

Quantum

Electron configurations:

- s - maximum of 1 orbital/states which can hold 2 electrons
- p- maximum of 3 orbitals/states which can hold 6 electrons
- d- maximum of 5 orbitals/states which can hold 10 electrons
- f- maximum of 7 orbitals/states which can hold 14 electrons

-Electron configurations describe the state of all electrons in a particular element.

-Filled shell configurations yields lowest energy (noble gasses are very stable)

-Valence electrons can be described in the outer unfilled shell

-Must fill lower energy shells first

-Each orbital holds one electron in each subshell before doubling up.

The first number represents the principal energy level ($n=1,2,3$) where s and p = n , d = $(n-1)$ and f = $(n-2)$.

The letter (s,p,d,f) corresponds to angular momentum number and describes the shape of the orbital.

The second number represents the number of electrons in that particular subshell.

General sequence is as follows:

$1s^2$

$2s^2 2p^6$

$3s^2 3p^6$

$4s^2 3d^{10} 4p^6$

$5s^2 4d^{10} 5p^6 \dots$

Orbital dot diagrams show the states of each subshell and of the electrons based on their electron configuration.

Cations (+) describe a loss of electrons whereas anions (-) will show electron gain.

Lower energy subshells in their valence shell always lose their electrons first.

For example, Titanium has a ground state valence electron configuration of $4s^2 3d^2$. Titanium 2+ will lose two of its electrons, and since the d subshell is higher energy than s, the s shell will lose its electrons preferentially before d. Therefore, titanium 2+ has a valence electron configuration of $4s^0 3d^2$ or just $3d^2$

There are some exceptions to electron configuration when it comes to transition metals.

Elements prefer to have a more stable state (filled or half-filled subshell) and may take electrons from lower energy subshells to become more stable.

For example, copper would normally have a valence configuration of $4s^2 3d^9$, however, as shown from an orbital dot diagram, in its 3d block, it is one electron away from achieving a fully stable $3d^{10}$ state. To achieve this, copper will take an electron from the lower energy 4s subshell and add it onto its 3d block. The resulting valence configuration at ground state is $4s^1 3d^{10}$. This scenario will occur for transition metals that are one away from a filled shell or half-filled such as Cr, Mo, Cu and Ag.

Periodicity

Effective Nuclear Charge

(Coulombic attraction, force of nucleus on valence electrons)

$$Z_{\text{eff}} = Z - S$$

$Z_{\text{eff}} = (\text{Atomic number} - \text{number of core electrons})$

-Increases going to the right of the periodic table as you increase in number of protons and the attraction

-Stays the same when you go down a column because each element is getting added the same set amount total electrons and core electrons and there will be no difference mathematically.

Atomic radii

(Measure of the center of the nucleus to outer electron cloud)

Generally decreases going left to right on the periodic table

-This is due to an increase of protons i.e., effective nuclear charge which will have a stronger pull on the valence electrons towards the nucleus

Generally increases going down the periodic table.

-You are adding principal energy levels ($n=1,2,3$) and adding additional valence shells

*Special Cases: * **Ionic radii for isoelectronic species**

Ions with the same number of electrons (electron configuration)

-ionic radii will decrease the more positively charged it is and increase the more negatively charged it is. This is because those that are more positively charged will have a larger number of protons (Z_{eff}) and those negatively charged have more electrons (shielding) (Z_{eff}). Ex) radius $\text{Ca}^{2+} < \text{Cl}^-$

* Ion vs atom with same Z_{eff}

-The atom with more electrons is larger

-The reason behind this is when you add more electrons you are increasing electron-electron repulsions/shielding effect. When the positively-charged nucleus pulls the outer negatively-charged valence shell closer to the negatively-charged core electrons, these like-charged forces repel and counteract the Z_{eff} . Adding more electrons will increase the repulsion and increase the radii.

Examples: S^{2-} is larger than S because even though they have the same number of protons (Z_{eff}) S^{2-} has 2 more electrons which will have more repulsion forces counteracting and lead to a larger electron cloud

A general rule is that anions are larger than the atoms from which they are formed, and cations are smaller than their parent atoms.

Electronegativity

(Affinity of an atom to attract an electron)

-Increases going to the right across a group- As atoms gain more valence electrons, they are getting closer to achieving noble gas configuration of 8 electrons

-Decreases going down a column- Going down a group increases atomic radii (increase in principal energy levels $n=1,2,3$) This puts the bonding electrons further away from the nucleus and ability to attract decreases.

