Lewis Structures and Darling Molecular Models

- Goal: Depict <u>all</u> the valence electrons of a covalent "species" (neutral or charged)
  ⇒ first count up the number of valence electrons in the species

- Always pair up electrons (one has $m_s = +½$, the other has $m_s = -½$)
  - Between atoms: "shared pair" (that is, a covalent bond!)
  - On one atom: "lone pair"

- Lewis structures, as interpreted by VSEPR theory, allow us to predict the <u>shape</u> of molecules, which largely determines their physical properties and reactivity!

<u>Rules for Drawing Lewis Structures</u>

(1) Give every atom a noble gas configuration (if possible)
H: duet (isoelectronic with He) All other main group atoms: octet

(2) Note that electrons are "double-counted" when checking the duet/octet rule
⇒ the very idea of a <u>covalent</u> bond: a shared electron pair "belongs" to each atom

(3) Make reasonable connections between atoms
(a) Know the common "valences" (that is, the number of connections):

Valence:	**1**	**2**	**3**	**4**
Groups:	**17**	**2 and 16**	**13 and 15**	**14**

(b) Put the atom with the highest valence at the center of the structure
(c) Some octet rule exceptions are stable (especially for Groups 2 and 13)

(4) **<u>Always</u>** label non-zero formal charge on each atom

formal charge = # of valence electrons - # of unshared electrons - # of shared electron pairs

(5) Sum of formal charges must equal overall (real) charge on species

(6) <u>Valence expansion</u> (also known as <u>hypervalency</u>) is allowed for atoms in the 3rd period (and below) of the periodic table (why?)

(7) Maximize bonding (that is, the number of shared electron pairs in the compound) and minimize formal charge without violating the octet/hypervalency rules

(8) Species with an odd number of electrons will have one unpaired electron
(a) Species is called a <u>radical</u> (or a monoradical)
(b) Location of unpaired electron directs reactivity

(9) Resonance structures

(a) Draw when there is an ambiguity in the location of electron pairs
(b) They are often required by the symmetry of the species
(c) A "movement" or "pushing" of electrons, not of nuclei

Rules for Building Molecules with the Darling Kits

(Note: You will be required to buy your own kit next fall if you go on to Organic I!)

Paradigm: Focus on the bonds between atoms; the atoms themselves are "merely" at the intersections or termini of bonds. (This convention, dominant in much of chemistry today, is very different from the one in your lab manual.)

Here are the Darling model color conventions:

Color	What It Represents
black	sp^3-hybridized C (or other Group 14 atom)
grey	sp^2- or *sp*-hybridized C
red	O (or other Group 16 atom)
blue	N (or other Group 15 atom)
green ball	Group 17 atom
white ball	H atom

Note that if an atom has four groups of electrons (either bonds or lone pairs) surrounding it, you need to snap together a pair of pieces to represent that atom.

Also note the small number of white balls in your kit. This follows the organic convention of drawing in hydrogen atoms explicitly only if it is bound to a so-called "heteroatom" (that is, some atom besides C or H).

e.g. methylammonia