AP Chemistry Unit 2

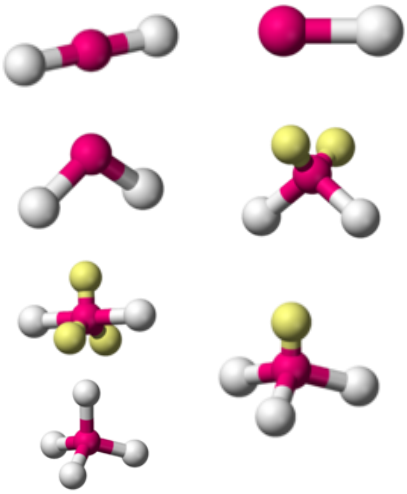
Unit 2.7 VSEPR and Hybridization

Learning Objectives

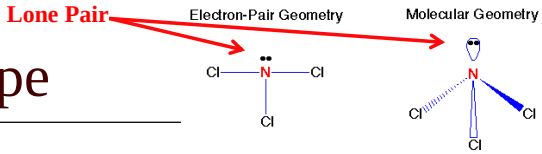
- Able to predict and explain the shapes of molecules using VSEPR theory
- Identify and describe the different types of molecular geometries
- Determine the bond angles in various molecular shapes
- Understand the concept of hybridization and how atomic orbitals mix to form hybrid orbitals,

VSEPR Model

- **Valence Shell Electron Pair Repulsion model**
- VSEPR is a model to predict the shape of molecules based on the idea that electron pairs around a central atom repel each other and arrange themselves as far apart as possible to minimize repulsion.
- The **shape of a molecule** determines many of its **physical and chemical properties**



Molecule Shape



- Molecular geometries take into account the **number of atoms** and the number of **Lone Pair electrons**
  - Electrons will distribute themselves to minimize repulsions between pairs of electrons
    - Causing the chemical bonds they form to stay as far apart as possible
- The main geometries without one pair elections are: VSEPR Video (11 mins)
  - Linear
  - Trigonal
  - Tetrahedral
  - Trigonal bipyramidal
  - Octahedral

VSEPR geometries

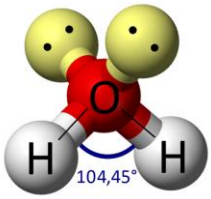
- **Depends on 2 factors**
  1. # of lone pair electrons
  2. # of atoms surrounding central atom

- **Steric Number** is the # of domains (atoms & lone electrons pairs) bonded to the central atom
  - Only worried about electron pairs on **Central Atom**

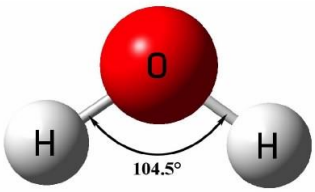
- **How to Determine Molecular Geometry – YouTube**: This video describes one method for quickly finding the major geometrical shapes for simple molecules. (20 Mins) On my Webpage

Structural vs Molecular Geometry

- We consider both lone electron pairs and bond electron pairs while determining the shape of the molecule in **Structural/electron geometry**.
- In **molecular geometry** only consider bond atoms.

