Guidelines for Drawing Lewis Structures

Rules

- 1. Determine the skeleton structure.
 - (a) H is always a terminal atom and has only one bond.
 - (b) In simple compounds, O and X (halogens) are terminal atoms. If X is bonded to O, O is terminal
 - (c) Oxygen atoms do not bond to each other except in (1) O_2 and O_3 molecules; (2) the peroxides, which contain the O_2^{2-} group; and the (3) the rare superoxides, which contain the O_2^{-} group.
 - (d) In ternary acids (oxoacids), hydrogen usually bonds to an O atom, not to the central atom. (Exceptions are phosphorous acid, H₃PO₃, where one H is bonded to P, and hypophosphorous acid, H₃PO₂, where two H are bonded to P.)
 - (e) The least electronegative atom is usually the central atom.
 - (f) For ions or molecules that have more than one central atom, the most symmetrical skeletons possible are used.
- 2. All the valence electrons must be accounted for.
- 3. Usually, each atom in a Lewis structure acquires an electron configuration with an outer-shell octet. (The outer shell of H has only 2 electrons.) Nonmetals of the third period and beyond may be surrounded by more than eight electrons (*expanded valence*). (The outer shell of Be has only four electrons, that of B only six electrons.)
- 4. Usually, all the electrons in a Lewis structure are paired.
- 5. 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 a single atom (coordinate covalent bond).
- 6. Sometimes, it is necessary to represent double or triple covalent bonds in a Lewis structure (C, N, O, P, S).

Lewis Structures

7. Sometimes, it is impossible to draw a single Lewis structure that is consistent with all the available data. In these instances the true structure can only be represented as a composite or hybrid of two or more plausible structures. This situation is called resonance.

Steps

- 1. Determine the number of available valence electrons, A. Add up the total number of valence electrons for all the atoms in the structure. For *anions*, *add* the charge of the ion. For *cations*, *subtract* the charge of the ion. This is the number of electrons that must appear in the Lewis structure.
- 2. Determine the number of valence electrons needed for *octets*, N. This number N equals the number of non-H atoms times eight plus the number of H-atoms times two. (Note the exceptions for Be and B.)
- 3. Determine the number of shared electrons, S.

S = N - A

The number of bond pairs is $\frac{S}{2}$.

- 4. Start with a plausible skeleton structure. This is a representation of the order in which atoms are bonded together. The skeleton structure consists of one or more central atoms with the other terminal atoms bonded to the central atom(s).
- 5. Place the bond pairs in the skeleton structure, starting with one bond pair between each pair of atoms. If bond pairs remain, form double or triple bonds.

If the number of bond pairs is less than the number needed to bond all atoms, then S is increased to the number of electrons needed. This generally indicates that the central atom displays expanded valence.

6. Determine the number of remaining valence electrons, A - S. Place these electrons as lone pairs, starting with the terminal atoms to complete the octets (exceptions!). If electrons are left over, place them on the central atom (expanded valence).

7. Use the concept of formal charge to assess the plausibility of the Lewis structure.

Formal Charge

Formal Charge: An atom in a molecule owns its lone pairs completely, but has an equal share in bonding electron pairs.

If this results in an atom having more electrons in the molecule than as a free, neutral atom, we say that the atom has a negative formal charge in the Lewis structure. If it has less electrons in the molecule, then it has a positive formal charge.

FC = number of valence electrons of free atom – number of lone-pair electrons $-\frac{1}{2}$ number of shared electrons

The sum of formal charges must equal zero for a neutral molecule and must equal the charge for ions.

Lewis structures with the lowest formal charges are most plausible.