Structure determination using the Lewis model

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The procedure for determining the correct three-dimensional structure of a molecular entity is given below. This skill is fundamental to all of chemistry and serves as a starting point for all other bonding models.

1. Count the total number of valence electrons in the molecular entity.
    a. Add the valence electrons from each atom; for example, in H_2O there are eight valence electrons, six from oxygen and one each from the two hydrogens: 6+1+1=8.
    b. For each overall negative charge (for example, NO_3^-), **add** one electron.
    c. For each overall positive charge (for example, H_3O^+), **subtract** one electron.
2. The atom with the ability to form the most bonds[1] is the central atom. There may be more than one central atom. If the atoms are in the same group, select the heaviest atom as the central atom. For oxygen-rich anions, the non-oxygen atom is the central atom.

    Connect all terminal atoms to the central atom(s) with a single bond (dash); each bond contains two electrons. Subtract twice the number of connections from the total number of electrons.
3. Distribute the remaining electrons, in pairs, to give all terminal atoms sufficient electrons to fill their valence shell (two electrons for elements in groups one and two; eight for elements in groups 13[2] through 18).
4. Distribute the remaining electrons around the central atom(s).
5. Determine formal charges for all atoms. This is done by counting the non-bonding electrons around an atom, then adding one electron for each bond to the atom, and subtracting the total from the atom's normal valence. For example, an oxygen atom (valence = six) with seven "local electrons" will have a formal charge of minus-one (six minus seven), while a nitrogen (valence = five) with four "local electrons" will have a formal charge of plus-one (five minus four).
6. If there are any non-zero formal charges, form multiple bonds to minimize the formal charges, typically by using lone pairs on terminal atoms to form bonds to the central atom. Repeat. The correct structure minimizes the number and magnitude of the formal charges[3] and distributes any remaining formal charges according to the atoms' electronegativity.
7. If there are two or more equivalent structures in 6, the true structure is the average: **resonance**.
8. Project into three dimensions using VSEPR. For ionic compounds, it is often convenient to look at entities as ions rather than neutral entities; for example, you would look at the ions in ammonium sulfate separately.

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[1] Boron forms three or four bonds, carbon forms four, nitrogen forms three or four, oxygen forms two or three, hydrogen and fluorine form only one. Elements in the periods below the second (C,N,O,F) row normally form the same number of bonds as the element above them, with some important exceptions such as the oxyanions (ClO_4^-, SO_4^{2-}, etc) and other hypervalent compounds (SF_6, PCl_5, SO_3, etc).

[2] Neutral boron compounds often show just six electrons for boron, but this is usually a consequence of boron being the central atom; see rules 4-6.

[3] Except for second-row elements such as boron or nitrogen, which **can <u>never</u>** form more than four bonds.