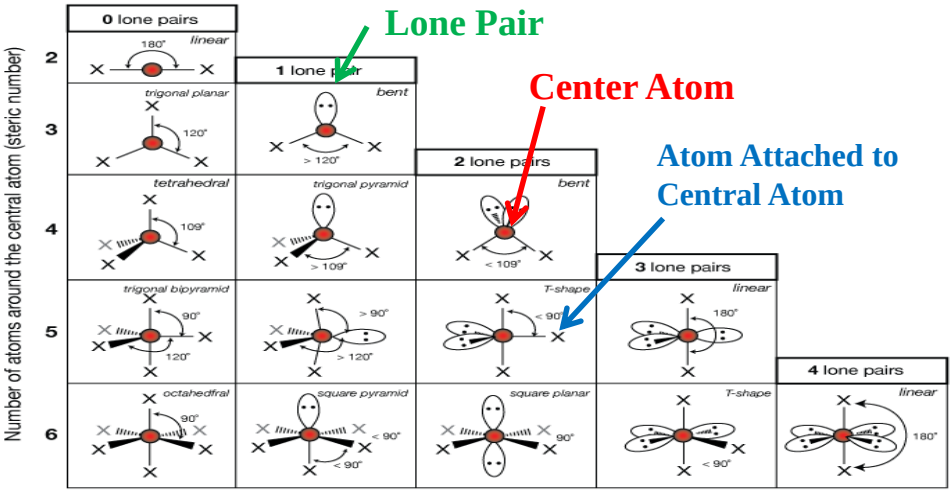


Structural/Electronic Geometry - Tetrahedral



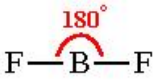
Molecular Geometry- Bent

VSEPR Model

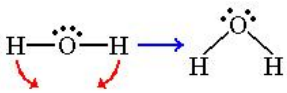


VSEPR Model

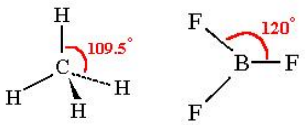
- Electron pairs repel each other and cause molecules to be in fixed positions relative to each other



- Unshared electron pairs also determine the shape of a molecule (LONE PAIRS)

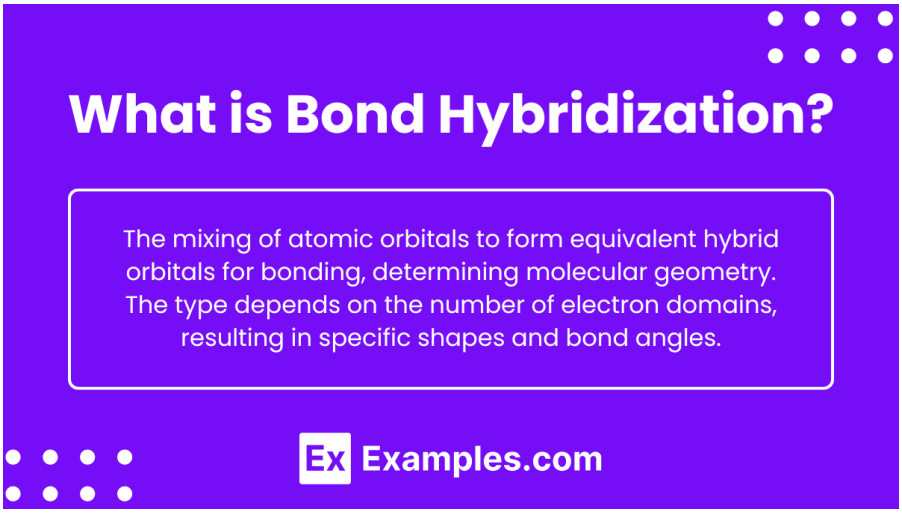


- Electron pairs are located in a molecule as far apart as they can be



Recap – Key Principles of VSEPR

- **Electron Pair Repulsion**: Electron pairs (bonding and lone pairs) around a central atom repel each other and seek to minimize repulsion by arranging themselves as far apart as possible.
- **Electron Domain Geometry**: The overall arrangement of regions of electron density (bonding pairs and lone pairs) around the central atom determines the electron domain geometry.
- **Molecular Geometry**: The shape of a molecule is determined by the positions of the atoms, which are influenced by the electron domain geometry. Lone pairs occupy more space than bonding pairs, affecting the final shape.
- **Lone Pair Effects**: Lone pairs repel more strongly than bonding pairs, causing bond angles to adjust and often become smaller than the ideal angles in a perfect geometry.
- **Steric Number**: The steric number, which is the sum of the bonding pairs and lone pairs around the central atom, helps determine the geometry:
  - 2 electron domains: Linear
  - 3 electron domains: Trigonal Planar
  - 4 electron domains: Tetrahedral
  - 5 electron domains: Trigonal Bipyramidal
  - 6 electron domains: Octahedral
- **Predictive Power**: By using the steric number and considering the repulsion between electron pairs, VSEPR theory allows for the prediction of molecular shapes and bond angles in various molecules.

