Course Name: Chemistry
Course NO: CHE1203

Chemical Bonds

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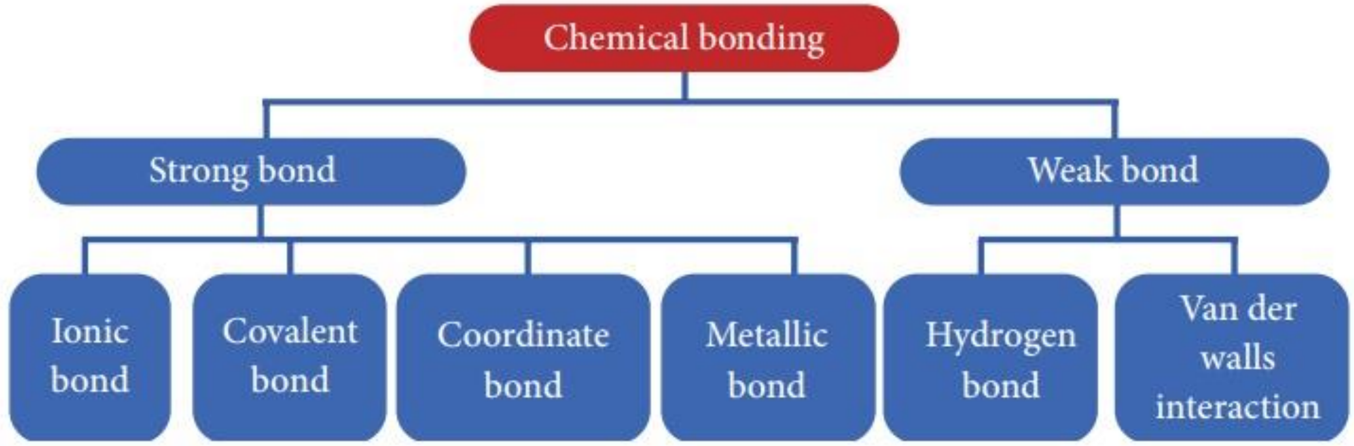
Chemical Bond

A chemical bond is the force that holds atoms together in a chemical compound. A chemical bond is a lasting attraction between atoms, ions or molecules that enables the formation of chemical compounds. The bond may result from the electrostatic force of attraction between oppositely charged ions as in ionic bonds or through the sharing of electrons as in covalent bonds



Electronic Theory of Chemical bonds

(i) Chemical combination between atoms of the same or different elements takes place due to the tendency by the outermost electron groups to attain the stable arrangement of the inert gases.

Name of the element	Atomic number	Shell electronic configuration
Helium (He)	2	2
Neon (Ne)	10	2,8
Argon (Ar)	18	2,8,8
Krypton (Kr)	36	2,8,18,8
Xenon (Xe)	54	2,8,18,18,8

(ii) The attainment of inert gas electronic configuration may take place by complete transference of electrons from one atom to another. The resulting electrically charged atoms (ions) are held together by electrostatic force of attraction.

(iii) The attainment of inert gas configuration may occur by sharing of electrons (in pair) between two atoms.

(iv) The attainment of electronic groupings of inert gases may also happen by both transference and sharing of electrons between atoms in pairs.

Ionic Bond

An ionic bond is a chemical bond formed by the electrostatic force of attraction between positive and negative ions. Ionic bonding is the complete transfer of valence electron(s) between atoms. It is a type of chemical bond that generates two oppositely charged ions. In ionic bonds, the metal loses electrons to become a positively charged cation, whereas the nonmetal accepts those electrons to become a negatively charged anion. Na atom losses electron and becomes a cation.

$$Na \rightarrow Na^{+} + e^{-} \text{ (loss of electron)}$$

The atom that gains electrons becomes an anion.