Ionization Energy

(Amount of energy required to remove an electron)

-Increases going to the right across a group

Increase in electronegativity and closer to noble configuration, element does not want to lose those electrons and will require more energy to take them away from the nucleus

-Decreases going down a column

Valence electrons are further out as you go down energy levels ($n=1,2,3$) and will be much further away from the nucleus and easier to give up.

***Exceptions to consider:** comparing elements right next to each other in the second or third row: Consider the energy required in breaking full shell/half shell orbitals. Electrons like this stability and may require more energy to break away from this, more than that of an element that is willing to lose an electron but may be closer to the right of the periodic table.

Example: Nitrogen vs Oxygen.

Nitrogen has 3 electrons in its p orbital and is pretty stable while half-filled; $1s^2 2s^2 2p^3$. It is not going to want to give up its stable half-filled state and lose an electron, so it requires more energy than normal

Oxygen has 4 electrons in its p orbital and is one away from obtaining a half-filled electron configuration: $1s^2 2s^2 2p^4$. When it loses an electron, it is going to become more stable because it is half-filled. It is going to favor losing an electron and not require as much energy

So even though Oxygen is further to the right of the table, it will have a lower first ionization energy than Nitrogen.

Keep in mind of when you are breaking half-filled/fully filled states, removing an electron from one subshell to another, and removing an electron from an entirely different principal energy level as these are usually cases where the trend in ionization energy breaks

Keep track of what is happening when considering 2^{nd} , 3^{rd} , 4^{th} etc. ionization energies in regards to the states that those electrons are in that are being taken away

Lewis Structures:

1. Count number of valence electrons in molecule you are drawing
2. Draw a draft Lewis Structure by drawing single bonds to the center atom (least electronegative atom) with the terminal atoms
3. Put lone pairs on all the terminal atoms to fulfill octet
4. Put lone pairs on center atom to fulfill octet*.
5. Count the electrons in the Lewis Structure and rearrange by adding single/double/triple bonds as necessary until total electrons equals those of step 1
6. Draw potential resonance structures and choose the most stable one

*Certain center elements break the octet rule. Boron and Beryllium, and some elements in group 3 of the p-block and down.

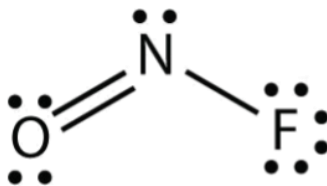
Resonance structures- recombination of bonds in a Lewis structure that yields the same structural molecule

Formal charge = Valence electrons - (#nonbonding Valence Electrons - $(\frac{1}{2})$ #bonding electrons))

Alternatively (and in my opinion, simpler)

Formal charge = Valence electrons - (#number of "things" around the atom)

Example:



Nitrogen: 5ve - [5 "things" (2 dots and 3 lines) around it] = 0 = FC

*You can also do 5ve - (2 nonbonding + $(\frac{1}{2})$ 6 bonding) = 0 FC (essentially same thing as above)

Oxygen: 6ve - 6 "things" = 0 FC

Fluorine: 7 ve - 7 "things" = 0 FC

-A way of checking that your formal charges/ structure is correct: Add up the formal charges of all the atoms on the molecule; they should equal the net charge of the molecule.

O=N-F has a net charge of 0

(Nitrogen FC+ Oxygen FC + Fluorine FC) = ONF total net charge

$$0 + 0 + 0 = 0$$

Which is the most stable Lewis Structure?

-Between several valid Lewis Structures, the most stable will have the smallest magnitude of formal charge on all the atoms. Ex: +1 and -1 is better than having +2 and -2

-If it is still a tie, look at the formal charge on the atom. If there is a negative formal charge, that atom is accepting an electron. The negative charge is going to prefer to go on an atom with a larger electronegativity (the more electron "hungry" atom) and will want the electron more. Vice versa for plus charges.

