Pharmaceutical analytical chemistry I

Lecture 3

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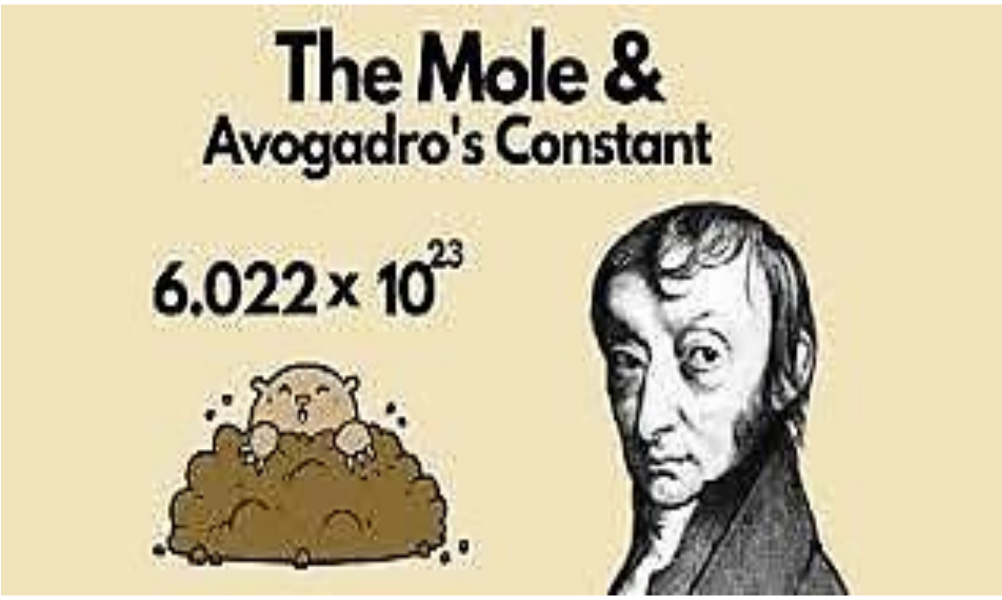


Avogadro's Number and the Molar Mass of an Element

In the SI system the *mole (mol)* is :the amount of a substance that contains as many formula units(atoms, molecules, or other particles) as there are in exactly 12 g (or 0.012 kg) of the carbon-12 isotope.

The actual number of atoms in 12 g of carbon-12 is determined experimentally. This number is called ***Avogadro's number (N_A),***

$$N_A = 6.022 \times 10^{23}$$

✓just as one dozen oranges contains 12 oranges, 1 mole of hydrogen atoms contains 6.022×10^{23} H atoms.

The mole: - 1 mole of carbon-12 atoms has a mass of exactly 12 g and contains 6.022×10^{23} atoms.

- 1 mole of O atoms contains 6.022×10^{23} O atom.
- 1 mole of O_2 molecules contains 6.022×10^{23} O molecules, that is 2 X 6.022×10^{23} O atoms .
- 1 mole of Na^+ contains 6.022×10^{23} Na^+ ions
- 1 mole Na_2CO_3 = 6.022×10^{23} Na_2CO_3 molecules = 2 X 6.022×10^{23} Na^+ ions and 6.022×10^{23} CO_3^{2-} ions.

