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Drawing Lewis Structures

SANTA FE COLLEGE Chemistry

The fact that a plausible Lewis structure can be drawn for a species is NOT proof that this is the true electronic structure. Experimental verification is always required.

Generalizations about Lewis Structures

1. **All** the valence electrons of the atoms in a Lewis structure must be accounted for.

2. **Usually**, each atom in a Lewis structure acquires an electron configuration with an outer-shell octet. (Hydrogen is limited to an outer-shell duet.)

3. **Usually**, all the electrons in a Lewis structure are paired.

4. **Often**, both atoms in a bonded pair contribute equal numbers of electrons to the covalent bond, but **sometimes**, both electrons in a bonded pair are derived from one atom. (Such a bond is referred to as a coordinate covalent bond.)

5. **Sometimes**, it is necessary to use double or triple bonds in a Lewis structure.

6. **Sometimes**, it is possible to draw more than one plausible structure (for a given formula) where the constituent atoms are in physically different locations with respect to one another. In these instances the different structures represent **different** chemical entities. (These different entities are called **ISOMERS**.)

7. **Sometimes**, it is impossible to draw only one structure that is consistent with **ALL** of the available data (that is, with the constituent atoms in exactly the same positions). In these instances the true structure can only be represented as a composite or **HYBRID** of the two or more plausible structures. (This situation is called **RESONANCE**.)

Strategies for Drawing Lewis Structures

1. Start with a plausible skeleton structure. This is a representation of the order in which the atoms are bonded. The skeleton consists of one or more central atoms with other atoms (called terminal atoms) bonded to the central atom(s). **Usually, the atom of lowest electronegativity is the central atom.**

2. Add up the total number of valence electrons for all atoms in the structure then add or subtract any electrons as indicated by the charge on the species. This is the number of electrons that **must** appear in the finished Lewis structure.

3. Starting with the **terminal** atoms, place the remaining electron pairs around the atoms to complete the valence shells of all atoms. If this is not possible with the number of electrons available **then** shift lone-pair electrons **from** terminal atoms to form multiple bonds to the central atoms in order to complete the valences of all atoms.

4. **If necessary**, use the **formal charge concept** to choose the best structure from among the possible Lewis structures. (See Formal Charge Concept on next page.)

THE FORMAL CHARGE CONCEPT

This is a method of electron "bookkeeping" that can help to choose among several possible structures. The method is based on the assignment of different numbers of electrons to atoms in different positions in a given structure. The number of assigned electrons is then compared to the number of electrons in the isolated atom and a charge is calculated for that given atom. This procedure is repeated until charges are assigned for each atom in all of the possible structures. **These calculated charges do not actually exist - they are only tools to help choose among the various structures.**

In this method the electrons are "counted" or "assigned" as follows:

i) Count all non-bonding electrons as belonging to the atoms on which they reside.

ii) Count all bonding electrons by dividing them evenly between the two bonded atoms.

The formal charge is calculated for each atom as follows:

F.C. is equal to the number of electrons on the isolated atom **MINUS** the number of electrons assigned above.

That is, F.C. = (# of valence e^-) — (# of assigned e^-)

USE OF THE FORMAL CHARGE CONCEPT

1. A Lewis structure in which there is **no formal charge** (i.e. where all formal charges equal zero) is better than one where formal charge exists. If all possible structure contain formal charge the best structure is that which contains **the smallest formal charges**.

2. In choosing among structures that contain formal charges with **the same magnitudes**, the better structure is that where the **negative formal charge is on the more electronegative atom.**

FINAL NOTES ON DRAWING LEWIS STRUCTURES

G. N. Lewis was one of the first to recognize the importance of the so called Noble Gas Configuration (sometimes referred to as a valence octet). In ionic compounds, ions tend to form with these same electron configurations. Lewis recognized that in molecules many atoms also achieve these configurations by sharing electron pairs between the two bonded atoms. Obviously, possessing a noble gas configuration enhances the stability of an atom but OTHER factors also enhance the stability. Even Lewis himself recognized this fact soon after he first proposed it. Two other factors which are known to affect the stability of atoms are formal charges and the number of bonds in the structure.

