Chemical Bonds

Chemical bond is an attraction between atoms or molecules and allows the formation of chemical compounds, which contain two or more atoms. A bond is a link that binds 2 or more atoms of elements together, to make a compound.

The strength of bonds varies considerably;
Two classes of bonds are identified in Biological Sciences:
- **Covalent bonds**
- **Non-covalent bonds**
    - **H-bonds**
    - **Ionic**
    - **Van der Waals forces**
    - **Hydrophobic**

Bonding

Two groups of bonds:

Primary Bonds----Covalent

- **Primary bonds consist of three types of bonds: ionic, covalent and metallic**

Secondary Bonds----- Non-covalent

- **Secondary bonds are weak bonds existing in many substances e.g. water and almost all biomolecules: e.g. H-bond, hydrophobic bond; Van der Waals forces; ionic bond.**

Valence

- The highest occupied electron shell is called the **valence shell**, and the electrons occupying this shell are called **valence electrons**.
- The number of valence shell electrons an atom must gain or lose to achieve a valence octet is called **valence.** In covalent compounds the number of bonds which are characteristically formed by a given atom is equal to that atom's valence , the following general valence assignments have been documented for the elements:

Atom	H	C	N	O	F	Cl	Br	I
Valence	1	4	3	2	1	1	1	1

1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A
								H 2.1								
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2

<1.0 | 1.5–1.9 | 2.5–2.9
1.0–1.4 | 2.0–2.4 | 3.0–4.0

Figure 9.9 Electronegativity values for the elements according to Pauling. Trends for electronegativities are the opposite of the trends defining metallic character. Nonmetals have high values of electronegativity, the metalloids have intermediate values, and the metals have low values.

Electronegativity Difference

- If the difference in electronegativities is between:
  - 1.7 to 4.0: Ionic
  - 0.3 to 1.7: Polar Covalent
  - 0.0 to 0.3: Non-Polar Covalent

Example: NaCl
Na = 0.8, Cl = 3.0
Difference is 2.2, so this is an ionic bond!

1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A
								H 2.1								
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2

<1.0 1.5–1.9 2.5–2.9
1.0–1.4 2.0–2.4 3.0–4.0

Figure 9.9 Electronegativity values for the elements according to Pauling. Trends for electronegativities are the opposite of the trends defining metallic character. Nonmetals have high values of electronegativity, the metalloids have intermediate values, and the metals have low values.

Electronegativity

- The ability of an element to attract or hold onto electrons is called **electronegativity**

Because of their differing nuclear charges, and as a result of shielding by inner electron

Electronegativity Values for Some Elements

H 2.20						
Li 0.98	**Be** 1.57	**B** 2.04	**C** 2.55	**N** 3.04	**O** 3.44	**F** 3.98
Na 0.90	**Mg** 1.31	**Al** 1.61	**Si** 1.90	**P** 2.19	**S** 2.58	**Cl** 3.16
K 0.82	**Ca** 1.00	**Ga** 1.81	**Ge** 2.01	**As** 2.18	**Se** 2.55	**Br** 2.96

Electronegativity

Electronegativity is the tendency of an atom to attract electrons.

If the electronegativity of an atom is high, then it attracts and holds on to electrons.

If the electronegativity of an atom is low, then it tends to give electrons away.