$$Cl + e^- \rightarrow Cl^- \text{ (gain electron)}$$

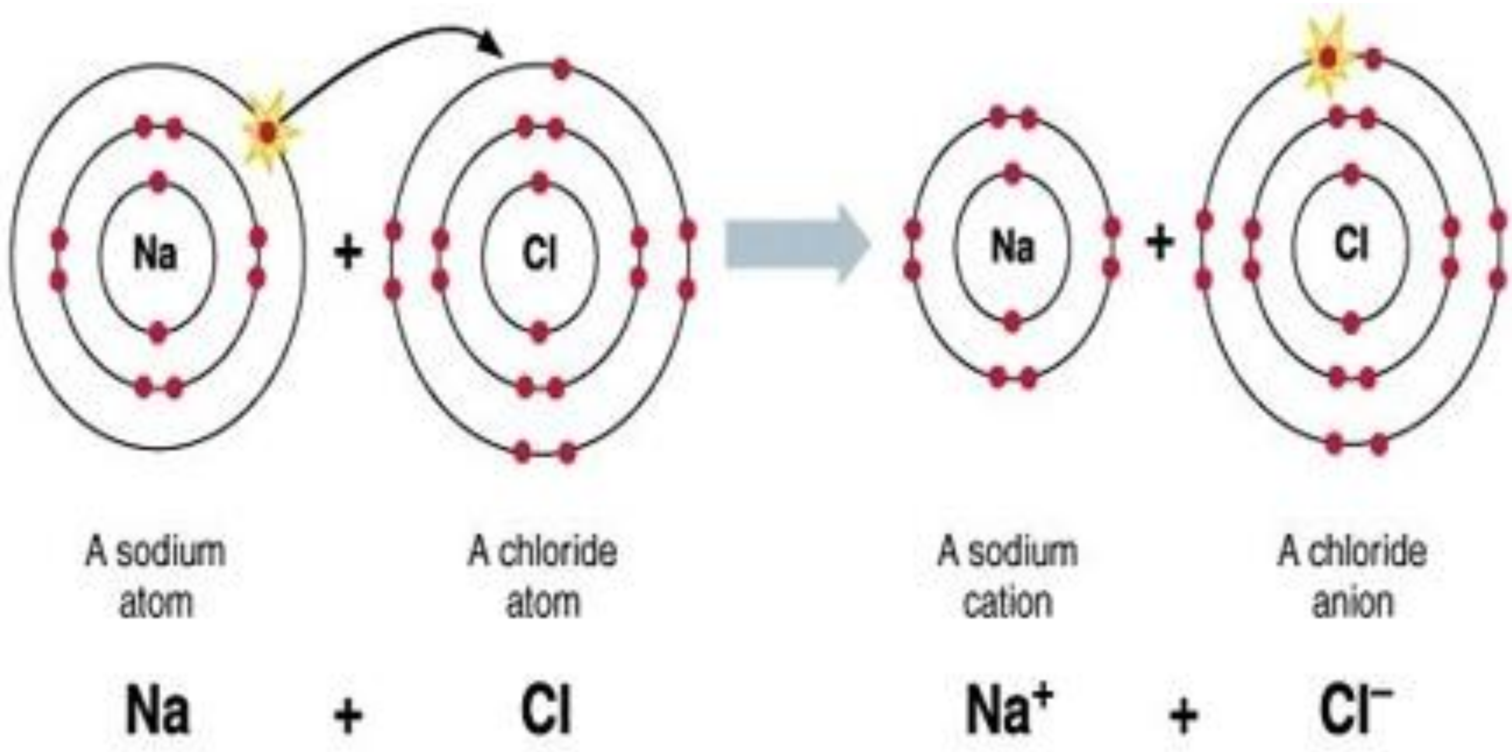


Fig. Schematic representation of ionic bond formation

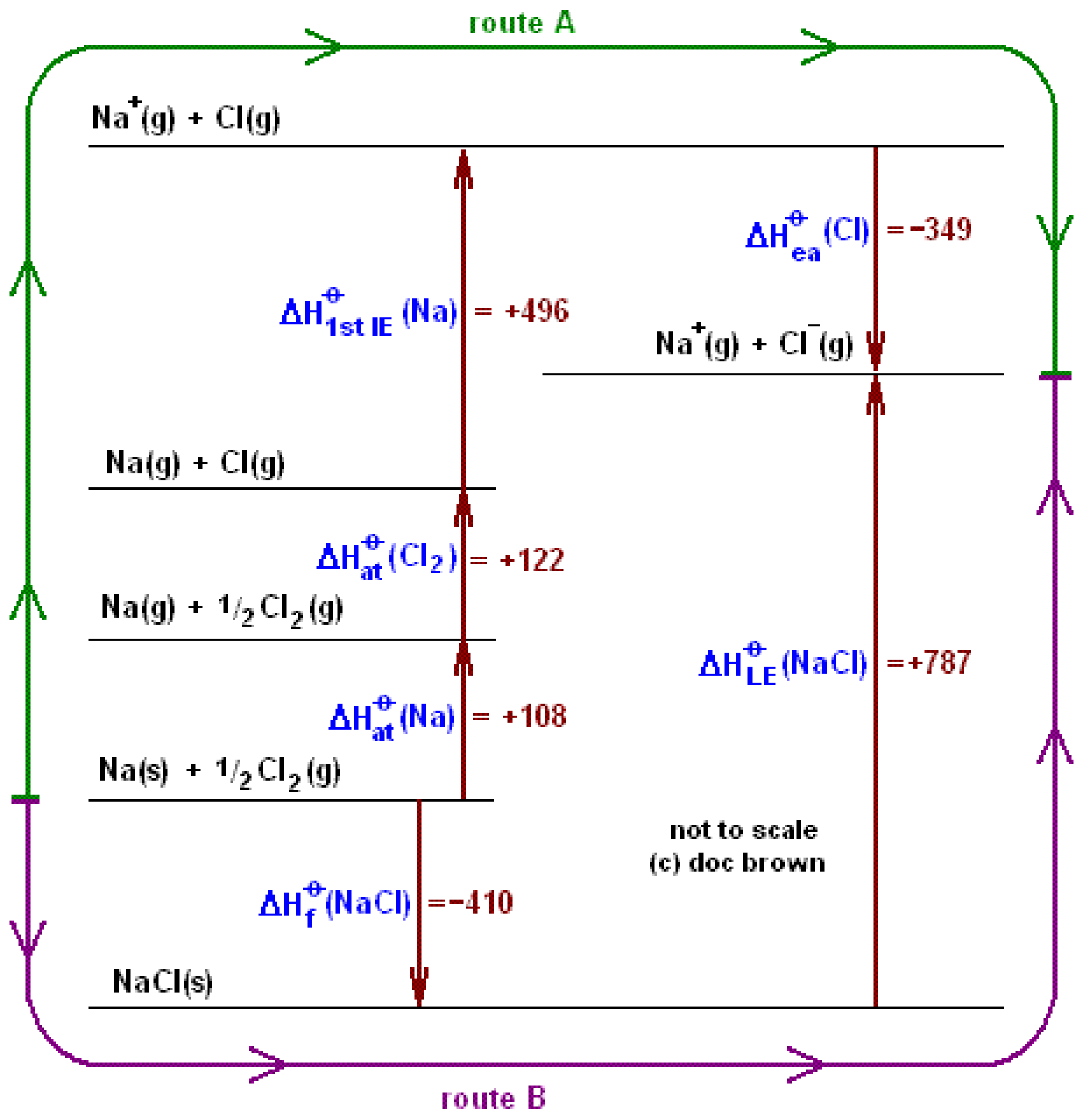
Energy involved in ionic Bond

Lattice Energy

The lattice energy is the change in energy that occurs when an ionic solid is separated into isolated ions in the gas phase. For example, NaCl, the process is

$NaCl(s) \rightarrow Na^{+}(g) + Cl^{-}(g)$

U= -786 KJ/mol



General Properties of Ionic Compounds

The properties of ionic compounds relate to how strongly the positive and negative ions attract each other in an ionic bond. Iconic compounds also exhibit the following properties:

They form crystals

Ionic compounds form crystal lattices rather than amorphous solids. At an atomic level, an ionic crystal is a regular structure, with the cation and anion alternating with each other and forming a three-dimensional structure based largely on the smaller ion evenly filling in the gaps between the larger ion.

They have high melting points and high boiling points

High temperatures are required to overcome the attraction between the positive and negative ions in ionic compounds. Therefore, a lot of energy is required to melt ionic compounds or cause them to boil.

They have higher enthalpies of fusion and vaporization than molecular compounds

Just as ionic compounds have high melting and boiling point, they usually have enthalpies of fusion and vaporization that can be 10 to 100 times higher than those of most molecular compounds.

They are hard and brittle

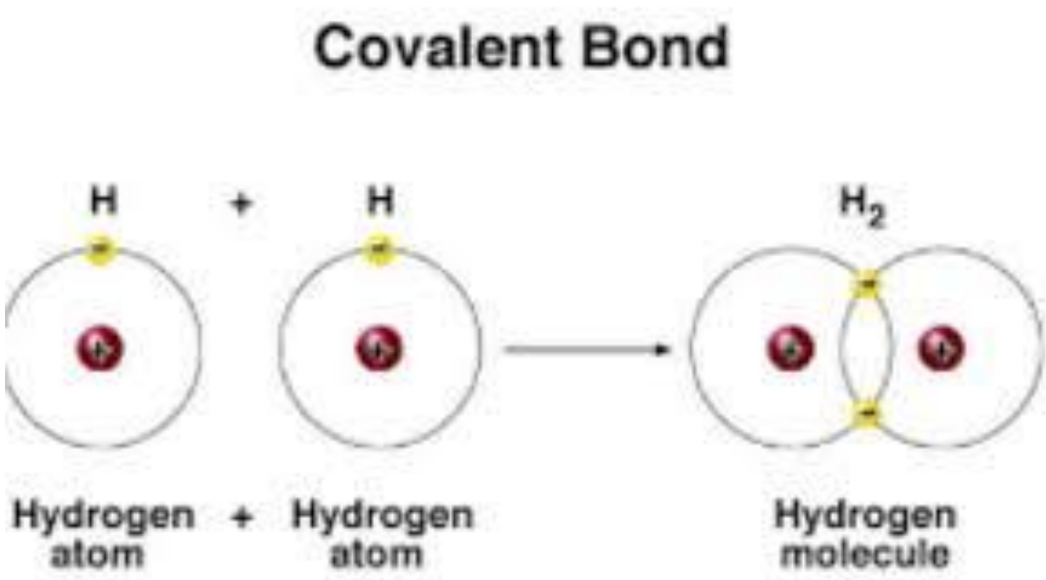
Ionic crystals are hard because the positive and negative ions are strongly attracted to each other and difficult to separate, however, when pressure is applied to an ionic crystal then ions of like charge may be forced closer to each other. The electrostatic repulsion can be enough to split the crystal, which is why ionic solids also are brittle.