The molar mass

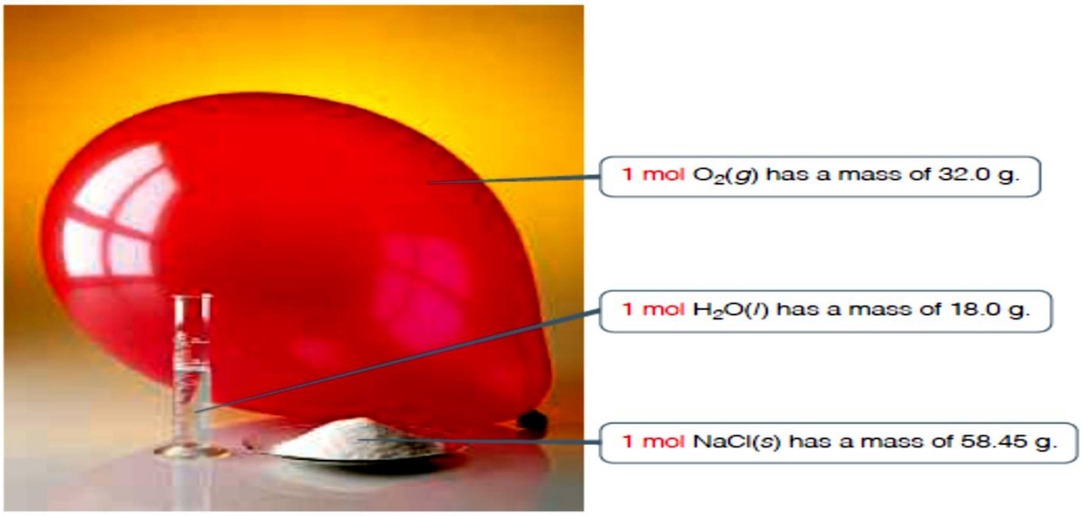
- Molar mass of a substance is **the mass of one mole of the substance.**
- Carbon-12 has molar mass exactly 12g.
- For This reason, molar mass in grams is also called gram formula weight or the gram molecular weight:

✓the atomic mass of sodium (Na) is 22.99 amu and its molar mass is 22.99 g.

✓ the atomic mass of phosphorus is 30.97 amu and its molar mass is 30.97 g; and so on.

An element's molar mass in grams per mole is numerically equal to the element's atomic mass in atomic mass units.

➢If we know the atomic mass of an element, we also know its molar mass.



▲ **One mole each of a solid (NaCl), a liquid (H_2O), and a gas (O_2).** In each case, the mass in grams of 1 mol—that is, the molar mass—is numerically equal to the formula weight in atomic mass units. Each of these samples contains 6.02×10^{23} formula units.

If you knew the molar mass and Avogadro's number

- we can calculate the mass of a single atom in grams.

- For example, we know the molar mass of carbon-12 (C^{12}) is 12.00 g and there are 6.022×10^{23} C^{12} atoms in 1 mole of the substance; therefore, the mass of one C^{12} atom is given by:

$$\frac{12.00\ g C^{12} atoms}{6.022 x\ 10^{23} C^{12}} = 1.993 \times 10^{-23}\ g$$

- Homework: Calculate the number of copper atoms in 2.45 mol of copper.

How to calculate the number of moles (n)

- $n = \frac{N}{N_A}$

n= number of moles.
N= number of molecules, ions or atoms.
N_A= Avagadro's number (6.022×10^{23})

or

- $n= \frac{m}{M.wt}$

n= number of moles.
m= mass in grams.
M.wt= molecular weight.

- We now have all the tools to count the number of atoms in a sample of an element by weighing it:
- First, we obtain the mass of the sample.
- Second, we convert it to an amount in moles using the element’s molar mass.
- Finally, we convert it to number of atoms using Avogadro’s number.

Example 1: **How many copper atoms are in a copper piece with a mass of 3.10 g? knowing that molar mass of copper is 63.55 gm**

Answer:

63.55 g Cu = 1 mol Cu (molar mass of copper)

6.022×10^{23} = 1 mol (Avogadro’s number)

$$\frac{3.10\ g\ Cu}{63.55\ g\ Cu} \times \frac{6.022 \times 10^{23}}{1\ mol\ Cu} = 2.94 \times 10^{22}\ Cu\ atoms$$

Example 2: How many gm of Cu in 2.55 mole of Cu ?

1mole of Cu has a mass of 63.5 g

1mole of Cu contains 63.5 g

(n = mass/ M.Wt)

2.55 mole contains x g

x = 63.5g x 2.55 mole / 1 mole = 162 g Cu

Example 3: How many mole of Al is present in 125 g of Al ?