Ionic Bonds

Ions and Ionic Bonds

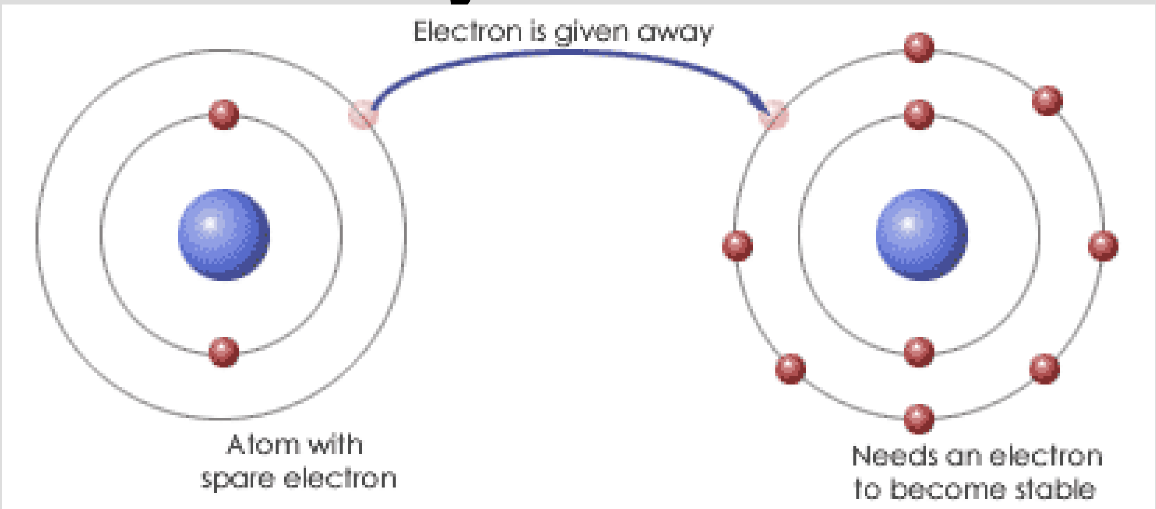
- Ion = a charged atom (can be + or -)

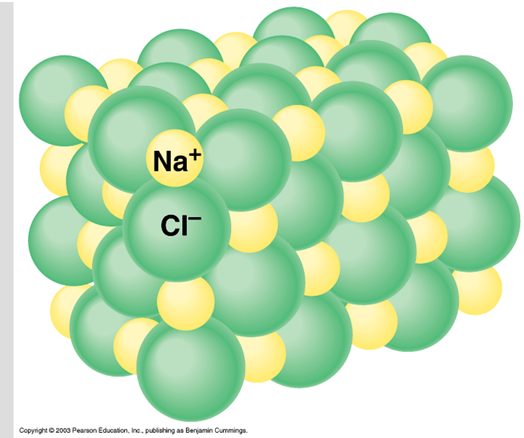
- Ionic bonds are fairly weak, and are formed by the attraction between a positively charged atom and a negatively charged atom.
- Example: NaCl

Ionic Bonding

- **<u>The Ionic Bond:</u>** Ionic bonds are formed when there is a complete transfer of electrons from one atom to another, resulting in two ions, one positively charged and the other negatively charged.
- For example, when a sodium atom (Na) donates the one electron in its outer valence shell to a chlorine (Cl) atom, which needs one electron to fill its outer valence shell, NaCl (table salt) results.
- Ionic bonds are often 4-7 kcal/mol in strength.

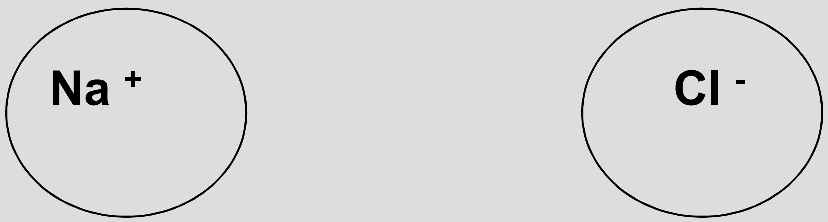
- Many metals have to gain several electrons to fill their outer shell and therefore find it easier to loose their electrons.
- In ionic bonding a metal gives an electron to an atom which needs extra electrons. This causes both atoms to be charged. One has a positive charge (it has more protons than electrons) and the other a negative charge.
- This causes an attraction between the atoms. Materials bonded this way are usually brittle with poor electrical conductivity.