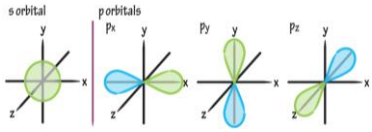


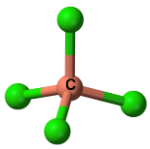
Hybridization

- **Hybridization** is a process in which atomic orbitals mix and form new, **Hybridized molecular orbital**

Atomic orbitals spd → **hybridization** → Hybridized molecular orbital

- **Hybridized molecular orbitals** have different shapes and energy levels than the atomic orbitals



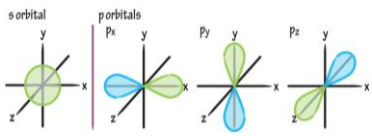


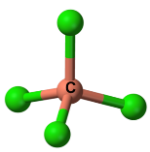
Hybridization

- **Hybridization** is a process in which atomic orbitals mix and form new, **Hybridized molecular orbital**

Atomic orbitals spd → **hybridization** → Hybridized molecular orbital

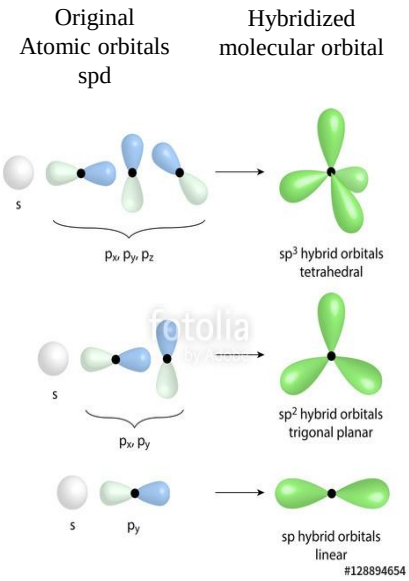
- **Hybridized molecular orbitals** have different shapes and energy levels than the atomic orbitals





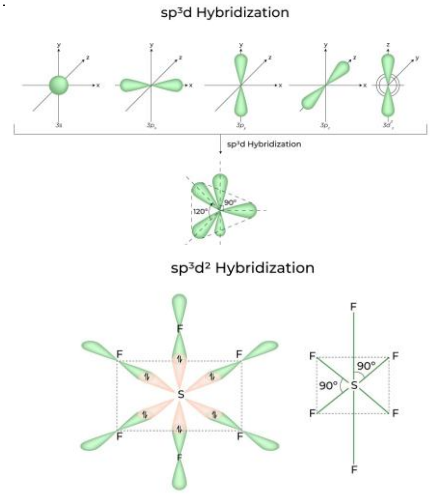
Types of Hybridization

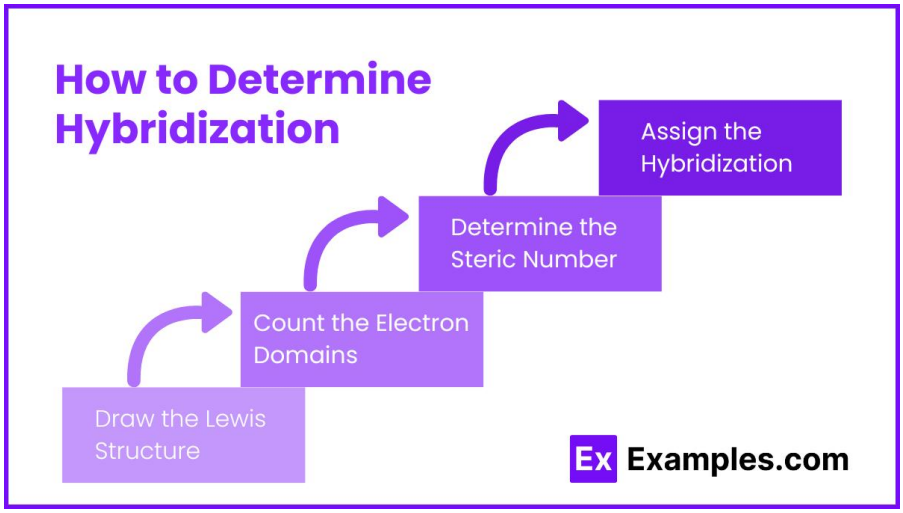
- **sp^3**
  - Mixing of s+p+p+p = 4 equivalent sp3 hybrid orbitals, tetrahedral geometry
- **sp^2**
  - Mixing of s+p+p = 3 equivalent sp^2 hybrid orbitals
  - Often associated with a double bond
- **sp**
  - mixing of 1 s orbital & 1 p orbital = 2 equivalent sp hybrid orbitals
  - Results in Linear geometry
  - Often associated with a triple bond



Types of Hybridization

- **sp^3 d**
  - Mixing of s+p+p+p + d = 5 equivalent sp^3d hybrid orbitals, tetrahedral geometry
- **sp^3d^2**
  - Mixing of s+p+p+d+d = 3 equivalent sp^3d^2 hybrid orbitals
  - Results in octahedral geometry, bond angles of 90°