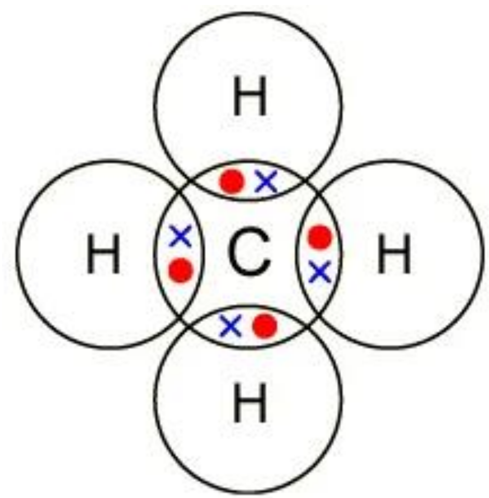
They conduct electricity in solution

When ionic compounds are dissolved in water the dissociated ions are free to conduct electric charge through the solution. Molten ionic compounds (molten salts) also conduct electricity.

Covalent Bond

A covalent bond is a chemical bond that involves the sharing of electron pairs between atoms. These electron pairs are known as shared pairs or bonding pairs, and the stable balance of attractive and repulsive forces between atoms, when they share electrons, is known as covalent bonding.





Recent Theory of Covalent Bond

When one hydrogen atom with its proton and electron combines with another hydrogen atom a several forces of attraction and repulsions are acting.

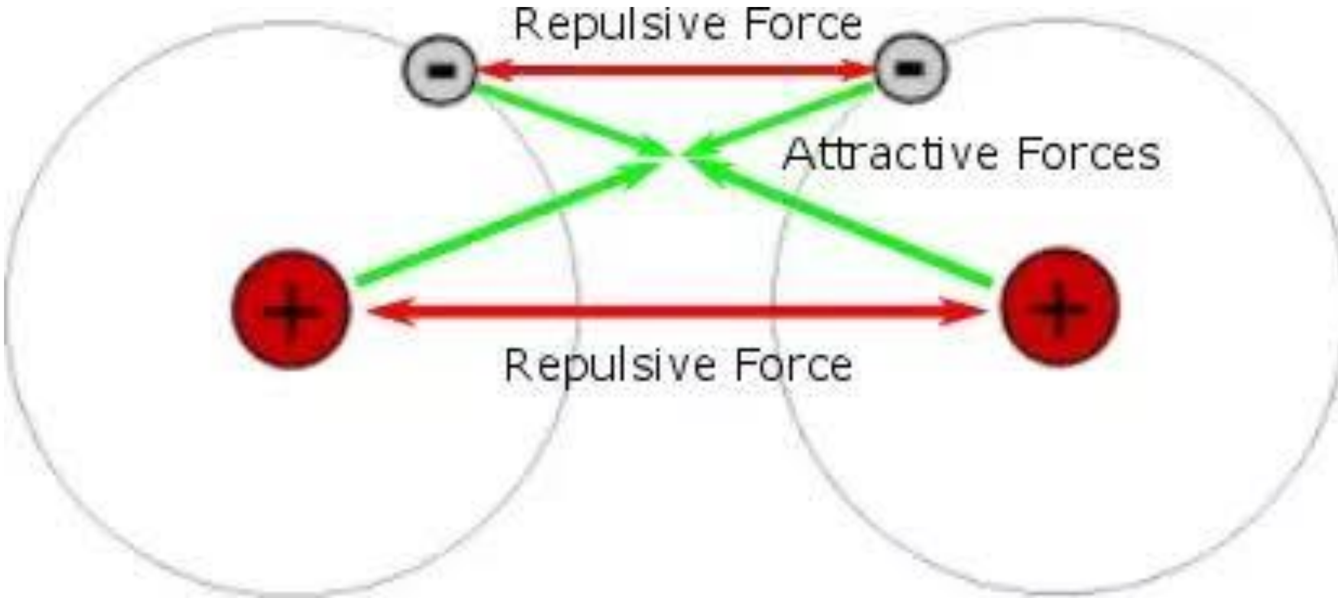
(i) Repulsion between electron and electron