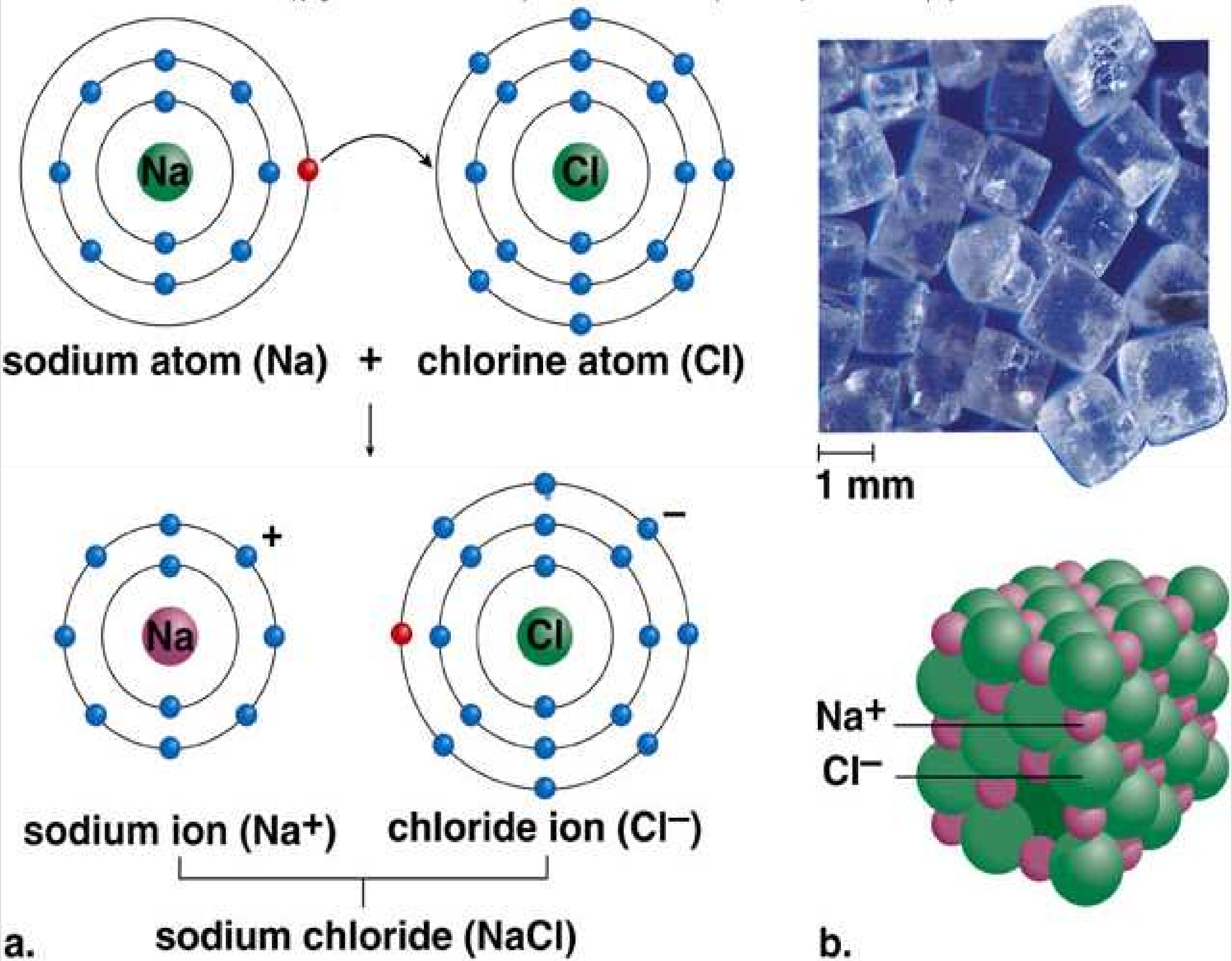
Ionic bonding

The sodium ion and the chloride ion will be attracted to each other and form an ionic bond.



The ionic bond is due to the attractive forces between the positively charged sodium & the negatively charged chloride.

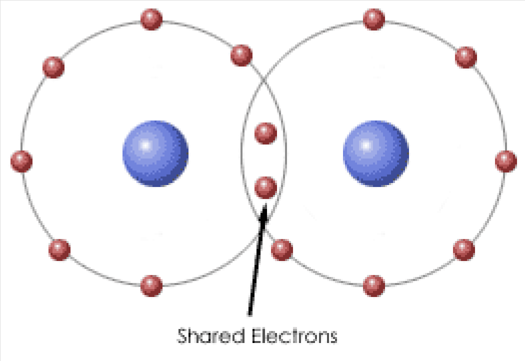
By looking at the periodic table, can you predict which atoms may form ionic bonds?


