

DRAWING LEWIS STRUCTURES or ELECTRON DOT DIAGRAMS

Introduction : Gilbert N. Lewis (1875-1946) because of his great work in chemical bonding became associated with a simple shorthand system for depicting the electrons involved in bonding. In writing Lewis structures **ALL** valence electrons must be shown. One of the most important ideas in chemistry is that each molecule has a particular shape, a minute architecture of atoms with specific distances and angles between them. The **VSEPR** Valence Shell Electron Pair Repulsion Theory can then help us to predict the shapes of molecules.

In drawing Lewis structures, we shall assume that the molecular "skeleton" (i.e. a plan of the bonding of specific atoms to other atoms) is known. In this respect, it helps to know that hydrogen and fluorine are always terminal atoms in Lewis structures, bonded to only one other atom. A systematic procedure for drawing Lewis structures can then be used, as expressed by the following rules:

Step 1: Count up the total number of valence electrons available by first using the group numbers to add up the valence electrons from all atoms present. If the species is a negative ion, *add* the absolute value of the total charge; if it is a positive ion, *subtract* the value of the charge.

Step 2: Calculate the total number of electrons that would be needed if each atom had its *own* noble gas shell of electrons around it (two for hydrogen, eight for carbon and heavier elements).

Step 3: Subtract the number in Step 1 from the number in Step 2. This is the number of shared (or bonding) electrons present.

Step 4: Assign two bonding electrons (one pair) to each bond in the molecule or ion.

Step 5: If bonding electrons remain, assign them in pairs by making some of the bonds double or triple bonds. In some cases there may be more than one way to do this. In general, double bonds form only between atoms of the elements C, N, O and S. Triple bonds are usually restricted to either C or N.

Step 6: Assign the remaining electrons as lone pairs to the atoms, giving octets to all atoms except hydrogen.

Step 7: Determine the formal charge on each atom and write it next to that atom. Check that the formal charges add to give the correct total charge on the molecule or polyatomic ion.

formal charge = group no. – no. of e⁻s in lone pairs – ½(no. of e⁻s in bonding pairs)

The last rule identifies structures that are undesirable because they imply large separations of negative from positive charge, and catches inadvertent errors (e.g. the wrong number of dots).

The use of these rules is illustrated by the following example.

EXAMPLE

Write a Lewis electron dot structure for phosphoryl chloride, POCl_3 .
Assign formal charges to all of the atoms.

Solution:

Step 1: Calculate the number of valence electrons available in the molecule.
For POCl_3 it is

$$5 \text{ (from P)} + 6 \text{ (from O)} + [3 \times 7 \text{ (from Cl)}] = 32$$

Step 2: Calculate how many electrons would be necessary if each atom were to have its own noble gas shell of electrons around it.

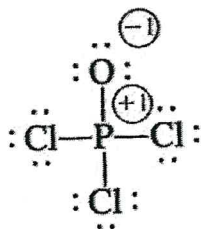
Because there are five atoms in the present case (none of them hydrogen),
 $5 \times 8 = 40$ electrons would be required.

Step 3: From the difference of these numbers ($40 - 32 = 8$), each atom can achieve an octet only if eight electrons are shared between pairs of atoms.

Step 4: Eight electrons correspond to four electron pairs, so each of the four linkages in POCl_3 , must be a single bond.

(Step 5): (If the number of shared electron pairs were *larger* than the number of bonds, double or triple bonds would be present.)

Step 6: The other $32 - 8 = 24$ electrons are assigned as lone pairs to the atoms in such a way that each achieves an octet configuration. The resulting Lewis structure is:



Step 7: Formal charges are already indicated in this diagram.

$$\text{formal charge} = \text{group no.} - \text{no. of } e^- \text{ in lone pairs} - \frac{1}{2}(\text{no. of } e^- \text{ in bonding pairs})$$

Phosphorus has group number 5, and it shares eight electrons with no lone pairs, so

$$\text{Formal charge on P} = 5 - 0 - \frac{1}{2}(8) = +1$$

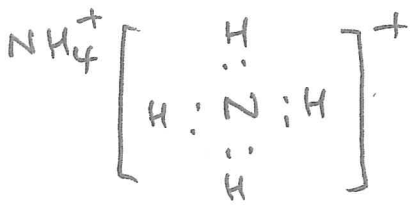
Oxygen has group number 6, with six lone pair electrons and two shared electrons, so