How to determine hybridization

- **Draw the Lewis Structure**
- **Count the Electron Domains**
  - This includes:
    - Bonding pairs (single, double, or triple bonds count as one region each)
    - Lone pairs of electrons
- **Determine the Steric Number**:
  - **Steric Number** is the # of domains (atoms & lone electrons pairs) bonded to the central atom
- **Assign the Hybridization**:
  - **2 Electron Domains**: sp hybridization
    - Example: BeCl2 (Linear geometry, 180° bond angles)

How to determine hybridization

- **Assign the Hybridization**:
  - **2 Electron Domains**: sp hybridization
    - Example: BeCl2 (Linear geometry, 180° bond angles)
  - **3 Electron Domains**: sp2 hybridization
    - Example: BF3 (Trigonal planar geometry, 120° bond angles)
  - **4 Electron Domains**: sp3 hybridization
    - Example: CH4 (Tetrahedral geometry, 109.5° bond angles)
  - **5 Electron Domains**: sp3d hybridization
    - Example: PCl5 (Trigonal bipyramidal geometry, 90° and 120° bond angles)
  - **6 Electron Domains**: sp3d2 hybridization
    - Example: SF6 (Octahedral geometry, 90° bond angles)

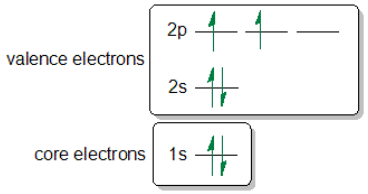
The following is more Hybridization info

- More than you probably need

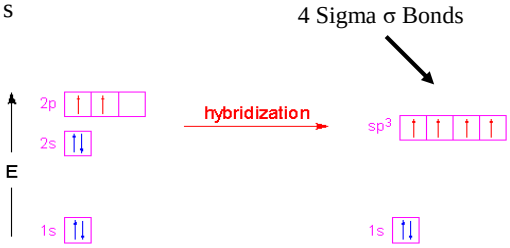
Hybridization

Orbitals of Carbon Atom

- Carbon, $1s^2\ 2s^2\ 2p^2$, often undergoes hybridization 3 different ways
  - sp^3
  - sp^2
  - sp

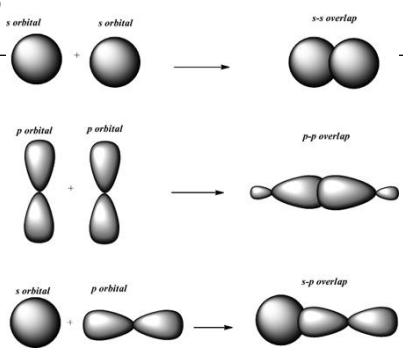


- an **sp3 orbital** formed from one s orbital and three p orbitals
  - Carbon Sigma Bond - overlapping orbitals
  - Hybridization – 4 orbitals

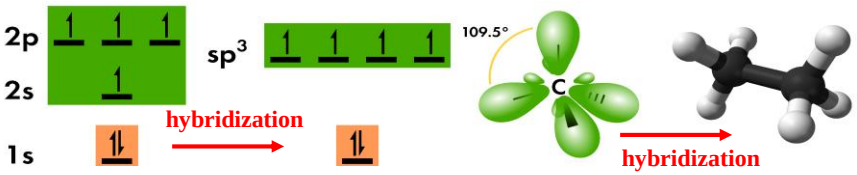


Hybridization - sp^3

- Sigma Bond σ
  - overlap of 2 s orbitals or s and p or p head to head



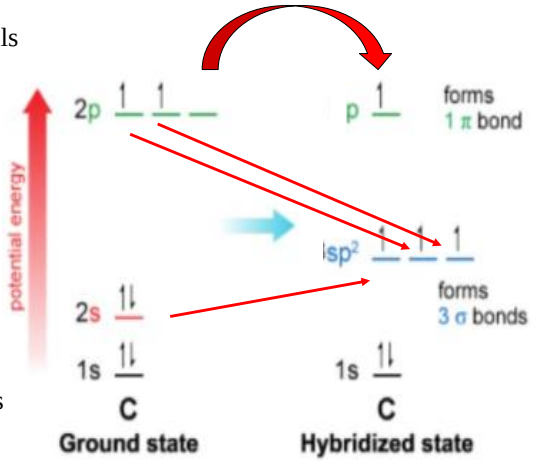
- Hybridization of sp^3



Hybridization - sp^2

- Sp^2 = s + p + p
  - Hydridization -3 orbitals
  - Unhydridization – 1 p
- 3 sites for boding
- Steric #= 3
- Double bond
- 3 Sigma & 1 Pi