(ii) Attraction between electrons and protons of each hydrogen atom

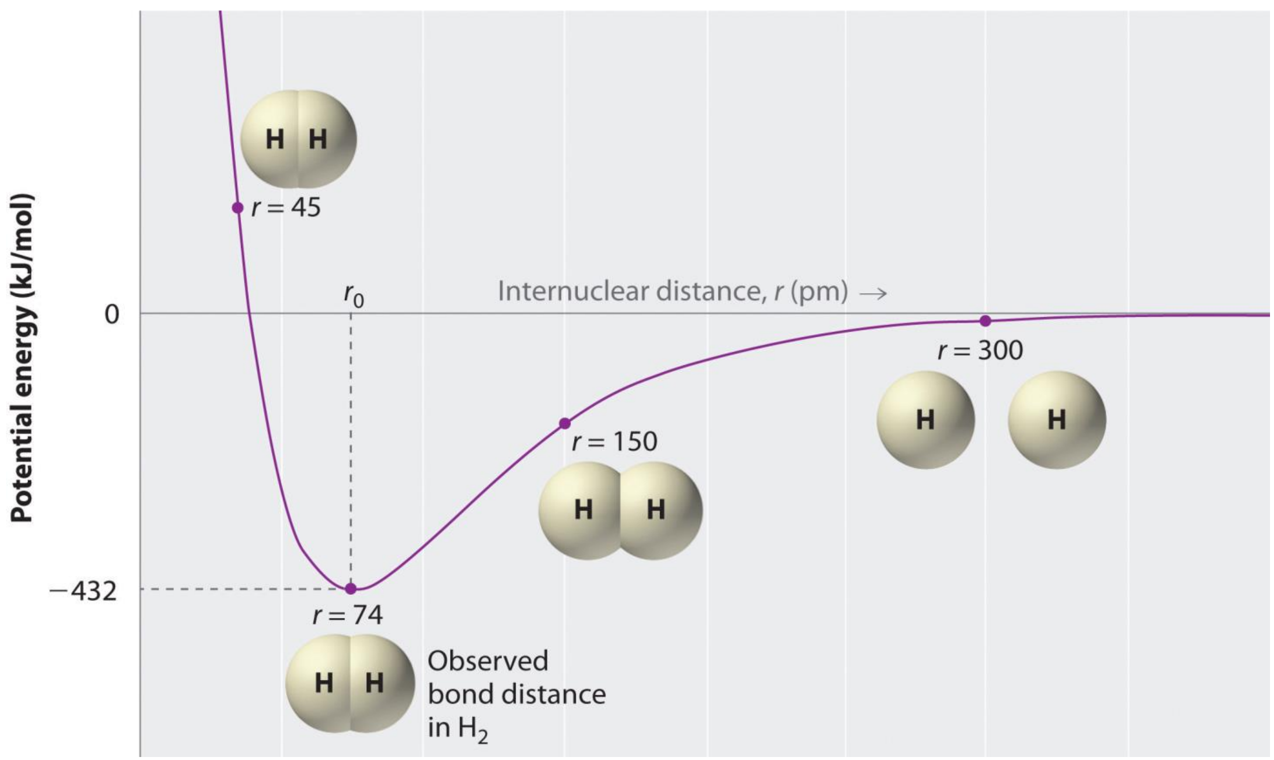
(iii) Repulsion between protons and protons

(iv) Electronic interactions between the two electronic systems

It is necessary to illustrate the potential energy diagram for the formation on of a chemical bond when two atomic systems approach each other.



Repulsive Force
Attractive Forces
Repulsive Force



Potential energy (kJ/mol)
0
−432
Internuclear distance, r (pm) →
r0
r = 45
r = 74
r = 150
r = 300
H
Observed
bond distance
in H2

Energy involved in Covalent bond

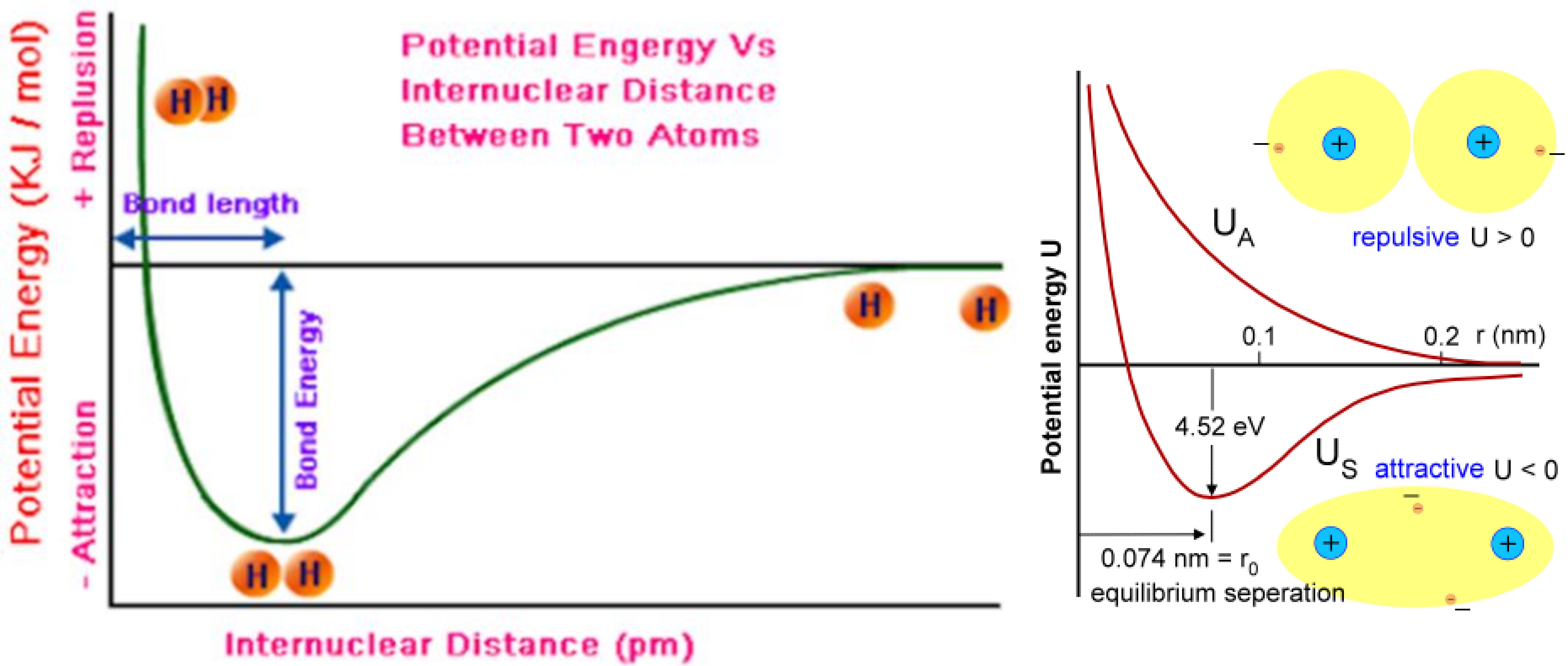


Fig. Potential energy diagram for the formation of diatomic molecule as a function of intermolecular distance