$$\text{Formal charge on O} = 6 - 6 - \frac{1}{2}(2) = -1$$

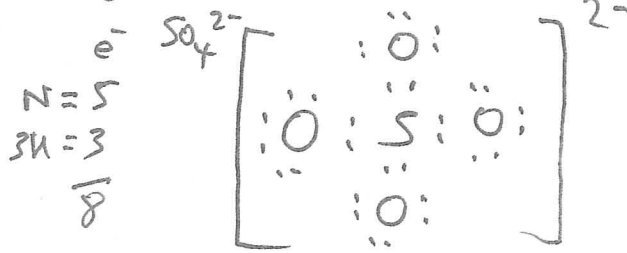
All three chlorine atoms have zero formal charge, computed by

$$\text{Formal charge on Cl} = 7 - 6 - \frac{1}{2}(2) = 0$$

Polyatomic electron arr.

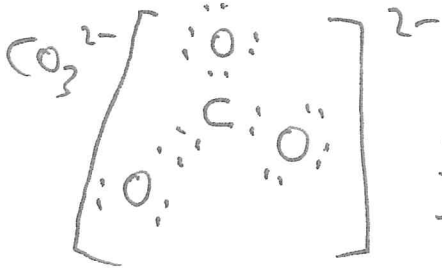


Tetrahedral.



Tetrahedral.

$$\begin{array}{r} e^- \\ S = 6 \\ 4O = 24 \\ + 2e^- = 2 \\ \hline 32 \end{array}$$



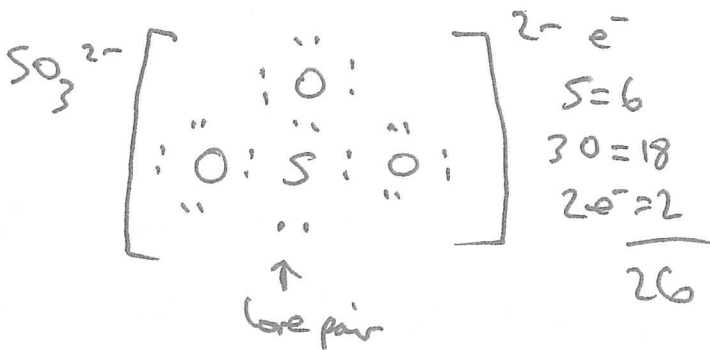
triangular planar 120°

$$\begin{array}{r} e^- \\ C = 4 \\ 3O = 18 \\ + 2e^- = 2 \\ \hline 24 \end{array}$$

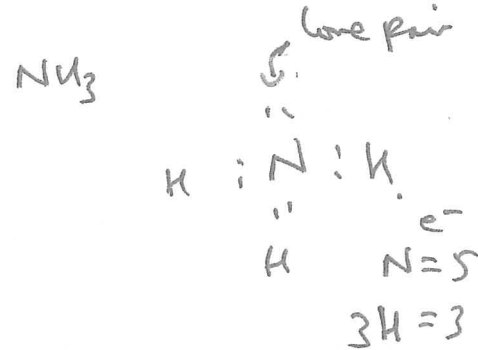


triangular planar 120°

$$\begin{array}{r} e^- \\ N = 5 \\ 3O = 18 \\ 1e^- = 1 \\ \hline 24 \end{array}$$