Na
Cl
sodium atom (Na) + chlorine atom (Cl)
Na
Cl
+
−
sodium ion (Na+)
chloride ion (Cl−)
sodium chloride (NaCl)
a.
1 mm
Na+
Cl−
b.

Therefore, ionic compounds are usually between metals and nonmetals (opposite ends of the periodic table).

The Covalent Bond

- **Covalent Bonds are the strongest chemical bonds,**
- **formed by the sharing of a pair of electrons.**
- **The energy of a typical single covalent bond is ~80 kilocalories per mole (kcal/mol). However, this bond energy can vary from ~50 kcal/mol to ~110 kcal/mol depending on the elements involved.**
- **Once formed, covalent bonds rarely break spontaneously.**



Covalent bonds are strong.

2 atoms share one or more electrons

Covalent Bonds

- Covalent bond may be formed between different elements. (Usually between non- metals).
- Shared electron pairs

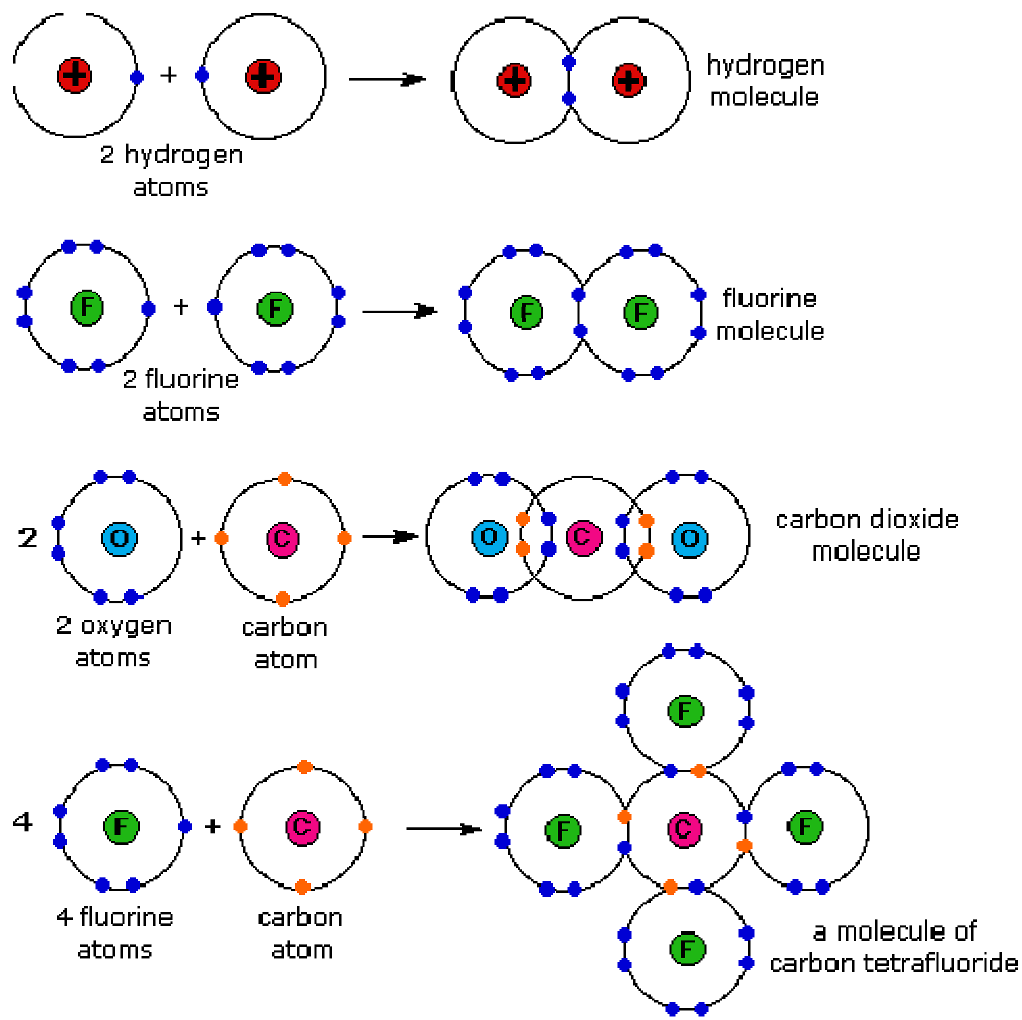
  Exs: CH4 , H2O
- Possible to have single bonds, double bonds, even triple bonds
- Exs: H-H (single bond); O=O or O=C=O (double bond); N N (triple bond)
- Number of bonds depends on valence