1mole of Al has a mass of 27.0 g

(n = mass/ M.Wt)

X mole ? of Al contains 125 g

x = 1mole x 125 g / 27 = 4.63 mole Al

Percent Composition of Compounds

- The formula of a compound tells us the numbers of atoms of each element in a unit of the compound.
- The ***percent composition by mass*** is the *percent by mass of each element in a compound:*

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

- Calculate the percent composition by mass of H, P, and O in phosphoric acid H_3PO_4 .[The molar mass of H_3PO_4 is 97.99 g]

- Solution:

- The percent by mass of each of the elements in H_3PO_4 is calculated as follows:

$$\%H = \frac{3(1.008\ g)\ H}{97.99\ g\ H_3PO_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\ g\ P}{97.99\ g\ H_3PO_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\ g)\ O}{97.99\ g\ H_3PO_4} \times 100\% = 65.31\%$$

- Homework: If the molar masses of H_2O_2, H, and O are 34.02 g, 1.008 g, and 16.00 g respectively. Calculate percent composition by mass of H and O

Stoichiometry

The quantitative relationships between reactants and products in a balanced equation are known as stoichiometry.

The chemical equation for the combustion of ethanol, C_2H_5OH

$$C_2H_5OH + 3\,O_2 \rightarrow 2CO_2 + 3H_2O$$

Tells us that 1 mole C_2H_5OH + 3 mole O_2 → 2mole CO_2 + 3 mole H_2O

In this example, we can write six equivalencies

1 mole C_2H_5OH ~ 3 mole O_2.

1 mole C_2H_5OH ~ 2 mole CO_2.

1mole C_2H_5OH ~ 3 mole H_2O.

3 mole O_2 ~ 2 mole CO_2.

3 mole O_2 ~ 3 mole H_2O.

2 mole CO_2 ~ 3 mole H_2O.

balanced equation provides quantitative relationship among reactants and products.

Stoichiometry

- a) How many moles of O_2 are needed to burn 1.8 mole C_2H_5OH?
- b) How many moles of water will form when 3.66 mole CO_2 are produced during the combustion of C_2H_5OH?

Solution:

$$C_2H_5OH \quad + \quad 3\,O_2 \rightarrow \quad 2CO_2 + 3H_2O$$

a) 1 mole C_2H_5OH ~ 3 mole O_2

1 mole C_2H_5OH needs 3 mole O_2

1.8 mole C_2H_5OH x ? mole O_2

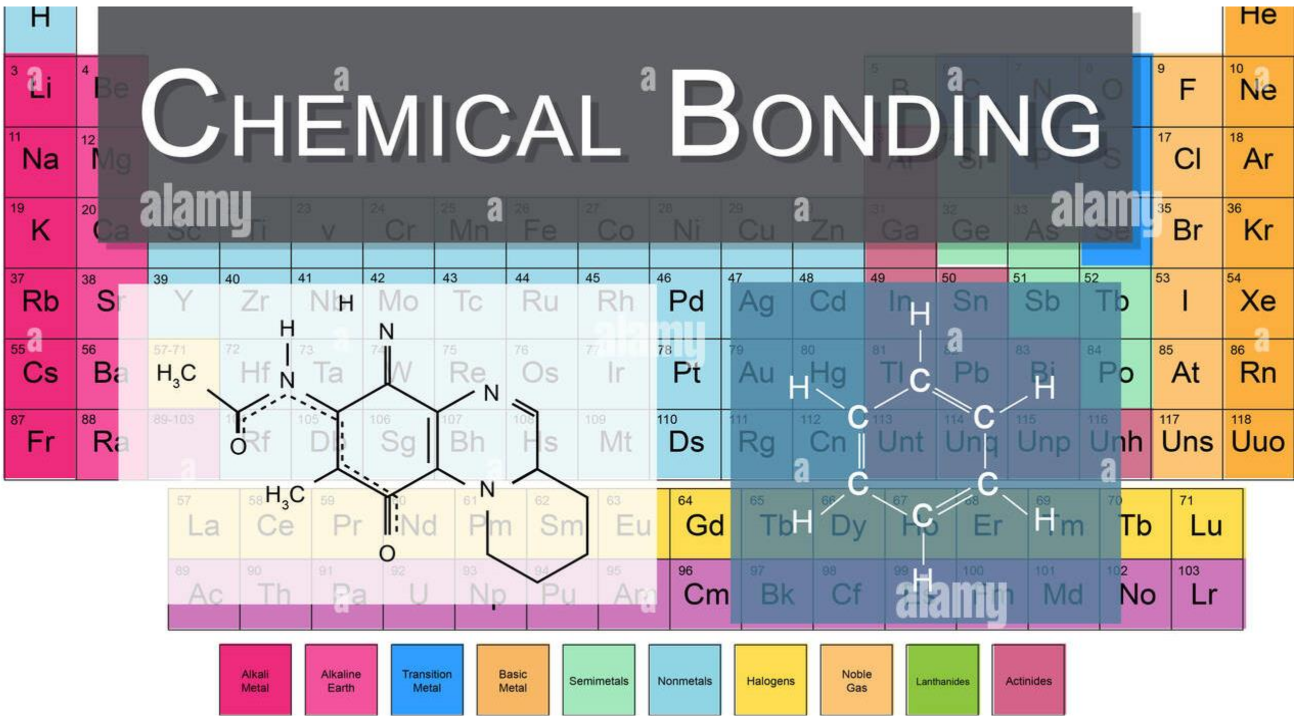
O_2 needed for combustion = 1.8 x 3 /1 = 5.4 mole O_2

