Lewis Dot Diagrams 2:
Formal Charges & Resonance Structures

Sometimes it is possible to draw multiple Lewis structures for a compound or an ion while still following the octet rule. These possible structures can differ in how the atoms within the molecule are connected to each other and/or with what bond type. In reality, only one of the structures can be correct: one structure will have less energy than the others and that's the structure that nature will favour. We can use **formal charges** to decide which of the possible structures would be favoured. Formal charges are a method of keeping track of where electrons come from in a molecule, and they are only useful for deciding between Lewis structures.

FORMAL CHARGES

The formal charge on an atom is calculated by finding **the number of valence electrons for an atom minus half the number of electrons in the atom's bonds within the Lewis structure**. The most favourable Lewis structure will have a formal charge of 0 on the most atoms possible, and after that, it will have the more negative formal charge on the more electronegative atom.

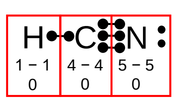
Example 1: Draw the Lewis structure for hydrogen cyanide.

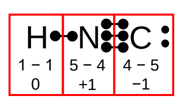
Solution: The cyanide ion consists of 1 carbon atom and 1 nitrogen atom. We know that hydrogen cannot be the central atom (since it can only bond once), but how can we decide between the other two?

First, we draw two Lewis structures, one with carbon as the central atom, and one with nitrogen as the central atom. There are 10 electrons to distribute, and after a bit of trial and error, we find that the only way to satisfy the octet rule for C and N is to have a triple bond between them:

H−C≡N: H−N≡C:

We compare the valence electrons for each atom to each atom's "share" of the electrons, assuming they all had the same electronegativity.





The structure with carbon as the central atom has formal charges of 0 for all atoms, so that's the more favourable structure.

Formal charges can also be used to decide between structures with different numbers of bonds between atoms and different numbers of lone pairs, but remember that the octet rule still takes precedence (except in the cases of beryllium, boron, and central atoms from the third period or higher which can have more than an octet). If there is still a choice between two equally viable-looking structures, the negative formal charges should appear on the atoms that are more electronegative.

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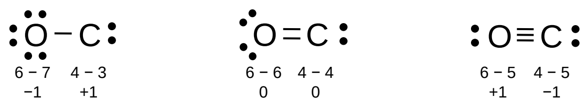
Example 2: Draw the Lewis structure of carbon monoxide, CO.

Solution: Since there are only two atoms, there's no question of which atoms are connected, but is the connection a single bond, a double bond or a triple bond? Let's draw the three structures and look at the formal charges. There are 10 electrons to distribute, and oxygen has more valence electrons. The three structures would look like this:



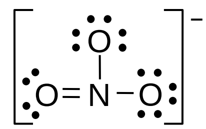
Formal charges would tell us that it's the structure in the middle that is most favourable. However, that structure doesn't give carbon a complete octet. Only the structure on the right follows the octet rule; we should remove the first two from consideration before examining formal charges. Therefore the structure on the right is the correct one.

RESONANCE STRUCTURES

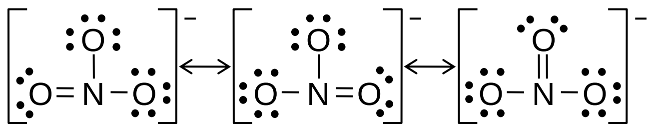
Sometimes there is more than one way to draw Lewis structures that satisfies the octet rule and keeps the formal charges close to zero. These cases exist where there is asymmetry among multiple bonds.

Example 3: Draw the Lewis structure for the nitrate ion, NO_3^-.

Solution: The ion has a charge of −1, and there are 24 electrons to distribute. The nitrogen atom is almost certainly the central atom, and a bit of playing around with the electrons might give us this diagram:

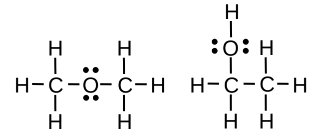


The bonds around the central nitrogen atom are symmetrical *except* for the double bond on one oxygen atom, but there's nothing special about that oxygen atom. The double bond could have been drawn on any of the three oxygen atoms. So which of the three is correct? All of them, and none of them. For the Lewis diagram, it doesn't matter where the double bond is and in fact, it's more correct to draw all three diagrams for the structure:



These three diagrams are called **resonance structures**. All three are representative of the true structure of the nitrate ion. The truth is that the bonds between the nitrogen and oxygen atoms are somewhere between single and double bonds in length. The bonds on the nitrogen atom are **delocalized bonds**: the electrons involved can move from one atom to another more freely than in single or double bonds.

In resonance structures, the configuration of the atoms remains the same. In other words, the atoms are not rearranged. The two diagrams at the right have the same numbers of atoms, but they are *not* resonance structures. They are two different compounds with different chemical properties.



EXERCISES

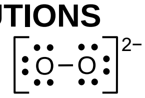
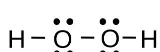
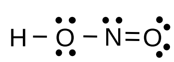
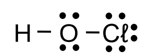
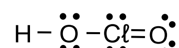
A. Draw the Lewis structures of the compounds and ions with the given numbers of atoms:

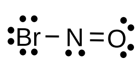
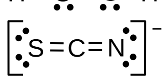
1) 2 O, anion (2−)
2) 2 H, 2 O, neutral compound
3) 1 H, 1 N, 2 O, neutral compound
4) 1 Cℓ, 1 H, 1 O, neutral compound
5) 1 Cℓ, 1 H, 2 O, neutral compound
6) 1 Br, 1 N, 1 O, neutral compound
7) 1 C, 1 N, 1 S, anion (1−)

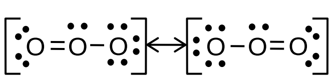
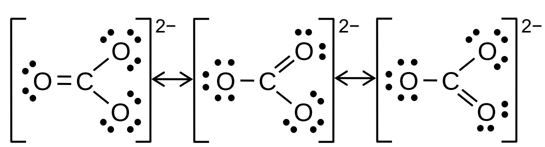
B. Draw all resonance structures for the following compounds:

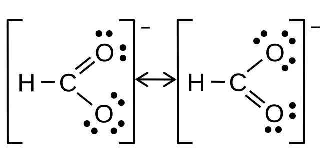
1) ozone, O_3
2) carbonate ion, CO_3^{2-}
3) formate ion, HCO_2^-
4) benzene, C_6H_6, where the carbons form a ring

SOLUTIONS

A. (1)  (2)  (3)  (4)  (5) 

(6)  (7) 

B. (1)  (2) 

(3)  (4)