Double & Triple Covalent Bonds

- **Double covalent bonds share two pairs of electrons.**
  - **CO_2 O=C=O**
- **Triple covalent bonds share three pairs of electrons.**
  - **N_2 :N≡N:**

Covalent bonding occurs by a sharing of valence electrons

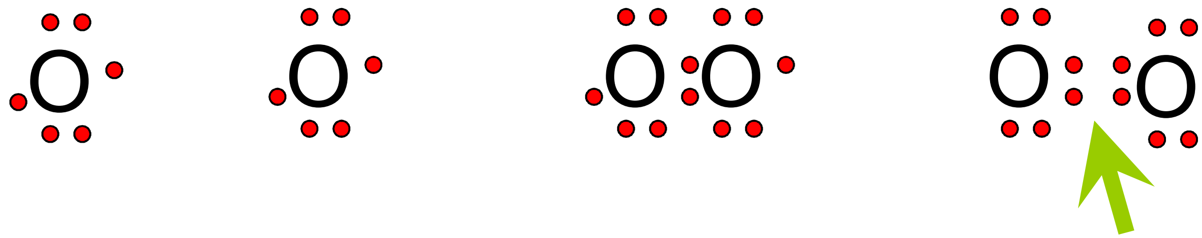
- **Examples of covalent bonding**



More sharing examples

O_2

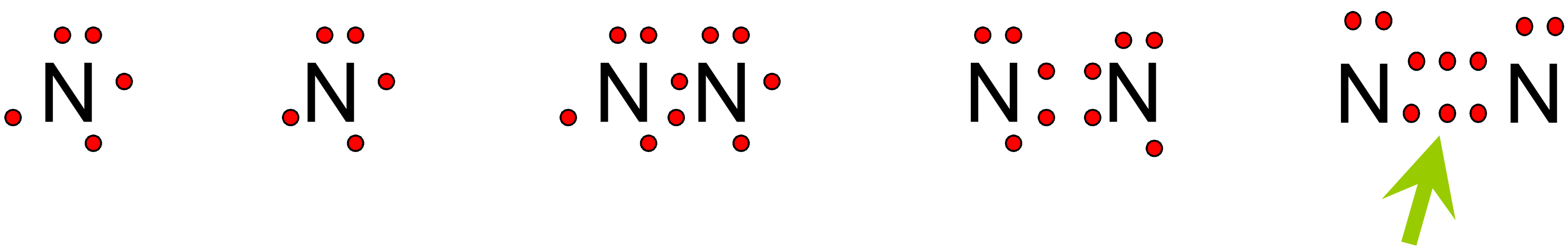
Share until octet is complete.



double bond (2 pairs)

