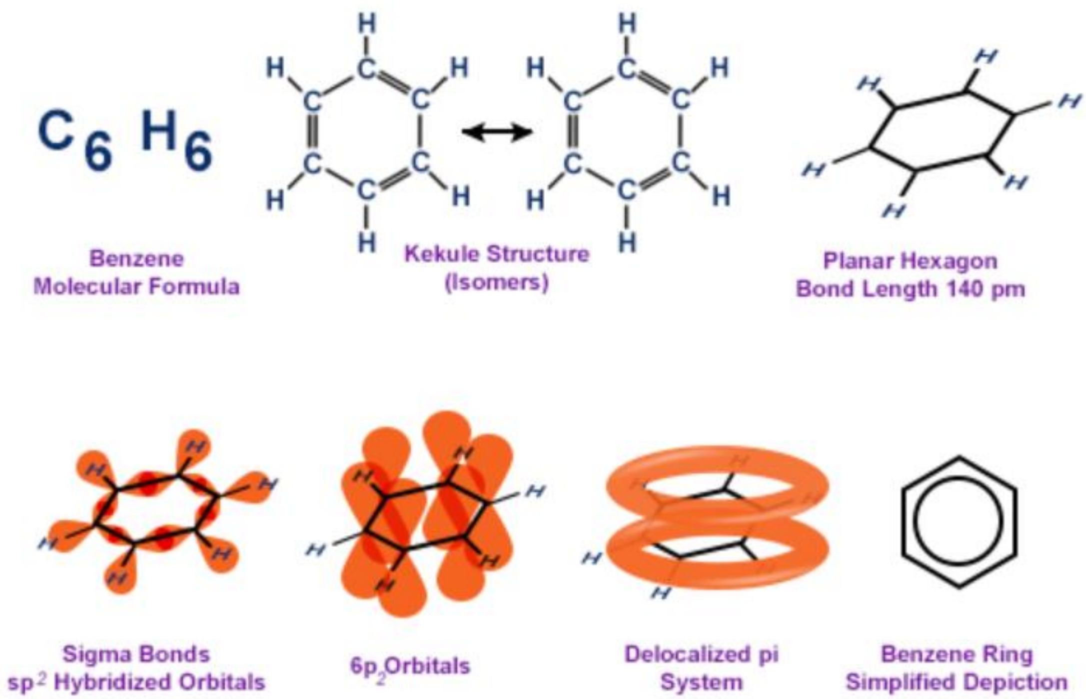
RESONANCE CONCEPT

Resonance, in chemistry, refers to contexts in which one or more electrons contribute to more than one bond in a molecule, and are not considered local to any one of the bonds they contribute to.

A most common example is found in the resonant bonds between the carbon atoms of benzene rings. When benzene is illustrated with a Lewis structure, each carbon is shown sharing a single bond with one neighboring carbon, and a double-bond with the other. There are two possible ways of illustrating the benzene ring by this description.

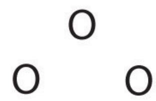
Each of these two possible ways is referred to as a contributing structure. Neither accurately depicts the reality of the molecule, as six of the electrons are delocalized across a pi system—a combination of the contributing structures, the combination placing associated electrons at a lower energy state than any one of the contributing structures would have the electrons in.



Resonance is a way of describing delocalized electrons within certain molecules or polyatomic ions where the bonding cannot be expressed by a single Lewis formula.

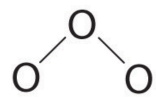
Such is the case for ozone (O3), an allotrope of oxygen with a V-shaped structure and an O–O–O angle of 117.5°. Let's motivate the discussion by building the Lewis structure for ozone.

1. We know that ozone has a V-shaped structure, so one O atom is central:



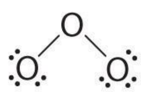
2. Each O atom has 6 valence electrons, for a total of 18 valence electrons.

3. Assigning one bonding pair of electrons to each oxygen–oxygen bond gives



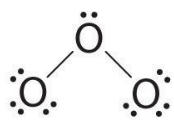
with 14 electrons left over.

4. If we place three lone pairs of electrons on each terminal oxygen, we obtain

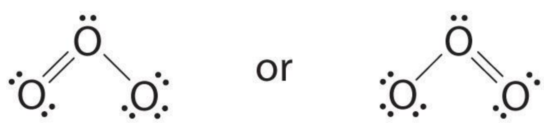


and have 2 electrons left over.

5. At this point, both terminal oxygen atoms have octets of electrons. We therefore place the last 2 electrons on the central atom:

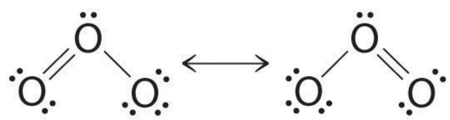


6. The central oxygen has only 6 electrons. We must convert one lone pair on a terminal oxygen atom to a bonding pair of electrons—but which one? Depending on which one we choose, we obtain either



Which is correct? In fact, neither is correct. Both predict one O–O single bond and one O=O double bond. As you will learn, if the bonds were of different types (one single and one double, for example), they would have different lengths. It turns out, however, that both O–O bond distances are identical, 127.2 pm, which is shorter than a typical O–O single bond (148 pm) and longer than the O=O double bond in O_2 (120.7 pm).

Equivalent Lewis dot structures, such as those of ozone, are called **resonance structures**. The position of the *atoms* is the same in the various resonance structures of a compound, but the position of the *electrons* is different. Double-headed arrows link the different resonance structures of a compound:



The double-headed arrow indicates that the actual electronic structure is an *average* of those shown, not that the molecule oscillates between the two structures.

Quantum mechanics reveals that the resonace hybrid possesses less energy than those calculated for anyone of the canonical structures. If A and B correspond to the calculated energies of the structures (a) and (b), and (c) stands for the energy state of the actual structure, the energy diagram assumes the following shape.

<u>Rules for estimating stability of resonance structures</u>

1. The resonance form in which all atoms have complete valence shells is more stable.
2. The **greater the number of covalent bonds**, the greater the stability since more atoms will have complete octets
3. The structure with the **least number of formal charges** is more stable
4. The structure with the **least separation of formal charges** is more stable
5. A structure with a **negative charge on the more electronegative atom** will be more stable
6. **Positive charges on the least electronegative atom** (most electropositive) is more stable
7. **Resonance forms that are equivalent have no difference in stability and contribute equally.** (eg. benzene)

<u>Documented By:-</u>

Niranjan Kumar Mandal