Lewis Dot Structures

1. Important points about Lewis Dot:

   a. Duet Rule: 2 electrons needed to satisfy valence shell.

      i. What follows this rule? Hydrogen and Helium

   b. Octet Rule: 8 electrons needed to satisfy valence shell.

      i. What follows this rule?

         C, N, O and F are the only elements that pretty much always follow the rule.

      ii. What can exceed the octet?

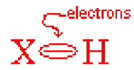
         Any element whose valence shell is in n=3 or higher have the ability to carry more than 8 electrons in their valence. This is because at n = 3, there are additional d orbitals available for bonding.

      iii. What can have less than the octet?

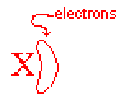
         Boron is happy with 6 electrons in its valence.

2. What are the two types of electron pairs?

   a. Bonding Pair – 2 electrons shared between two atoms in a molecule. These electrons are confined to the area between the two atoms sharing them.



b. Lone Pair – 2 unshared electrons that are found on one atom. These electrons take up more room than a bonding pair and tend to push bonding pairs closer together.



3. Steps for drawing a Lewis Dot structure

a. Add up all valence electrons available using the periodic table.

b. Draw a skeleton structure.

c. Give all atoms in the compound the need duet or octet.

d. Add up all electrons in use. Compare the number of electrons used to the number available. Remember you cannot exceed or go below the valence available. You must use the exact value.

e. If you have used too many electrons you will need to make a double bond between two atoms. When you add the double bond pull a lone pair off each of the atoms participating in the double bond. Continue this process until you have used the correct number of electrons.

f. If you have too few electrons, you will typically add them to the central atom.

4. Draw the Lewis Dot for CH_2O

<u>Step 1 – Count up valence electrons</u>

Based on the periodic table we can see that:

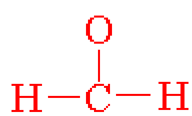
C – 4 valence, H – 1 valence, O – 6 valence

Adding them all up we get:

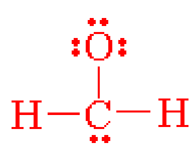
$$\overbrace{4}^{C} + \overbrace{2(1)}^{2H} + \overbrace{6}^{O} = 12$$
$$\text{valence electrons available}$$

Step 2 – Build a skeleton

If carbon is in a structure it is typically the central atom.



Step 3 – Give all atoms octet/duet



Step 4 – Add up electrons in Lewis

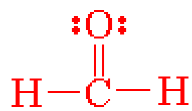
Each bond counts for 2 electrons and each lone pair counts for 2 electrons. In this structure there are 3 bonds and 4 lone pairs:

$$3(2e^-) + 4(2e^-) = 14e^- \text{ in use}$$

This value exceeds the 12e$^-$ available so we are going to have to make additional bonds.

<u>Step 5 – replace lone pairs with bonds</u>

The only place we can add additional bonds is between carbon and oxygen (hydrogen does not make more than one bond). When we make this bond we will have to remove one lone pair from oxygen and one lone pair carbon.



We needed to remove a lone pair from each because they share the bond and thus the bond counts as 2 electrons for both.

We now recount the number of electrons in use to see if it matches the number of electrons available.

There are a total of 4 bonds and 2 lone pairs:

$$4(2e^-) + 2(2e^-) = 12e^- \text{ in use}$$

As this value matches the original valence count – this is a valid Lewis structure.

5. What do you do if there is more than one viable Lewis Structure?

You need to look at the formal charges on the atoms in the compound and see which Lewis structure gives the “best” formal charges.

a. How do you determine the formal charge?

(# of valence electrons) – (# of actual electrons in compound) = formal charge

"# of valence" is the value you get from the periodic table.

When counting the "actual electrons" remember that:
lone pair = 2 e^-
bonding pair = 1e^-

b. What are "favorable" formal charges?

1. Values close to zero.
2. Negative formal charges on the most electronegative atom.
3. Positive formal charges on the least electronegative atom.

6. Draw the Lewis Dot with the best formal charges for

a. OCN^-

<u>Step 1 – Count up valence electrons</u>

Based on the periodic table we can see that:

C – 4 valence, N – 5 valence, O – 6 valence

Adding them all up we get:

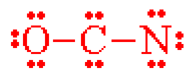
$$\underbrace{\overset{C}{4}+\overset{N}{5}+\overset{O}{6}+\overset{\substack{-1\\ \text{charge}}}{1}=16}_{\text{valence electrons available}}$$

Step 2 – Build a skeleton

If carbon is in a structure it is typically the central atom.

O–C–N

Step 3 – Give all atoms octet/duet



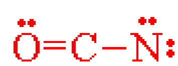
Step 4 – Add up electrons in Lewis

Each bond counts for 2 electrons and each lone pair counts for 2 electrons. In this structure there are 2 bonds and 8 lone pairs:

$$2(2e^-) + 8(2e^-) = 20e^- \text{ in use}$$

This value exceeds the $16e^-$ available so we are going to have to make additional bonds.

Step 5 – replace lone pairs with bonds



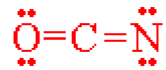
We needed to remove a lone pair from each because they share the bond and thus the bond counts as 2 electrons for both.

We now recount the number of electrons in use to see if it matches the number of electrons available.

There are a total of 3 bonds and 6 lone pairs:

$3(2e^-) + 6(2e^-) = 18e^-$ in use

We are still over our valence electron limit – this means that we are going to have to make another bond.

