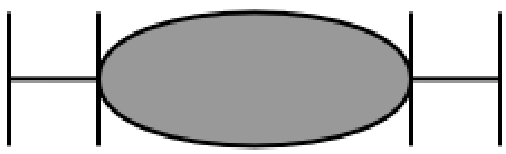
Introduction

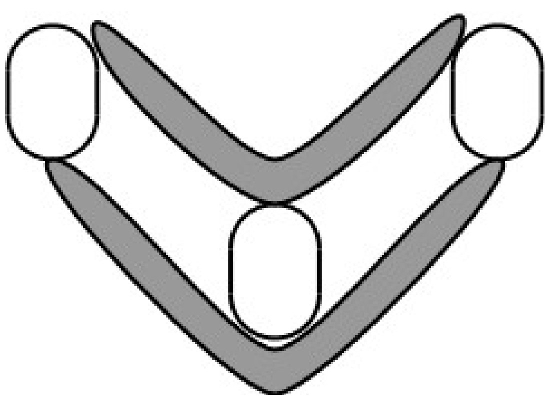
In the previous note pack, we learned how to write Lewis structures fir simple compounds. We can use the four simple rules we discussed in most situations to get a good structure. However, there are some things to watch for when drawing Lewis structures. One is the phenomenon of **resonance** (caused by electrons being shared by more than two atoms). We will discuss resonance in this note pack.

Delocalization and bonding

When you think of a covalent bond (involving the sharing of electrons), you most likely think of a picture like this:

	• The shaded area represents the likely location of the shared pair of electrons. • The bonded electrons are located in between the atoms being bonded.
Illustration 1: Cartoon diagram of a covalent bond in H_2.	

With many bonds, this is indeed a correct picture of how the electrons are distributed between atoms. In some cases, though, electrons are shared by more than two atoms. The shared electrons aren't necessarily located between two of the atoms all the time - they are spread out over several other atoms. These spread-out electrons are said to be **delocalized**. You can picture delocalized electrons this way:

	• The shaded area represents the likely location of the shared pair of electrons. • The bonded electrons are **not** located simply between two atoms - they're shared by a group. • These electrons are **delocalized** - they are shared by more than two atoms.
Illustration 2: Cartoon diagram of delocalized electrons in O_3.	

An extreme case of delocalization is the **metallic bond**, where some electrons are shared by **all** atoms in a solid piece of metal.

Resonance

How can we tell when **delocalization** occurs in a compound? How do we show this **delocalization** in a **Lewis structure**? We'll do an example to illustrate.

Let's examine the carbonate (CO_3^{2-}) ion. First, we draw a Lewis structure the way we learned previously.

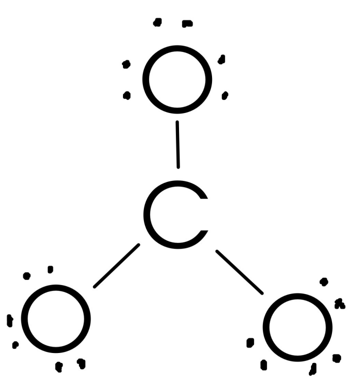
1) *Count the number of valence electrons*:

Atom	***Number of valence electrons***	***Number of atoms in molecule***	***Total valence electrons***
Carbon (C)	4	1	4
Oxygen (O)	6	3	18
Overall charge -2	2		2
Total			***24***

So, CO_3^{2-} has a total of 24 valence electrons.

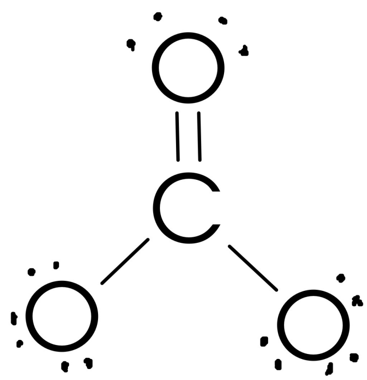
2) *Draw the skeletal structure*. Carbon goes in the middle. Carbon is less electronegative than oxygen, and needs to gain more electrons.

3) *Distribute electrons on the atoms - outside first, inside last*. Once each oxygen is assigned three lone pairs of electrons, there are no more electrons left. Carbon is assigned no extra electrons.