b) 2 mole CO_2 ~ 3 mole H_2O

2 mole CO_2 is produced with 3 mole H_2O

3.66 mole CO_2 is produced with x ? mole H_2O

H_2O mole formed = 3.66 x 3 /2 = 5.49 mole H_2O



Chemical bonds

- Bonds are forces that hold groups of atoms together and make them function as a unit.
- Most chemical bonds into two types: ionic and covalent.

- *Ionic bonds*—which occur between metals and nonmetals and involve the *transfer* of electrons from one atom to another.

- *Covalent bonds*—which occur between two or more nonmetals and involve the *sharing* of electrons between two atoms.

Remember that:
-charged particles show electrostatic forces on one another: like charges repel and opposite charges attract. These forces are responsible for chemical bonding.

Why do elements tend to form bonds?

✓ **Molecules are formed because each atom is trying to attain a stable electron configuration (Nobel gas configuration).**

- **The Octet Rule:**

✓ **"Any atom other than hydrogen tends to form bonds until it is surrounded by eight valence electrons".**

1- Ionic bond

when a metal interacts with a nonmetal

it can transfer one or more of its electrons to the nonmetal.

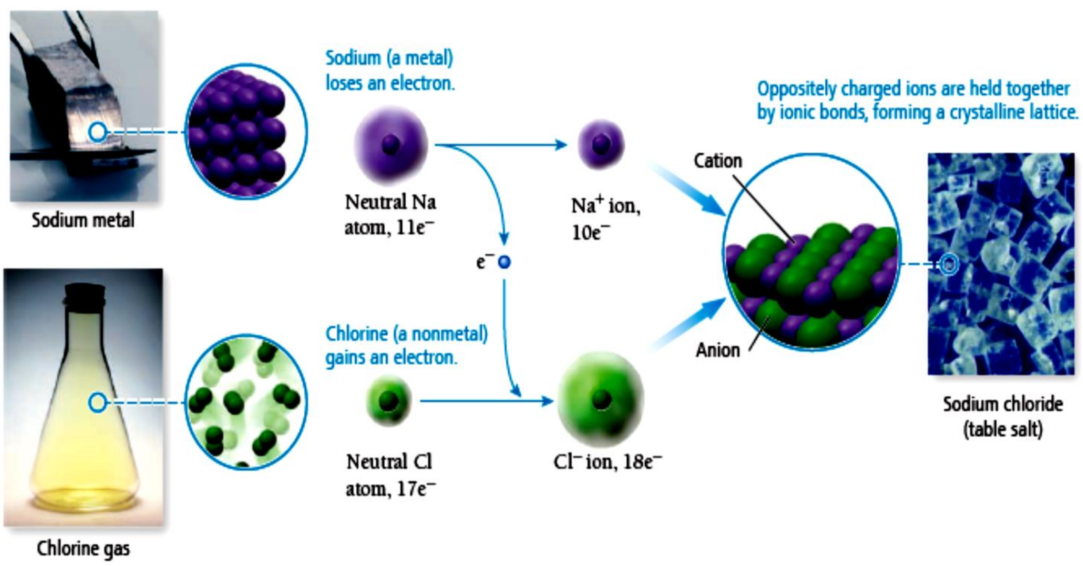
The metal atom then becomes a *cation* (a positively charged ion)

The nonmetal atom becomes an anion (a negatively charged ion),

These oppositely charged ions **attract** one another by electrostatic forces and form an **ionic bond**.