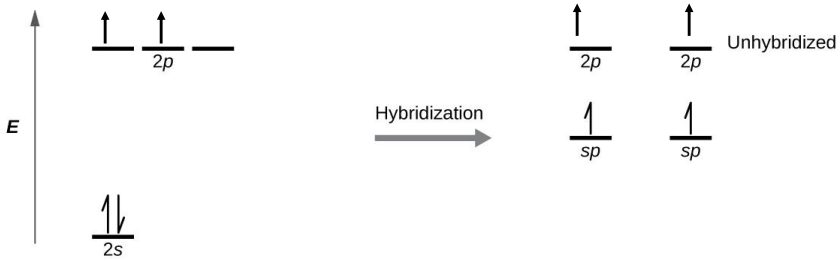
- PI bond π
  - Pi bonds form from unhydridized P orbitals



Hybridization - sp

- Sp = s + p
  - Hydridization – 2 orbitals, 2 + p
  - Unhydridization – 2 p orbitals
- 2 sites for boding
- Steric #= 2
- Triple bonds

- 2 pi bonds
- 2 sigma bonds



Hybridization

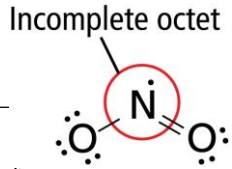
Type of Hybridization	Electron Geometry	# of Electron Groups
sp	Linear	2
sp^2	Trigonal Planar	3
sp^3	Tetrahedral	4
dsp^3	Trigonal bipyramidal	5
d^2sp^3	Octahedral	6

Review: Main Idea's

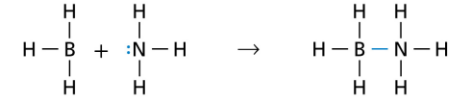
- Specific rules are used when naming binary molecular compounds and binary acids
- Atoms gain stability when they share electrons and form covalent bonds
- Structural formulas show the relative positions of atoms within a molecule
- The VSEPR model is used to determine molecular shape
- Electronegativity: the relative ability of an atom to attract electrons in a chemical bond
- A chemical bond's character is related to each atom's attraction for the electrons in the bond

Review

Exceptions to Octet Rules



- Some molecules do not obey the octet rule
- A small group of molecules might have an odd number of valence electrons.
- NO_2 has five valence electrons from nitrogen and 12 from oxygen and cannot form an exact number of electron pairs
- A few compounds form stable configurations with less than 8 electrons around the atom—a suboctet.
- A **coordinate covalent bond** forms when one atom donates both of the electrons to be shared with an atom or ion that needs two electrons.

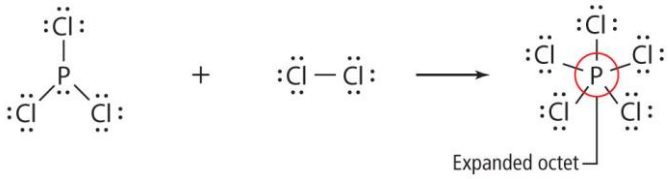


The boron atom has no electrons to share, whereas the nitrogen atom has two electrons to share.

The nitrogen atom shares both electrons to form the coordinate covalent bond.

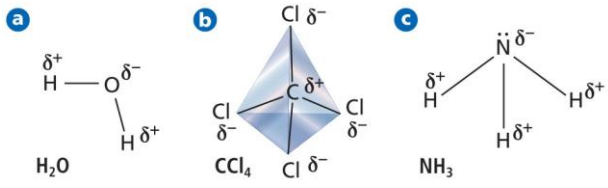
Exceptions to the Octet Rule (cont)

- A third group of compounds has central atoms with more than eight valence electrons, called an expanded octet
- Elements in period 3 or higher have a d-orbital and can form more than four covalent bonds



Polar Covalent bonds

- Compare Water and CCl_4
  - Both are polar by subtracting electronegativities
  - But only water is a polar molecule because of the shape of the molecule



The bent shape of a water molecule makes it polar.