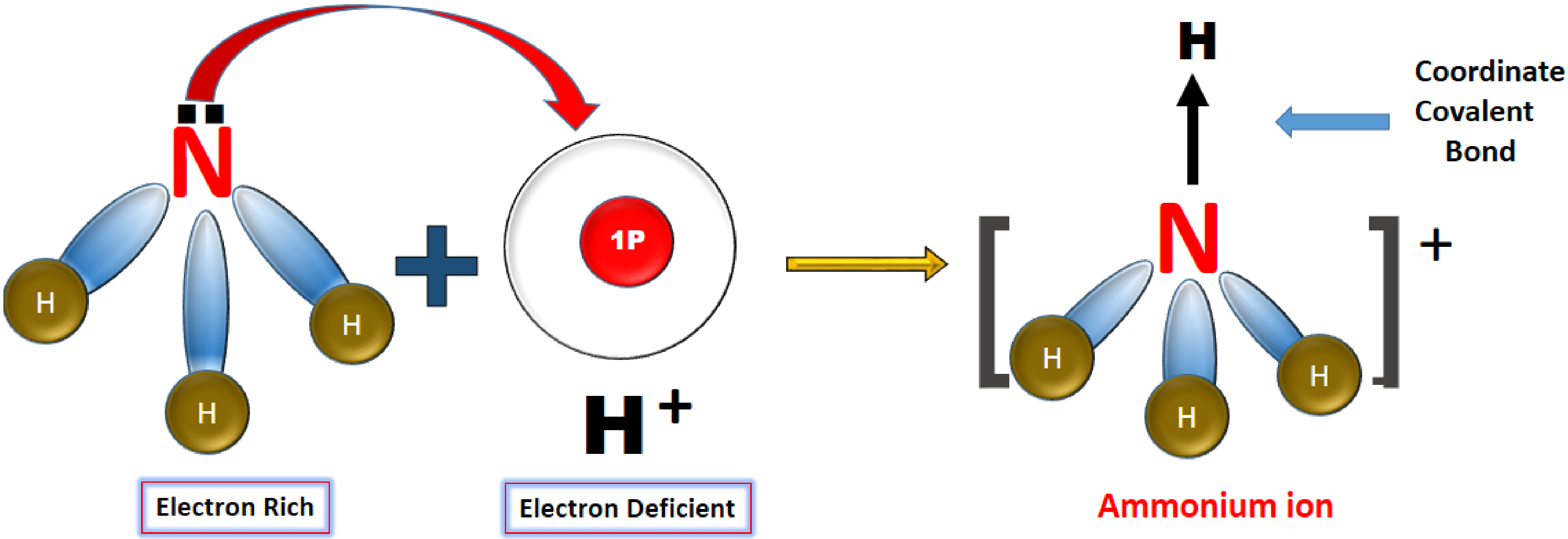
As the atom approach each other and if there is no chemical bond formation, the energy required to force the two atoms to come close to each other will be very high as indicated by upper curve I right Fig. This shows increasing external energy to force them near to each other. On the other hand, the formation of chemical bond between the two atomic system through electronic interaction leads to the rearrangement of the electron clouds giving rise to the lowering of energy as shown by the curve in same Fig. Two atomic systems form a molecule with increased stability at the equilibrium internuclear distance between the two atoms.

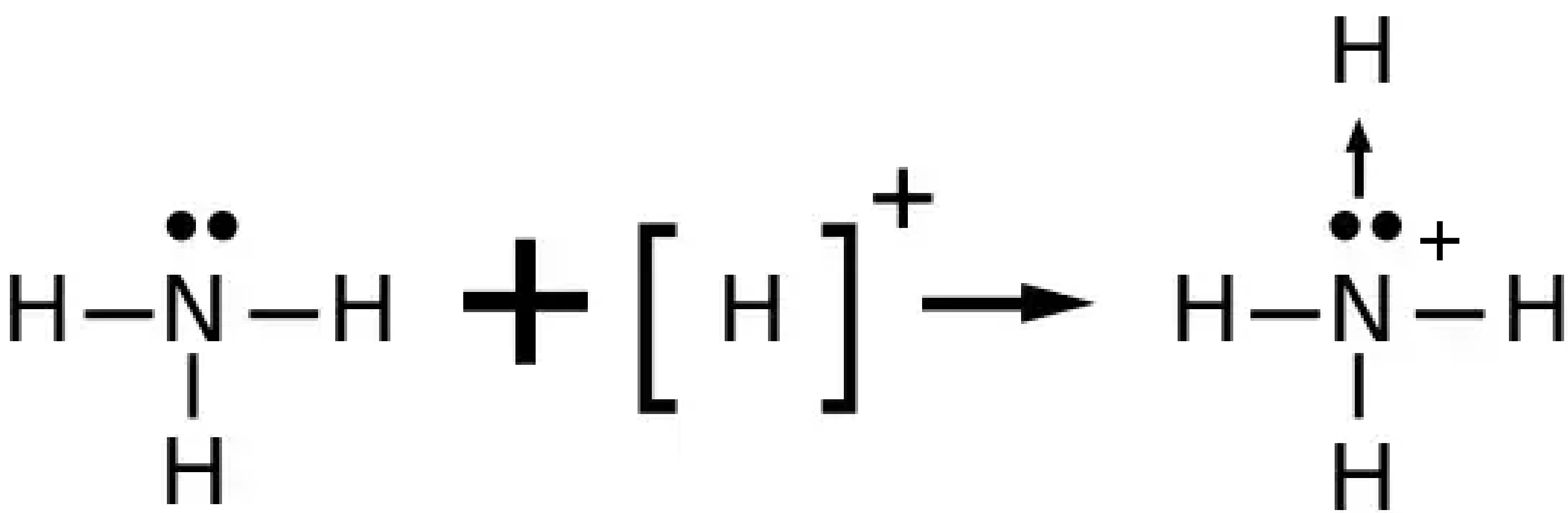
The lowering of energy occurs in chemical bond formation because of the rearrangement of electron clouds of the two systems. The formation of a stable molecule through initially excited states also involves lowering of energy as indicated by Fig.

Coordinate Covalent bonds

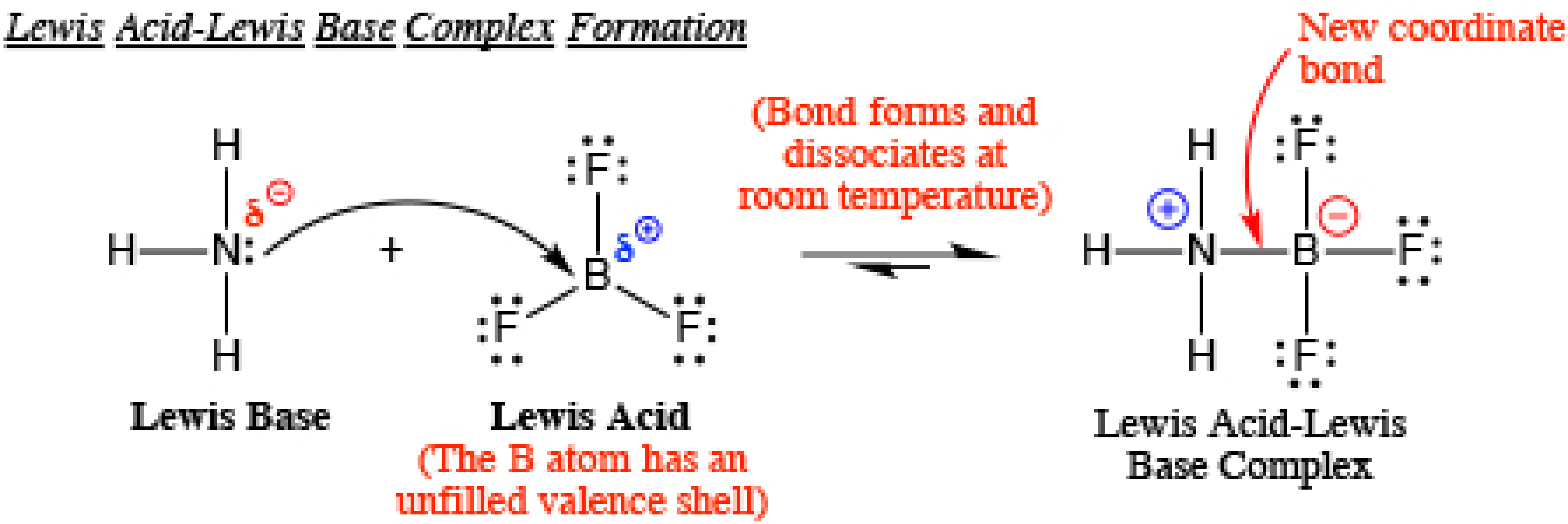
A coordinate bond (also called a dative covalent bond) is a covalent bond in which both electrons come from the same atom. A covalent bond is formed by two atoms sharing a pair of electrons. The atoms are held together because the electron pair is attracted by both of the nuclei.