The result is an **ionic compound**,

The Formation of an Ionic Compound



2- covalent bond

When a nonmetal bonds with another nonmetal

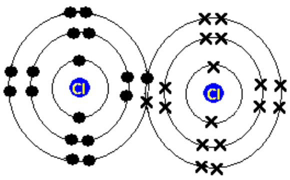
neither atom transfers its electron to the other.

Instead the bonding atoms ***share*** some of their electrons.

The bond is a **covalent bond**, and the covalently bound atoms compose a molecule. Each molecule is independent of the others, the molecules are themselves not covalently bound to one another. Therefore, we call covalently bonded compounds **molecular compounds.**

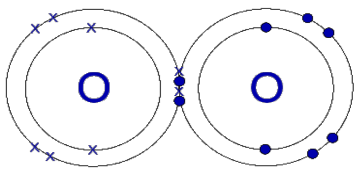
Types of covalent bonds

a) Single covalent bond



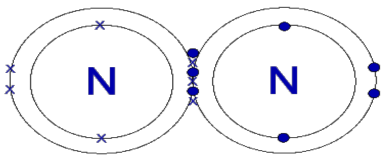
if two electrons are shared (that is, there is one bond) e.g. Cl_2 molecule.

b) Double covalent bond

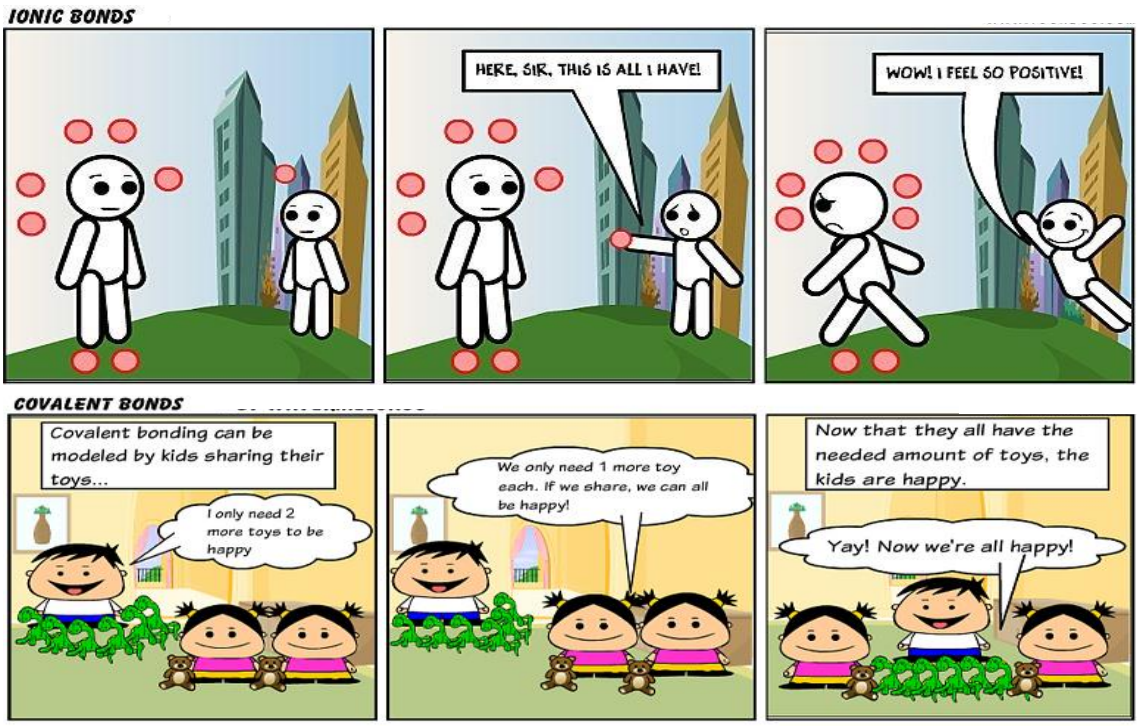


if four electrons are shared (that is there are two bonds e.g. O_2 molecule.