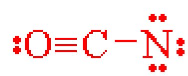


Once again, I need to add up the electrons in use – there are four bonds and 4 lone pairs.

$4(2e^-) + 4(2e^-) = 16e^-$

We are using the correct number of valence electrons – so this is a valid Lewis structure… but is it the best?

Couldn't we, just as easily, have drawn the structure as:



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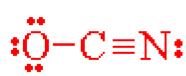
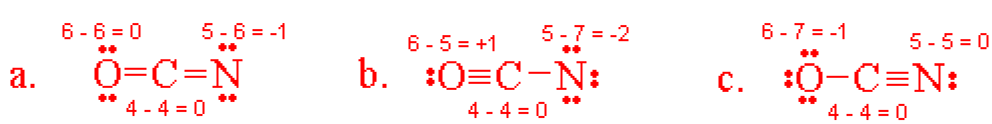


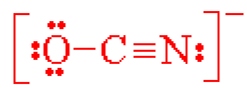
At this point we have 3 valid Lewis structures (valid meaning that octet/duets are satisfied and proper number of electrons have been used).

<u>Step 6 – Compare formal charges</u>



Looking at the formal charges, structure b is definitely *not* the correct structure, a formal charge of -2 on nitrogen would be too high energy. Comparing structure a and c the difference between their formal charges is the atom on which the negative charge is located.

Remember that oxygen is more electronegative than N. This means that it would be preferential for the negative charge to be located on oxygen. This leads us to the conclusion that structure c is the best Lewis structure. Thus our final answer would be:



When your compound has an overall charge it is important to remember to bracket the structure and place the charge outside.

b. NO

<u>Step 1 – Count up valence electrons</u>

Based on the periodic table we can see that:

N – 5 valence, O – 6 valence

Adding them all up we get:

$$\overbrace{5}^{N} + \overbrace{6}^{O} = 11$$

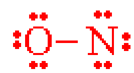
valence electrons available

<u>Step 2 – Build a skeleton</u>

If carbon is in a structure it is typically the central atom.

$$N - O$$

Step 3 – Give all atoms octet/duet



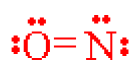
Step 4 – Add up electrons in Lewis

Each bond counts for 2 electrons and each lone pair counts for 2 electrons. In this structure there is 1 bond and 6 lone pairs:

$$1(2e^-) + 6(2e^-) = 14e^- \text{ in use}$$

This value exceeds the $11e^-$ available so we are going to have to make additional bonds.

Step 5 – replace lone pairs with bonds

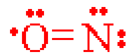
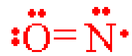


We now recount the number of electrons in use to see if it matches the number of electrons available.

There are a total of 2 bonds and 4 lone pairs:

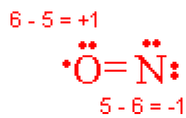
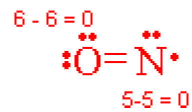
$$2(2e^-) + 4(2e^-) = 12e^- \text{ in use}$$

We are still over our valence electron limit – but only by one electron – this means that we cannot make a bond. We need to remove one electorn from either O or N and form a radical (a radical is a compound that contains an unpaired electron). This means we can form

 or 

At this point we have 2 valid Lewis structures.

<u>Step 6 – Compare formal charges</u>

a.  b. 

Looking at the formal charges, structure b is the best Lewis dot. Al formal charges are equal to zero.

7. What is resonance?

Resonance is a situation in which there are more than one valid structure for a molecule such that the actual compound is some combination of all resonance structures.

a. How do you know if you should "pick the best structure" or draw all resonance structures?

In a case where all formal charges are equal you will have to draw each resonance structure out. When there is a case where there are variations in formal charges (as in the example above) you will pick the "best" structure.

8. Draw the Lewis Structure for NO_3^-.

<u>Step 1 – Count up valence electrons</u>

Based on the periodic table we can see that:

N – 5 valence, O – 6 valence

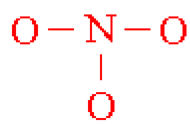
Adding them all up we get:

$$\overbrace{5}^{N} + \overbrace{3(6)}^{3\,O} + \overbrace{1}^{\substack{-1 \\ \text{charge}}} = 24$$

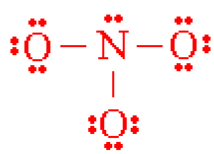
valence electrons available

<u>Step 2 – Build a skeleton</u>

If carbon is in a structure it is typically the central atom.



<u>Step 3 – Give all atoms octet/duet</u>



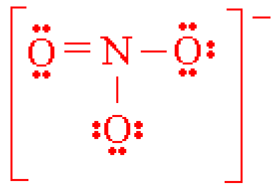
<u>Step 4 – Add up electrons in Lewis</u>

In this structure there is 3 bond and 10 lone pairs:

$$3(2e^-) + 10(2e^-) = 26e^- \text{ in use}$$

This value exceeds the 24e$^-$ available so we are going to have to make additional bonds.

<u>Step 5 – replace lone pairs with bonds</u>



We now recount the number of electrons in use to see if it matches the number of electrons available.

There are a total of 4 bonds and 8 lone pairs:

$$4(2e^-) + 8(2e^-) = 24\ e^-\text{ in use}$$

We are using the correct number of electrons. But now we have to consider that there is no reason why the N has to be double bonded to one oxygen over another. This is a resonance case. That double bond is equally valid between the N and any of the oxygens. There is no difference in formal charges – so all structures must be drawn: