

A First Year blog on Lewis Structures and Formal Charges (for the week commencing the 20th of October 2019)

If you start from the basic dot-and-cross diagrams of GCSE Chemistry, then (in theory) it is possible to construct different alternative structures for the same molecular formula. However, only one of them would normally be the “correct” structure for that particular molecule, and all the others would be unstable and disintegrate on forming. The rules that govern the stable configuration of a molecule are those formulated by the great G. N. Lewis and thus bear his name (“Lewis Structures”), while the rules of Formal Charges spring from the work of John Slater and Linus Pauling.

Lewis Structures

- Dot-and-cross diagrams take up a lot of space, and (unless you are artistic) they are cumbersome to draw correctly. Chemists therefore use two representational systems (bond-line diagrams and Lewis diagrams) to show the bonding in covalent substances, and I show below the basic rules for drawing Lewis structures. However, before you can draw a Lewis structure you need to know how to calculate the number of “Valence Electrons” in a substance, and Dr Wayne Breslyn of the University of Maryland is exceedingly good at explaining how to do this at <http://www.thegeoexchange.org/chemistry/bonding/Valence-Electrons/index.html>
- Dr Breslyn then covers the subject of Lewis structures superbly on *youtube* and his website is <http://www.thegeoexchange.org/chemistry/bonding/Lewis-Structures/>
He suggests the following steps for writing Lewis structures
 1. Find the total number of valence electrons for the molecule.
Examples: [H₂S](#), [NCl₃](#), [OH](#)
 2. Put the least electronegative atom in the center. (NB H always goes on the outside.)
Examples: [NOCl](#), [CF₂Cl₂](#), [HCN](#)
 3. Put two electrons between the atoms to form a chemical bond.
Examples: [CH₄](#), [NH₃](#), [I₂](#)
 4. Complete the octets on the outside atoms. (NB H needs and can take only two valence electrons.)
 5. If the central atom does not have an octet, then move electrons from the outer atoms to form double or triple bonds.
Examples: [O₂](#), [N₂](#), [C₂H₄](#)
 6. If there are any extra electrons after the steps above, then add them to the central atom. (NB Elements in Period 3, and usually S, P, or Xe, can have more than eight valence electrons.)
Examples: [ClF₃](#), [SF₄](#), [XeH₄](#)
 7. Check the Formal Charges to make sure you have the best Lewis Structure possible.
Examples: [SO₄²⁻](#), [N₂O](#), [XeO₃](#)

Notable Exceptions to the Octet Rule

- H needs only 2 valence electrons.
- S and P sometimes have more than 8 valence electrons and thereby create ‘*expanded octets*’.
- Elements in Period 3/4/5/etc (in the Periodic Table) can hold more than 8 valence electrons i.e. they can have ‘*expanded*’ octets.
- Be and B do not need 8 valence electrons. They can have ‘*diminished*’ instead of ‘*expanded*’ octets.

Let us see how this works in practice.

Lewis Structures

1 Find the total number of electrons in the outermost shells of each of the reactants

In Chemistry these are called the “**valence**” electrons, and the Roman Numeral number of the **Group** in which the element lies will tell you how many outermost electrons there are.¹

NB The number of valence electrons for an individual atom is the same as the old Roman Numeral number of its Group in the Periodic Table (**NOT** the modern IUPAC number for the Group!), e.g.

No of valence electrons for N or for P = 5

No of valence electrons for O or for S = 6

No of valence electrons for F or for Cl = 7

..... and so on.

For example, the number of valence electrons

| | | | | | | | | |
|------------------------------------|---|-------------------------------|---|-------------|---|------------|---|----|
| for H ₂ O | = | 2 x 1 for H | + | 1 x 6 for O | = | 2 + 6 | = | 8 |
| for CO ₂ | = | 1 x 4 for C | + | 2 x 6 for O | = | 4 + 12 | = | 16 |
| for SO ₂ | = | 1 x 4 for S | + | 2 x 6 for O | = | 4 + 12 | = | 16 |
| for O ₃ | = | 3 x 6 for O | | | = | | = | 18 |
| for BF ₃ | = | 1 x 3 for B | + | 3 x 7 for F | = | 3 + 21 | = | 24 |
| for HNO ₃ | = | [(1 x 1) + (1 x 5) + (3 x 6)] | | | = | 1 + 5 + 18 | = | 24 |
| for H ₂ SO ₄ | = | [(2 x 1) + (1 x 6) + (4 x 6)] | | | = | 2 + 6 + 24 | = | 32 |
| and H ₃ PO ₄ | = | [(3 x 1) + (1 x 5) + (4 x 6)] | | | = | 3 + 5 + 24 | = | 32 |

2 Now start to draw the resulting structures by putting the least electronegative element at the very centre of the structure

All that you need to know is that ignoring the Noble Gases

- as you go up the Periodic Table, the elements become more electronegative, and
- as you go from left to right across the Periodic Table, the elements become more electronegative, therefore Fluorine is the most electronegative element that there is on earth. OK, all that you need to do now is to look at a Periodic table to decide which element in the substance that you are considering has the least electronegativity, and then build the atoms of all the other elements in the substance around that atom.

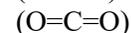
2a However, at ‘A’ Level we now need another rule viz. **put all the H atoms on the periphery of your construction**, for example

HCl has only 2 atoms therefore there can be no ‘centre’ to it

H₂O H atoms go on the periphery therefore the O atom must be at the centre



CO₂ C is less electronegative than O, therefore the C atom must be at the centre



SO₂ S is less electronegative than O, therefore the S atom must be at the ‘centre’



BF₃ B is less electronegative than F, therefore the B atom must be at the centre



BCl₃ B is less electronegative than Cl, therefore the B atom must be at the centre

¹ There are exceptions to this rule, but I am not going to go into that now.

- 3 *Something* has to hold the substance together (and if the substance is a molecular one then the inter-molecular binding force is a *molecular/covalent* bond), therefore now **start putting pairs of electrons in between the atoms.**
- 4 Now, go back to Rule 1 where you will see the number of valence electrons in the atom of each element, and start counting your valence electrons. **If you as yet do not have the correct number of valence electrons, then put in pairs of electrons on the atom until you have the correct number of valence electrons.**
- 6 Now **complete the Noble Gas stability configuration of 8 electrons in the outermost shell of each species in the substance.**
- 7 **If necessary, use dative bonding.**

OK, before we can draw any of the structures we need to talk about “Formal Charges”.

Formal charges

Formal Charges must be calculated for EACH INDIVIDUAL ATOM as well as for the whole species. The objective of the exercise will be to draw a Lewis structure that minimises the formal charges for the individual atoms and for the whole species.

- Most of the entries for Chemistry in Wikipedia are from eminent people in their fields, and Wikipedia is therefore a reasonable starting point if you want to look something up. On Formal Charges, Wikipedia says “In Chemistry, a **formal charge (FC)** is the charge assigned to an atom in a molecule, assuming that electrons in all chemical bonds are shared equally between atoms, regardless of relative electronegativity. When determining the best Lewis structure (or predominant resonance structure)² for a molecule, the structure is chosen such that the formal charge on each of the atoms is as close to zero as possible.”
- In Chemistry, the place in a species where it will react with another species is often determined by the spot where there is a concentration of electrostatic charge in the species, and “Formal Charges” are a good rule-of-thumb method for calculating where there could be such a concentration of electrostatic charge.
- The rules for the calculation of Formal Charges are as follows

The FC = (No. of valence electrons) - (half the No. of bonded electrons) - (No. of NON-bonded electrons)

and this is the same as

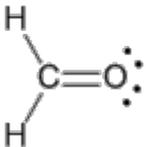
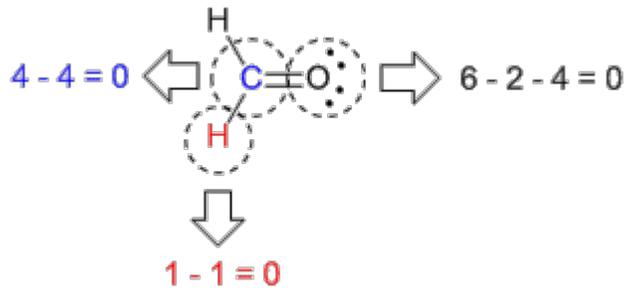
FC = (No of valence e⁻s) - (½ the number of bonding e⁻s) - (total number of lone e⁻s).

- The following example for the substance Formaldehyde (which we will talk about when we get to Organic Chemistry) comes from the University of Calgary.

² We will talk about “Resonance” next year.

- **The Diagrammatic or visual method** visually compares the number of valence electrons in an isolated neutral atom (which can be determined from the older style group number of the [periodic table](#)) with the atom in the molecule. It is a visual equivalent of the equation based method described above.
 - Draw a circle around the atom of interest
 - Count the number of electrons in the atoms circle (electrons in covalent bonds are shared)
 - Formal charge = group number of atom of interest - electrons in the circle of atom of interest

NB H.COOH is Methanoic Acid.

| | |
|--|--|
|  | <p>Example molecule of interest</p> |
|  | <p>Formal charge on oxygen: Group number = 6 Number of covalent bonds = 2 Number of lone pair electrons = 4</p> |
|  | <p>Formal charges for all the different atoms</p> |

Source: University of Calgary

ALL the Formal Charges are 'zero' therefore the structure is 'correct'.

- OK, you now know all the rules, so could you please draw the most stable Lewis structures for

H₂O
 CO₂
 SO₂
 O₃
 BF₃
 HNO₃
 H₂SO₄
 H₃PO₄