VSEPR Theory

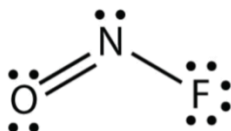
Regions of Electron Density	0 lone pairs	1 lone pair	2 lone pairs	3 lone pairs
2 EG: Linear hybridization: sp	MG: Linear Bond angle: 180			
3 EG: Trigonal planar Hybridization: sp^2	MG: Trigonal planar Bond angle: 120	MG: Bent Bond angle: <120		
4 EG: Tetrahedral Hybridization: sp^3	MG: Tetrahedral Bond angle: 109.5	MG: Trigonal Pyramidal Bond angle: 109.5	MG: Bent Bond angle: $<<109.5$	
5 EG: Trigonal Bipyramidal hybridization: sp^3d	MG: Trigonal Bipyramidal Bond angle: 120, 90	MG: See-Saw Bond angle: $<120, <90$	MG: T-Shaped Bond angle: <90	MG: Linear Bond angle: 180
6 EG: Octahedral hybridization: sp^3d^2	MG: Octahedral Bond angle: 90	MG: Square Pyramidal Bond angle: <90	MG: Square Planar Bond angle: 90	

Polarity: Think of tug of war. Symmetrical molecules will have pulling forces (dipole moments) based on electronegativity that are equal and opposite and negate net dipole moments; therefore, they will be non-polar. Those that are not symmetrical or have acting lone pairs that contribute to dipole moments will have a net dipole in the direction of the difference in EN and be polar.

Hybridization is mixing of atomic orbitals. This depends on the number of electron dense regions since this describes the used and available bonding orbitals around atom that electrons occupy. The number of electron dense regions should equal the number of orbitals available; 5 dense e^- regions will have sp^3d^1 .

Pi and sigma bonds: Every single bond contains a sigma bond. Every additional bond after a single bond comes from unhybridized p orbitals. This creates lateral overlap and what are known as “pi” bonds.
 single bond = 1 sigma bond double bond = 1 sigma, 1 pi triple bond = 1 sigma, 2 pi bonds

Ex) This molecule's center has 3 electron dense regions, one of which is a lone pair. Therefore, its EG is trigonal planar, its MG is Bent with a bond angle of about 117 degrees. It has net dipole moments (the pull of fluorine onto nitrogen is greater than that of oxygen to nitrogen) so the overall net dipole is towards the direction of fluorine and the molecule is polar. Since it has 3 electron regions, its hybridization is sp^2 . In this molecule, there are 2 sigma bonds and 1 pi bond. Note this structure does have resonance, but the molecule shown will have the lowest magnitude of formal charges (zero) and is the most stable.



CH 231 Midterm 2 Concept Review Sheet

Empirical Formula:

“Percent to grams, (out of fractional 100%)
 Grams to mole, (convert each to gram)
 Divide by small (all by the smallest mole calculated above)
 Times until whole” (multiply until whole number is reached)

Naming:

Case 1: using prefixes

When you have **2 nonmetals** Ex H₂O is dihydrogen monoxide

Mono, di, tri, tetra, penta, hexa, hepta, octa, nona, deca

Case 2: **Metal with non-metal** “just name it”.

Keep in mind criss-crossing charges of your alkali metals (cations) and non-metals (column 6 or 7 or a polyatomic) (anion) this yields a neutral charge on the subscript of the other molecule and reduced down.

The “big seven” diatomic molecules (H,N,O,F,Cl,Br,I) will have “ide” ending

Remember these polyatomics:

Sulfate	SO ₄ ²⁻	Permanganate	MnO ₄ ⁻	ex) MgF ₂ is magnesium fluoride
Carbonate	CO ₃ ²⁻	Chromate	CrO ₄ ²⁻	ex) Ca ₃ (PO ₄) ₂ is calcium phosphate
Acetate	C ₂ H ₃ O ₂ ⁻	Hydroxide	OH ⁻	
Nitrate	NO ₃ ⁻	Cyanide	CN ⁻	
Phosphate	PO ₄ ³⁻	Chlorate	ClO ₃ ⁻	

Case 3: **When using transition metal:** keep in mind criss-crossing the charge of the molecules. The charge of the molecule is placed as a subscript on the other molecule as neutral and reduced down.

Ex) Nickel (II) is Ni²⁺

Ex) Ni(SO₄)₂ is nickel (IV) sulfate because it is the reduced form of Ni₂(SO₄)₄ where when you reverse criss-cross, your starting elements are Ni⁴⁺ and SO₄²⁻

Molecular Orbital Theory

MO diagrams: tell you about covalent bonding between atoms and likelihood of them existing.

Bond order = (bonding electrons - antibonding electrons)/2

Proposed structures with BO greater than 0 are stable and can exist. Those that are 0 or smaller will not exist

Paramagnetic: Magnetism occurs; at least one non-fully paired electron

Diamagnetic: Magnetism “dies”; all electrons are fully paired