Formation of NH_4^+ by coordinate covalent bond



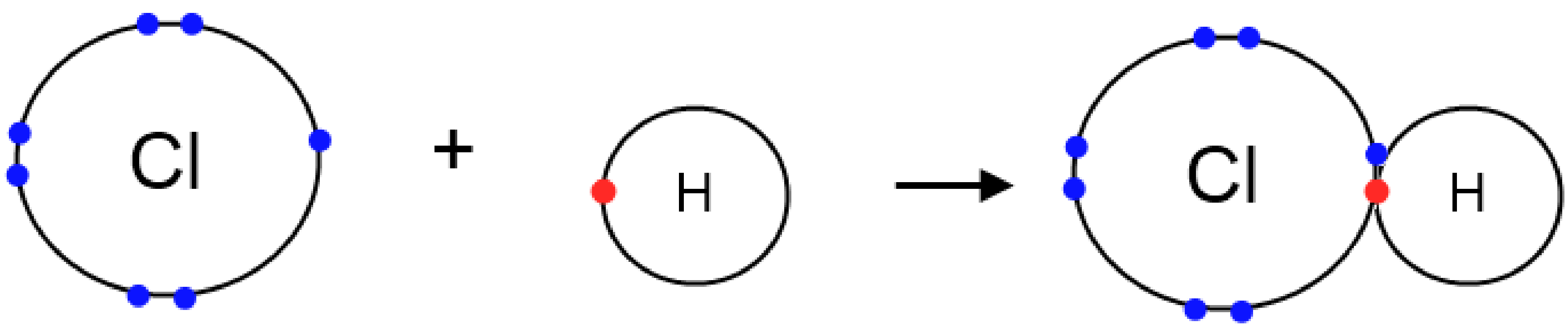


Formation of NH_3BF_3 by coordinate covalent bond



Octet Rule

The octet rule is a chemical rule of thumb that reflects the theory that main group elements tend to bond in such a way that each atom has eight electrons in its valence shell, giving it the same electronic configuration as a noble gas.

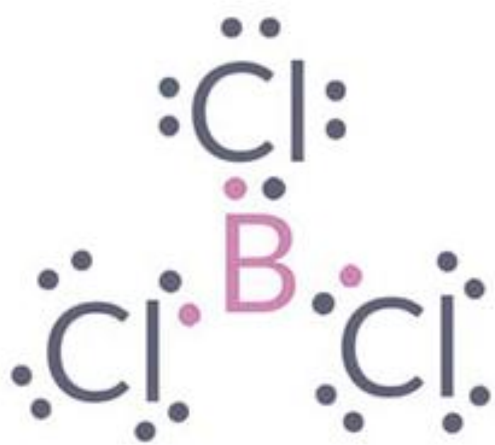


Exceptions to the Octet Rule

There are three types of molecules or ions that are exceptions to the octet rule:

- Electron-deficient molecules
- Molecules with expanded valence shells
- Molecules with an odd number of electrons