c) Triple covalent bond



if six electrons are shared (that is there are three bonds) e.g. N_2 and acetylene molecule

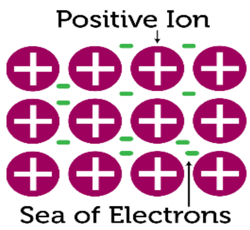


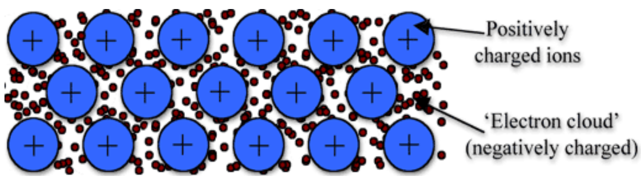
3- Metallic bond

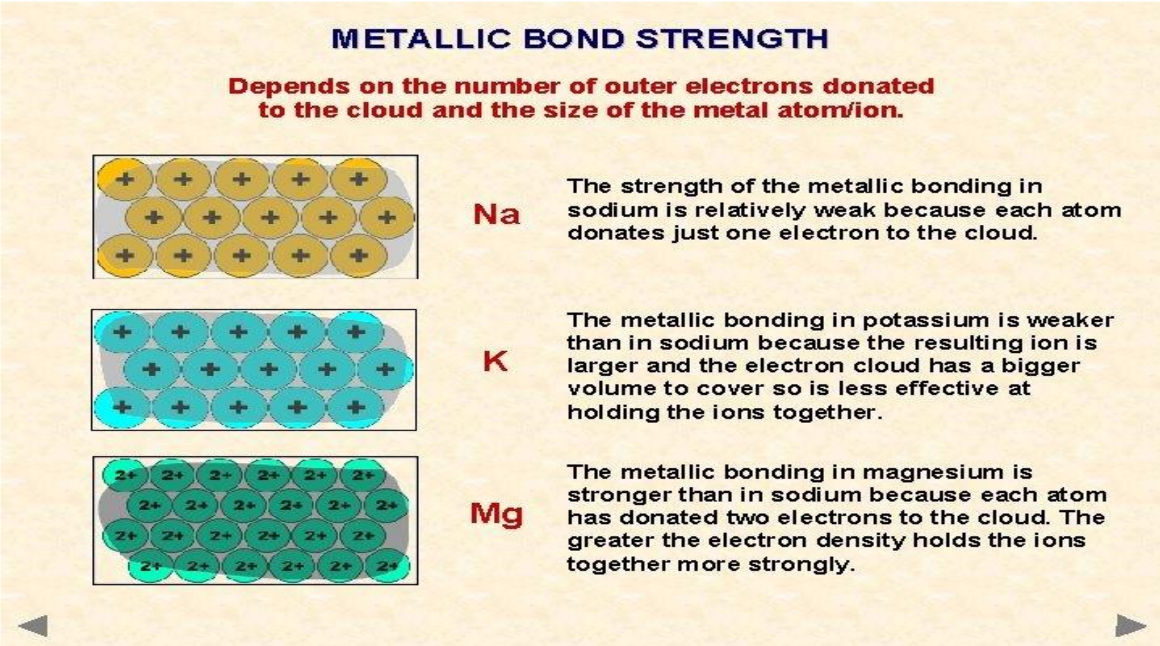
- **Metallic bonds occur among metal atoms. Metallic bonding joins a bulk of metal atoms (same or different metals).**

❑How is metallic bond formed?

❑Formation of metallic bond: When metallic bonds form, the S and p electrons delocalize, they form a "sea of electrons" surrounding the positive metal ions.







- The delocalized nature of the electrons explains a number of unique characteristics of metals:

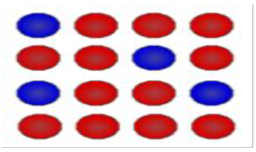
1. Metals are good conductors of electricity

2. Metals have very high melting and boiling points (Metallic bonding is very strong).

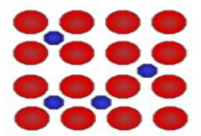
How is alloy formed?