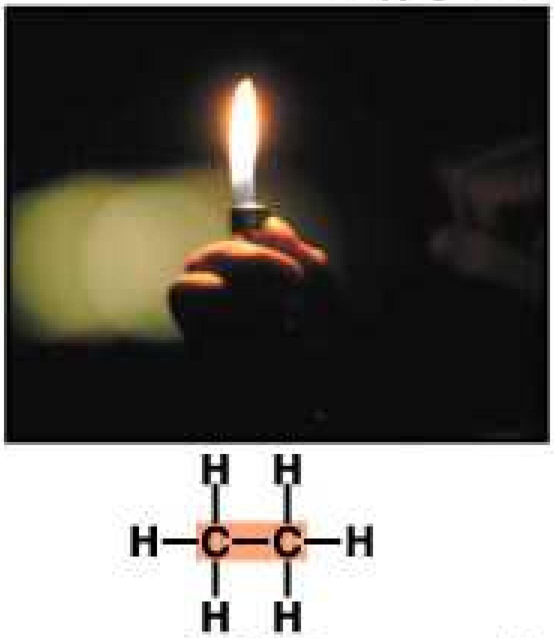
N_2

octet complete



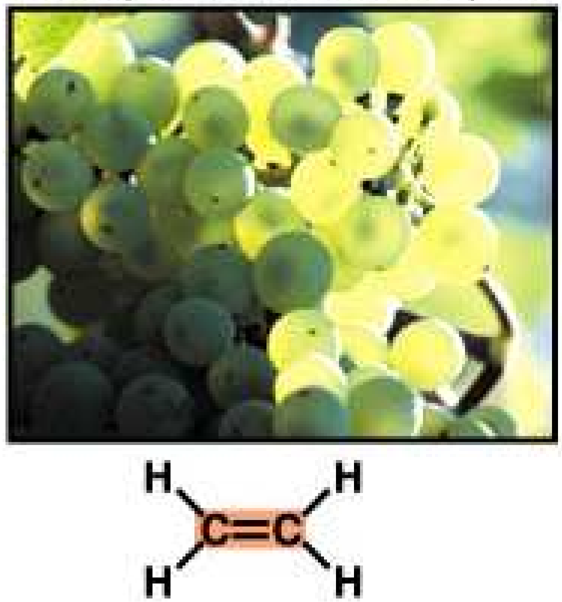
triple bond (3 pairs)

Carbon forms covalent bonds



Ethane

A

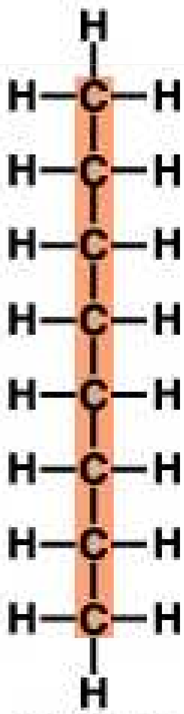


Ethylene

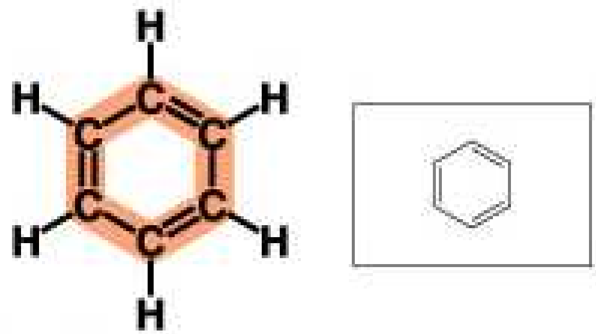
B

Acetylene

C



D Octane

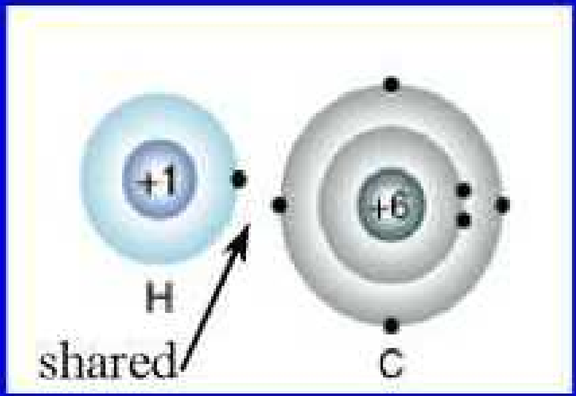


E Benzene

Other examples

C-H covalent bond

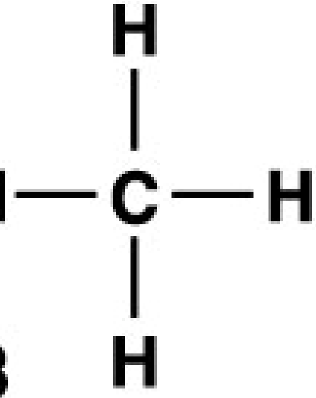
- H has one outer electron needs one
  - H_2 has 1 single covalent bond
- C has four outer electrons
  - C forms four covalent bonds
  - CH_4 sharing one electron pair with each H