The symmetry of a CCl_4 molecule results in an equal distribution of charge, and the molecule is nonpolar.

The asymmetric shape of an ammonia molecule results in an unequal charge distribution and the molecule is polar.

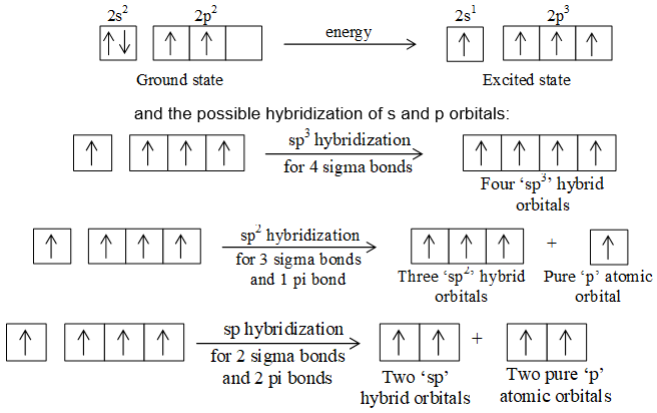
Ionic Bonding and Coulomb's Law

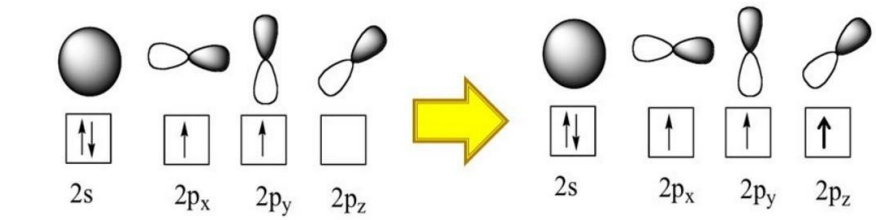
So how strongly "bonded" are things in ionic solids?

It depends on:

1. How + or - things are (the greater the difference in charge, the stronger the attraction)
2. How close together things are (the lower the radius, the stronger the attraction)

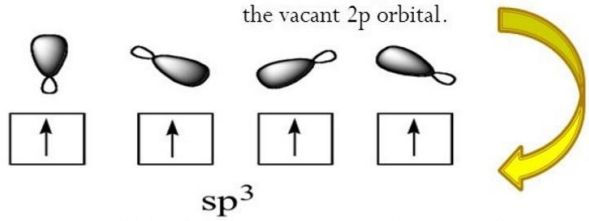
You can predict everything you need to know about an ionic solid based off this.





Electron configuration of carbon at in most stable state.

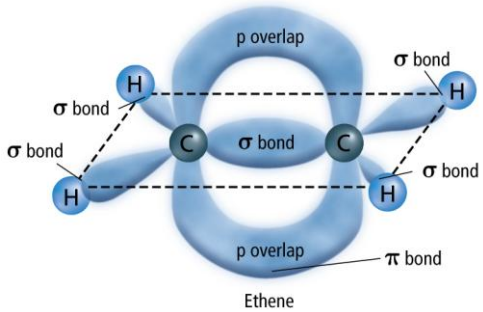
An electron is promoted from the 2s orbital to the vacant 2p orbital.



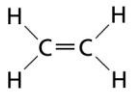
The 2s orbital and the three orbital 2p orbital are combine to give a set of four equal-energy sp^3 hybridized orbitals, each of which contains one electron.

Double & Triple Bonds

- A **pi bond** is formed when parallel orbital's overlap and share electrons
  - A Double & Triple bond consists of one sigma bond and at least one pi bond
  - Electrons being shared from **S and P subshells** (Reason called pi Bond)



Ethene



Extra - Chemical Bonding

- Ionic Bonding results from cations and anions in a regular array called a crystal lattice.
  - Water must overcome the ion-ion attractions to dissolve ionic substance.
    - Size and charge affect this.
  - Lattice energy is the energy contained in the crystal lattice.
    - Can be calculated by:

$$\text{Lattice Energy} = k\left(\frac{Q_1 Q_2}{r}\right)$$

    - K is a proportionality constant that depends on the structure of the solid and the electron configurations of the ions.

Sigma and Pi Bonds

Pi (π) bonds exist in the region above and below a line drawn between two bonded atoms.

Single bond	**1 sigma bond**
Double Bond	**1 sigma, 1 pi bond**
Triple Bond	**1 sigma, 2 pi bonds**