	• Connect the oxygen atoms to the central carbon atom using single bonds. • We run out of electrons after satisfying all the oxygen atoms.
Illustration 3: Skeletal structure of CO_3^{2-}	

4) *Check the structure and use multiple bonds if atoms do not have an octet of electrons (or two electrons for hydrogen)*. Look in the structure in Illustration 3. The central

carbon atom has a share in only **six** electrons. So we use a lone pair on one of the oxygen atoms to make a double bond to the carbon atom:



- The structure checks - all atoms are satisfied.
- One of the oxygen atoms is bonded differently than the others. This should be an observable difference!
- We'll still need to indicate the charge of the ion in the final structure.

Illustration 4: A possible Lewis structure of CO_3^{2-}

According to our rules, we're done and Illustration 4 (with the addition of the ion's charge) is the Lewis structure of CO_3^{2-}. It's odd that one oxygen would have a double bond while the two others have a single bond. There's no other difference between the oxygens - they're all bonded to the same atom and no others.

We should be able to tell experimentally that one oxygen atom is bonded differently from the other two. However, experimental data for carbonate ion shows that all carbon-oxygen bonds in the molecule are the same length. There is a degree of **delocalization** in the bonds. Some bonding electrons are shared by all the atoms in the molecule.

How do we represent the fact that all the carbon-oxygen bonds are the same **and** still draw a "correct" Lewis structure showing all atoms with filled valence shells? We draw alternate structures with the double bond to the other two oxygen atoms. In essence, we draw **three** Lewis structures for carbonate ion and say that the real structure is a combination of all three: These structures are called **resonance structures**

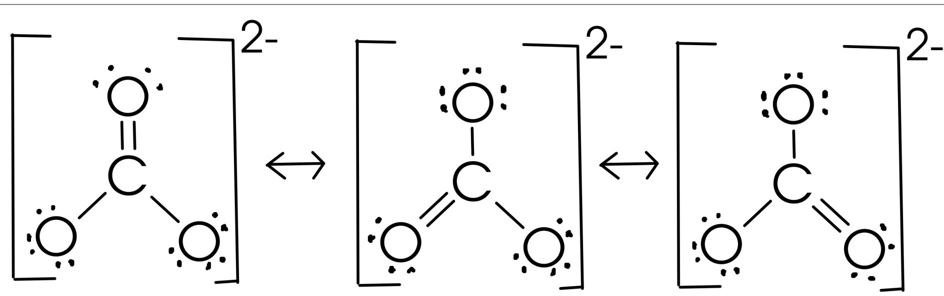


Illustration 5: The resonance structures of CO_3^{2-}

Some notes on Illustration 5:

- The proper way to draw the Lewis structure of carbonate ion is to draw all three of the above structures separated by double-headed arrows. Simply drawing one isn't adequate!
- The double-headed arrows are used to show that all three structures **together** are a representation of CO_3^{2-}'s true structure.
- Don't visualize the carbonate ion as having a double bond that flips around. Visualize it as having a pair of electrons shared by **all** the atoms.

How do we tell if a molecule has delocalized bonds in the first place - without experiment? We can tell from the Lewis structure. First, look at any double bonds in the structure you've drawn. If there's an **identical** atom you could have made that double bond to in your molecule, you are dealing with a molecule that probably has delocalized bonds. In the carbonate ion example above, we expect delocalized bonds because the double bond could have been assigned to any of three **identical** oxygen atoms around the carbon atom.

For a compound with delocalized bonding, it is not technically correct to draw only one Lewis structure. There's not **actually** a double bond between carbon and one of the oxygen atoms. In reality, that pair we draw in the double bond is shared by all the atoms in the structure. Because of this, the single structure we drew in Illustration 4 isn't enough to give us the true picture of the CO_3^{2-} ion, We need to draw all three possibilities, as we did in Illustration 5. These possibilities are called **resonance structures**, and the correct way to draw the structure of CO_3^{2-} is to draw all three of the possible resonance structures and connect them with double-headed arrows. This indicates that the three structures are resonance structure and that the true carbonate ion structure is really something in between all three.

<u>Summary</u>

We've dealt with molecules that exhibit **delocalized bonding**, where electrons are shared by more than one atom. We discovered that you can tell when delocalization occurs by trying to write a Lewis structure for a molecule and looking at the double or triple bonds. Since a single Lewis structure is not able to show this delocalization, we drew multiple **resonance structures** and wrote them with double-headed arrows between them to indicate that the real structure of the molecule was somewhere in between. Next, we will discuss the concept of **formal charge** and how you can use it to choose between several possible structures for a molecule.