Thus when drawing Lewis structures one must keep in mind these **three factors**:
1) **minimizing formal charges** on all atoms.
2) **maximizing the number of bonds**. (Since it requires energy to break bonds then it follows that making bonds must release energy and is therefore a favorable factor)
3) **possession of a noble gas configuration**.

1. Draw the Lewis structure for N_2H_4.

   Start with a plausible skeleton.

   a) H—H—N—N—H—H

   b)
   ```
   H—N—N—H
     |   |
     H   H
   ```

   Structure a) is not a plausible skeleton since two of the hydrogen atoms are shown with two other atoms attached to them. Hydrogen has only one valence orbital (the 1s orbital) and therefore can only share two valance electrons and not four as shown in structure a). It is possible for nitrogen atoms to share more than two electrons as they possess four valence orbitals (the 2s and the three 2p orbitals) and can share UP TO eight electrons. Thus structure b) is the more plausible skeleton and is the one to be used in completing the structure for N_2H_4.

   Next, count up the valance electron for all of the atoms in the formula. This totals 14 electrons in the example. These 14 electrons must appear somewhere in the final structure. In the skeleton shown in part b) above there are only 10 electron depicted. Thus an additional four electrons are needed. Normally these "extra" electrons are placed on the terminal atoms but as mentioned previously, H atoms can only share two electron each and in our skeleton the H atoms already have two shared electrons. Therefore the electron must be placed around the N atoms to complete the structure. Now the N atoms have achieved the same configuration as the noble gas, Ne, while the H atoms possess the He configuration.

   I.e.,
   ```
     ••  ••
   H—N—N—H
     |   |
     H   H
   ```

2. Draw the Lewis structure for CHN.

   There are only two plausible skeletons for CHN.

   a) H—N—C

   or

   b) H—C—N

   Note that both C and N atoms **CAN** be bonded to more than one atom at a time as they both have four valence orbitals (the 2s and the three 2p orbitals). There are a total of ten valence electrons for these three atoms. There are only four electron shown in each of the two structures. Thus, six more electron must be added to each structure. It is best to begin by placing then around the terminal atoms and then if there are still remaining electron to be added they are added to the central atom.

Beginning with structure a) the six remaining electron are added to the C atom;

a) H—N—C:

Next, the electron are moved around so that each atom shares a total of eight electron (this allows each atom to achieve a noble gas configuration. In this example four electrons on the C atom are moved so that the N atom in the center can share them.

a) H—N≡C:

Moving on to structure b) the six remaining electron are added to the N atom;

a) H—N—C:

Next, the electron are moved around so that each atom shares a total of eight electron (this allows each atom to achieve a noble gas configuration. In this example four electrons on the N atom are moved so that the C atom in the center can share them.

b) H—C≡N:

Which of these structures is the correct one? We will use the formal charge concept to determine the more plausible structure.

In structure a) the N atom has a +1 formal charge. After dividing the bonds in half the N atom is assigned a total of four electrons. This is one short of the total number of valence electron in a normal N atom, hence the +1 charge. The C atom has a −1 charge. After dividing the bonds in half the C atom is assigned a total of five electrons. This is one more than the total number of valence electron in a normal C atom, hence the −1 charge.

In structure b) both atoms have no charge on them. After dividing the bonds in half the N atom is assigned a total of five electrons. This is equal to the total number of valence electron in a normal N atom, hence no charge. After dividing the bonds in half the C atom is assigned a total of four electrons. This is equal to the total number of valence electron in a normal C atom, thus the carbon atom has no charge either.

A structure in which there is no formal charge is more plausible than a structure that has formal charges. Thus, structure b) is the more plausible structure. As predicted, experiments have verified that indeed the C atom is in the center and the N atom is triply bonded to the C atom.