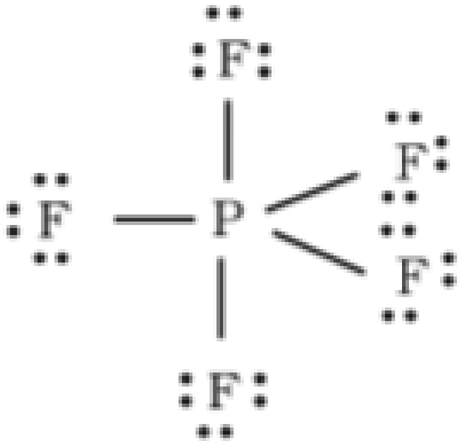
$BeCl_2$



BCl_3

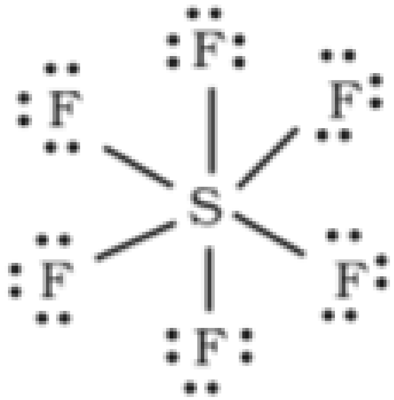
Electron deficient molecules

Molecules with expansion of octet rule



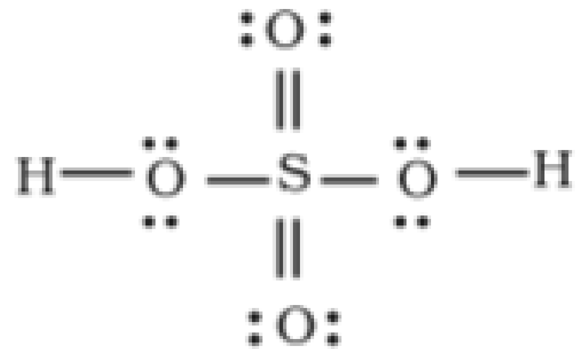
PF_5

10 electrons around the P atom



SF_6

12 electrons around the S atom



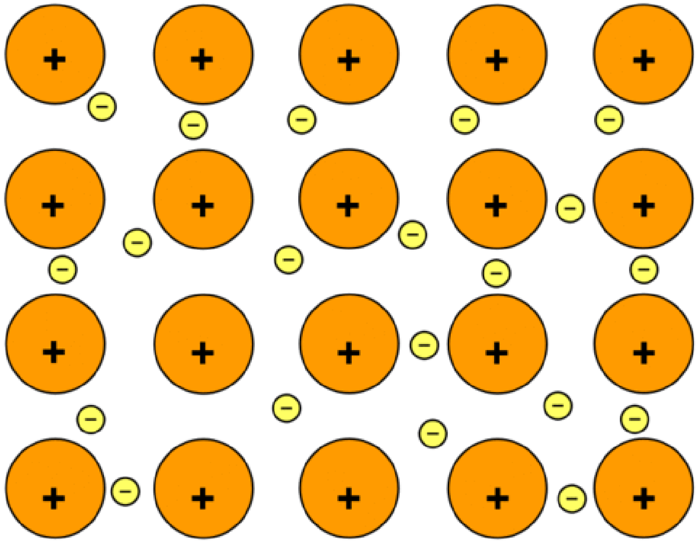
H_2SO_4

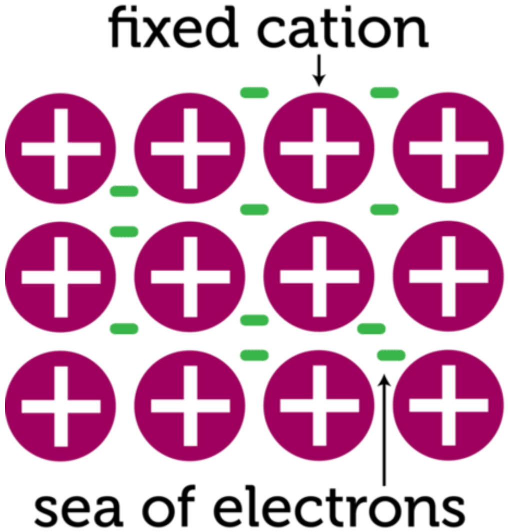
12 electrons around the S atom

Molecule with odd number of electrons

Metallic Bonds

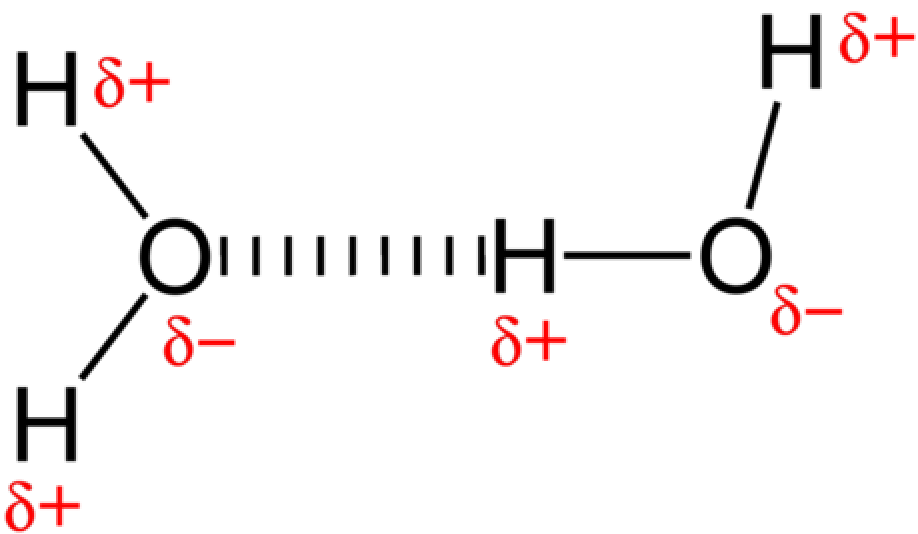
- The chemical bonding that results from the attraction between metal cations and the surrounding sea of electrons.
- Vacant p and d orbitals in metal's outer energy levels overlap, and allow outer electrons to move freely throughout the metal.
- Valence electrons do not belong to any one atom.



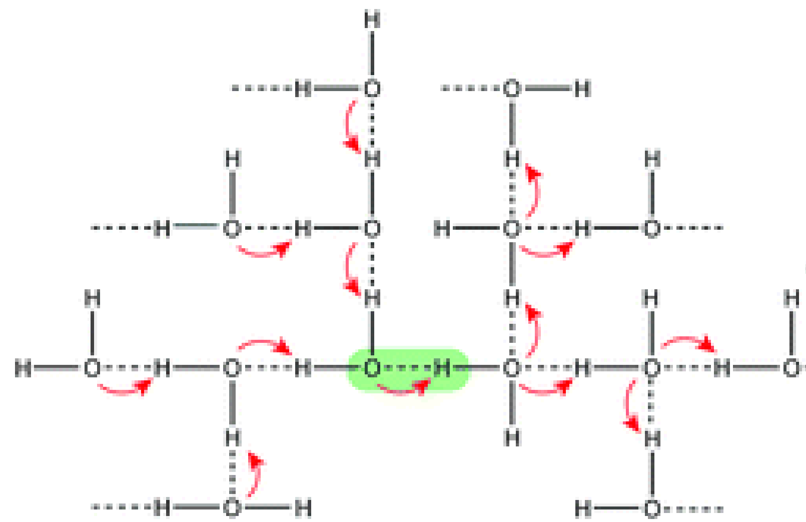


Hydrogen Bond

A hydrogen bond (H-bond) is a primarily electrostatic force of attraction between a hydrogen (H) atom which is covalently bound to a more electronegative atom or group, particularly the second-row elements nitrogen (N), oxygen (O), or fluorine (F)-the hydrogen bond donor (Dn)-and another.



H-bond in water

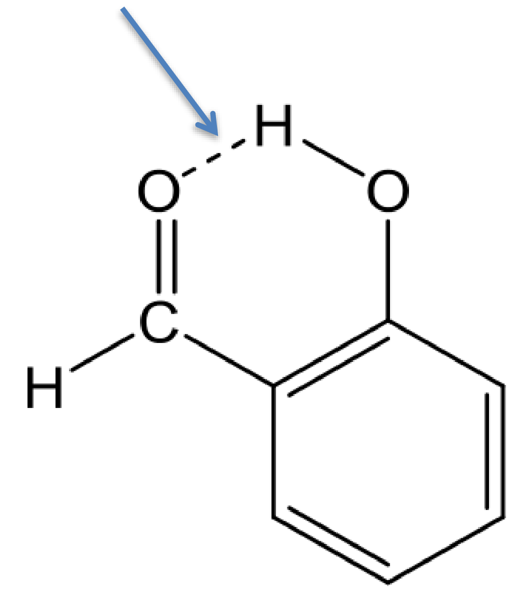


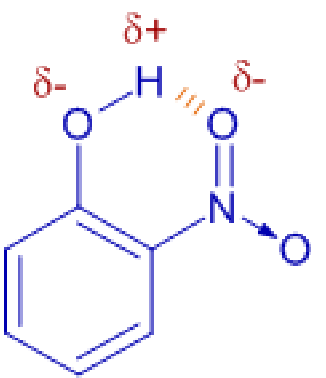
Types of Hydrogen Bonds

(1) Intramolecular hydrogen bond

- ❑Occur within one single molecule
- ❑Occurs when two functional groups of a molecule can form hydrogen bonds with each other
- ❑Both a hydrogen donor and acceptor must be present within one molecule

For example, salicyldehyde between its carbonyl and hydroxyl groups.