Metallic bonds can occur between different elements.
A mixture of two or more metals is called an alloy. سبيكة

Depending on the size of the atoms being mixed, there are two different kinds of alloys that can form:



1. Substitutional alloy



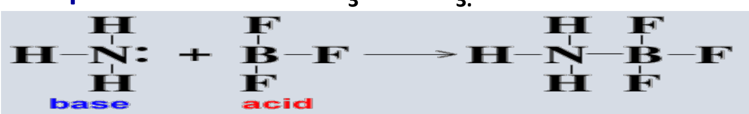
2. Interstitial alloy

The resulting mixture will have a combination of the properties of both metals involved.

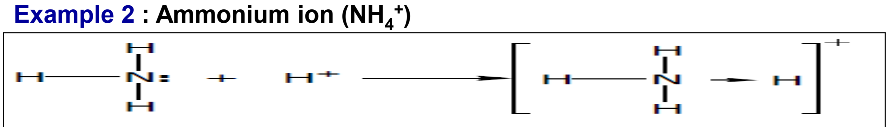
4- Coordinate bond

- **sharing of lone pair of electrons from one atom called donor (Lewis base) to another atom called acceptor (Lewis acid).**
- **Lewis acid: electron pair acceptor e.g. H^+, $AlCl_3$, $FeBr_3$, BF_3.**
- **Lewis base: electron pair donor e.g. compounds containing heteroatoms (O, S, N) e.g. NH_3, H_2O**

Example 1: reaction of NH_3 and BF_3.



Example 2 : Ammonium ion (NH_4^+)



Coordinate bond: is a sharing of lone pair of electrons from one atom called donor (Lewis base) to another atom called acceptor (Lewis acid).

Lewis acid: electron pair acceptor e.g. H^+, $AlCl_3$, $FeBr_3$, BF_3.

- Lewis base: electron pair donor e.g. compounds containing heteroatoms (O, S, N) e.g. NH_3, H_2O

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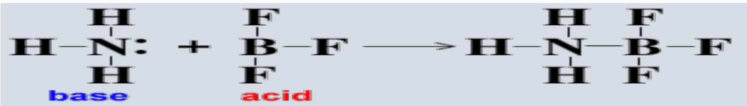

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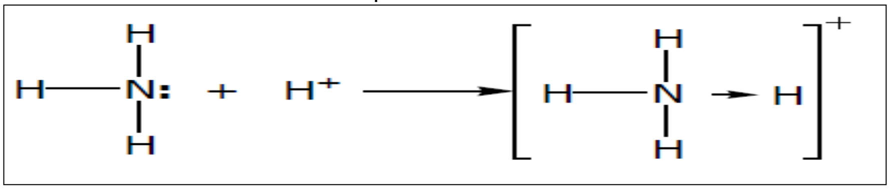
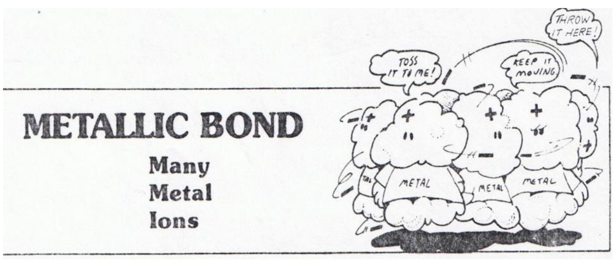


Co-ordinate covalent bond



- **Metallic bonds** occur when valence electrons drift from one metal atom to another. These **"delocalized"** electrons therefore do not belong to any particular metal atom but instead can be thought of as belonging to all the metal atoms.

Types of Intramolecular Bonds

Ionic Bond	Covalent Bond	Metallic Bond	Coordinate Bond
Formed between electropositive element (metal) and electronegative element (nonmetal) e.g. Na Cl, $CaCl_2$ $CaCl_2$	Formed between electronegative element and electronegative one e.g. Cl_2 H_2	Formed between two electro-positive elements (Two metals) e.g. Fe, Mg.	Bonds between electron rich molecules and electron deficient molecules between NH_3 with H^+ to form NH_4^+