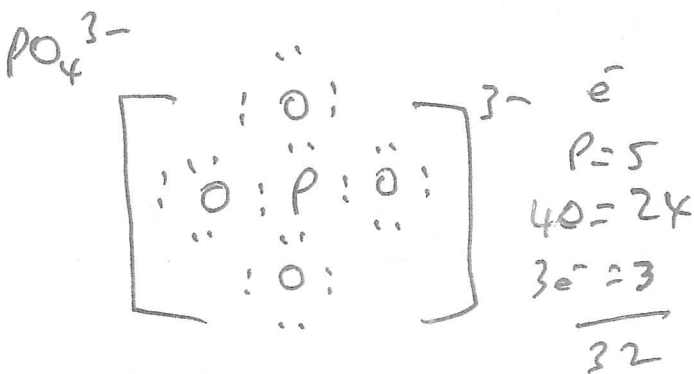


↑ lone pair
trigonal pyramidal



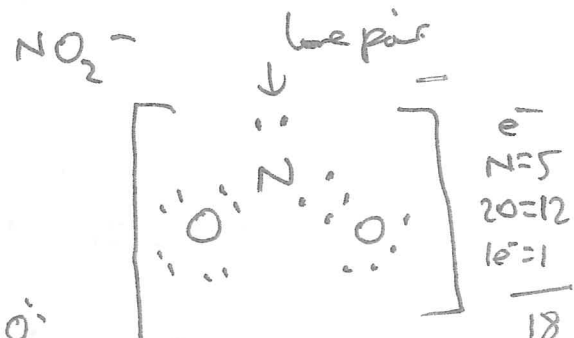
trigonal pyramidal

$$\begin{array}{r} e^- \\ N = 5 \\ 3H = 3 \\ \hline 8 \end{array}$$



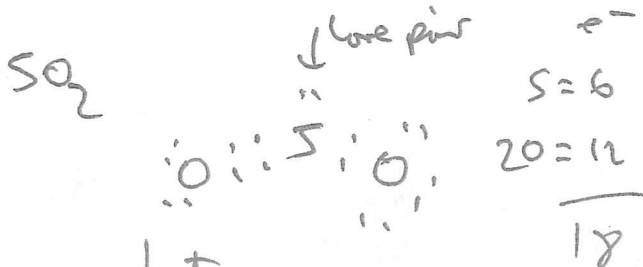
tetrahedral.

$$\begin{array}{r} e^- \\ P = 5 \\ 4O = 24 \\ 3e^- = 3 \\ \hline 32 \end{array}$$



↑ lone pair
bent

$$\begin{array}{r} e^- \\ N = 5 \\ 2O = 12 \\ 1e^- = 1 \\ \hline 18 \end{array}$$



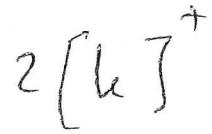
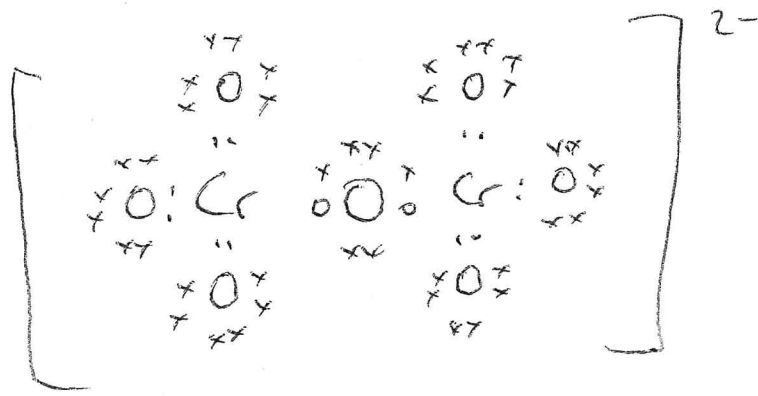
bent

$$\begin{array}{r} e^- \\ S = 6 \\ 2O = 12 \\ \hline 18 \end{array}$$



Trigonal planar

$$\begin{array}{r} S = 6 \\ 3O = 18 \\ \hline 24 \end{array}$$



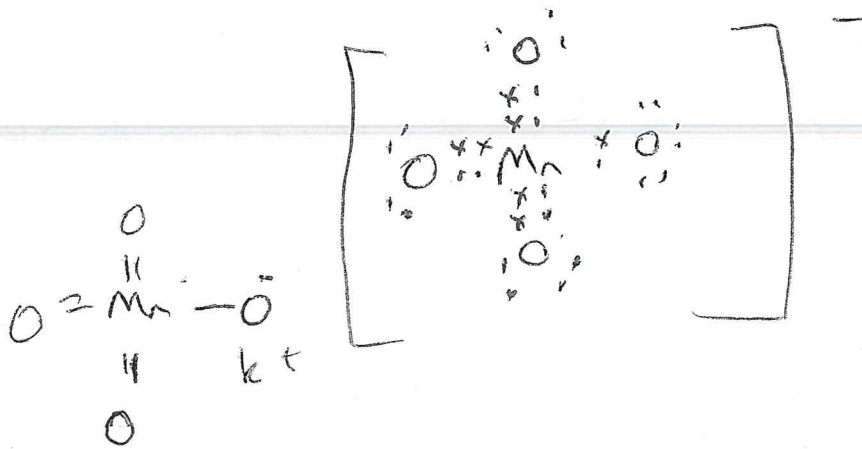
$$7 \times 8 = 56$$

$$O \quad 7 \times 6 = 42$$

$$Cr^{6+} \quad 2 \times 6 = 12$$

$$2e \quad = 2$$

$$56$$



$$O \quad 4 \times 6 = 24$$

$$Mn \quad 7 = 7$$

$$1e \quad = 1$$

$$32$$

If the atoms group no. add to even charge -2

If the atoms group no. add to odd charge -1,