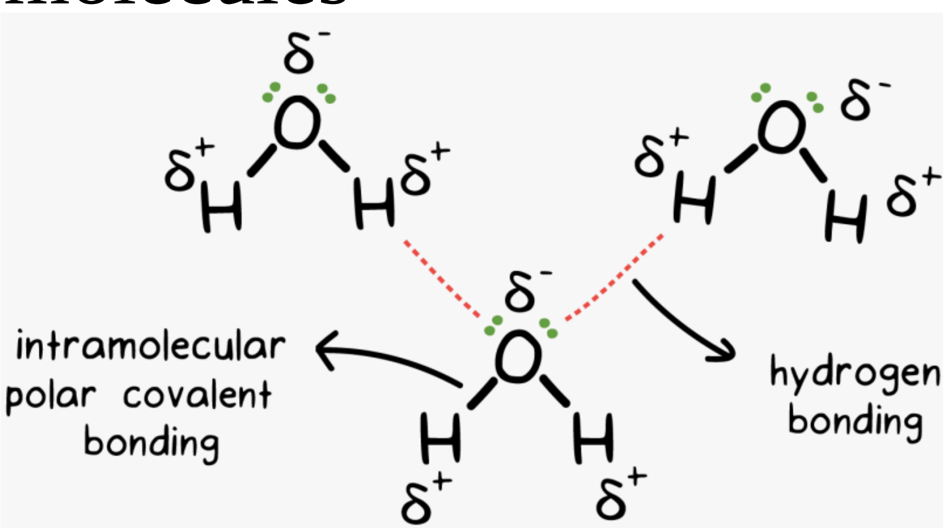


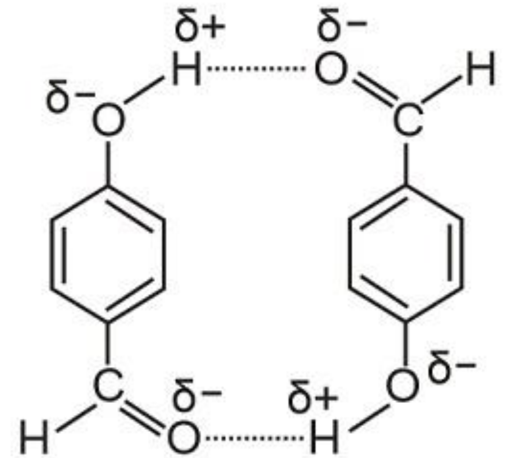
Intramolecular hydrogen bonding in ortho nitrophenol

(2) Intermolecular hydrogen bond

- Occur between separate molecules in a substance
- Occur between any number of like or unlike molecules as long as hydrogen donors and acceptors are present in a positions in which they can interact

For example, between H_2O molecules alone, between NH_3 molecules alone, or between H_2O and NH_3 molecules



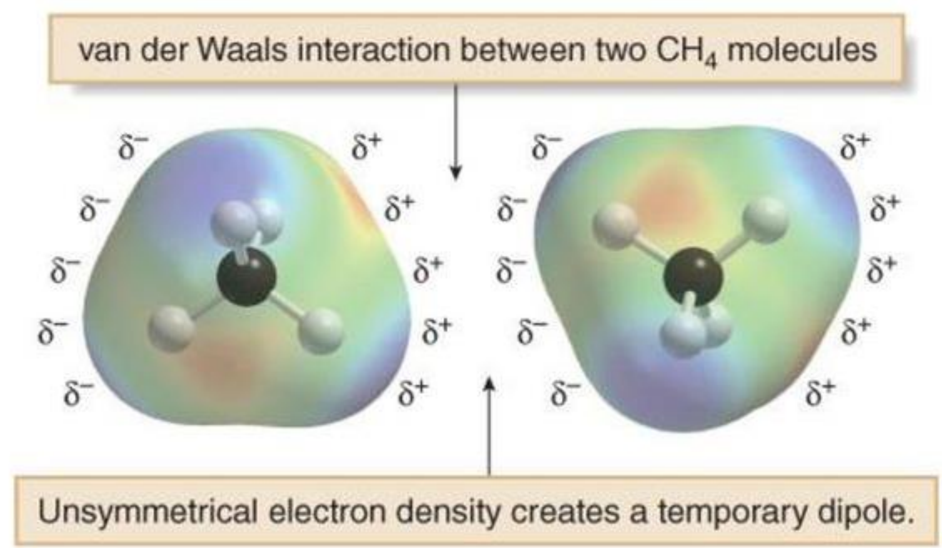


Intermolecular hydrogen bonding in para hydroxy benzaldehyde

Van der Waal's Force

- Van der Waal's forces are also known as London forces
- They are weak interactions caused by momentary changes in electron density in a molecule
- They are the only attractive forces present in nonpolar compounds.

Even though CH_4 has no net dipole, at any one instant its electron density may not be completely symmetrical, resulting in a temporary dipole. This can induce a temporary dipole in another molecule. The weak interaction of these temporary dipoles constitutes van der Waals forces.



Fajans's Rule

The ability of a cation (M^+) to polarize a nearby anion (X^-) is called its polarizing power and the tendency of an anion to get distorted or polarized by a cation is called its polarizability. Factors affecting the magnitude of polarizing power of a cation and polarizability of an anion is suggested by Fajans and is called Fajans's rule.

The factors those affect on the polarizing power of a cation to polarize a nearby anion and the polarisability of an anion are:

(i) Charge on cation or anion

The cation with higher positive charge attracts the electron cloud of the anion more strongly towards itself than the cation with smaller positive charge. For example, in LiCl, $BeCl_2$, BCl_3 and CCl_4 molecules, the polarizing power of Li^+, Be^{2+},B^{3+} and C^{4+} cations to polarize Cl^- anion increases with the increase of positive charge on them. Therefore, $Li^+ < Be^{2+} < B^{3+} < C^{4+}$

On the other hand higher the negative charge on the anion, more strongly it will be polarized by a given anion. For example, in CH_4, NH_3, H_2O and HF molecule, the polarizability of C^{4-}, N^{3-}, O^{2-} and F^- anions to be polarized by H^+ cation decreases from C^{4-} to F^-. Therefore, $C^{4-} > N^{3-} > O^{2-} > F^-$

(ii) **Size of the cation**

The smaller is the size of the cation, higher is the polarizing power to polarize a given nearby anion. For example, $BeCl_2$, $MgCl_2$, $CaCl_2$, $SrCl_2$ and $BaCl_2$ molecules the polarizing power of Be^{2+}, Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} cations to polarize Cl^- anion decreases with the increase of their size. $Be^{2+} > Mg^{2+} > Ca^{2+} > Sr^{2+} > Ba^{2+}$

(iii) **Size of anion**

Larger is the size of anion, more strongly or easily it will be polarized by a given anion.

Halide	MF MCl MBr MI
Halide ions	F^- Cl^- Br^- I^-
Size of halide ions	$1.36 < 1.81 < 1.95 < 2.16$
Polarizability of ions	F- <Cl- <Br- <I-