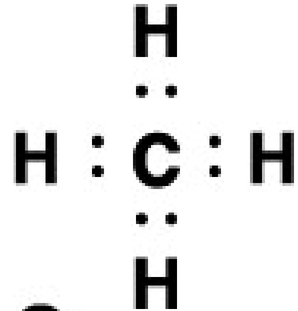
Ways to represent molecules

CH_4

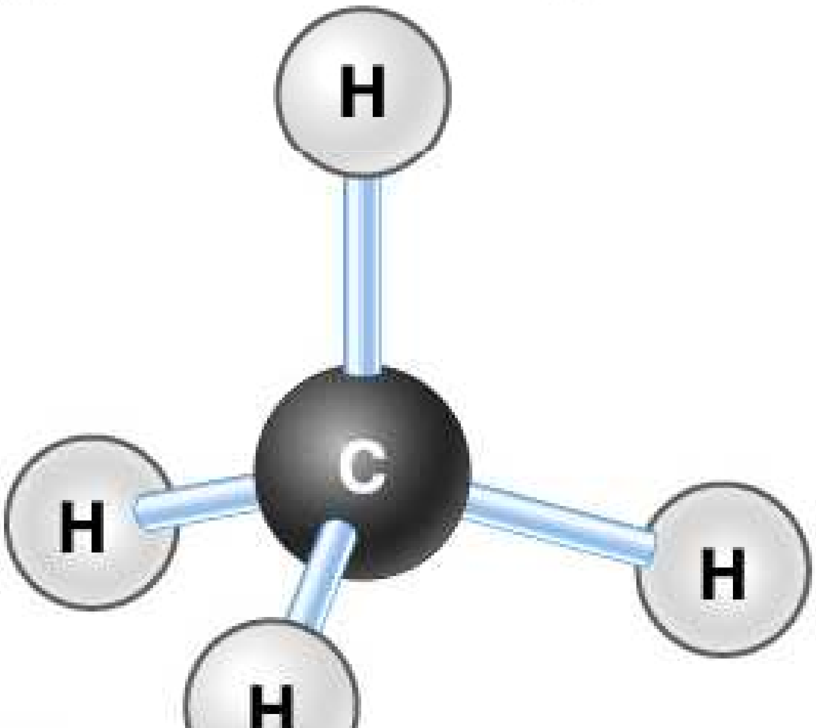
A



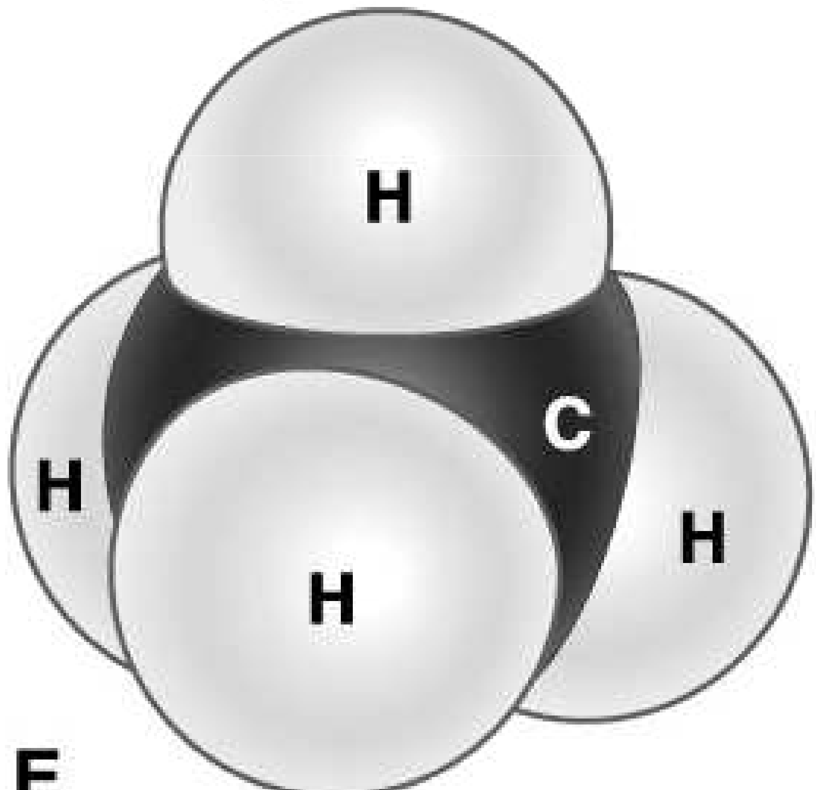
B



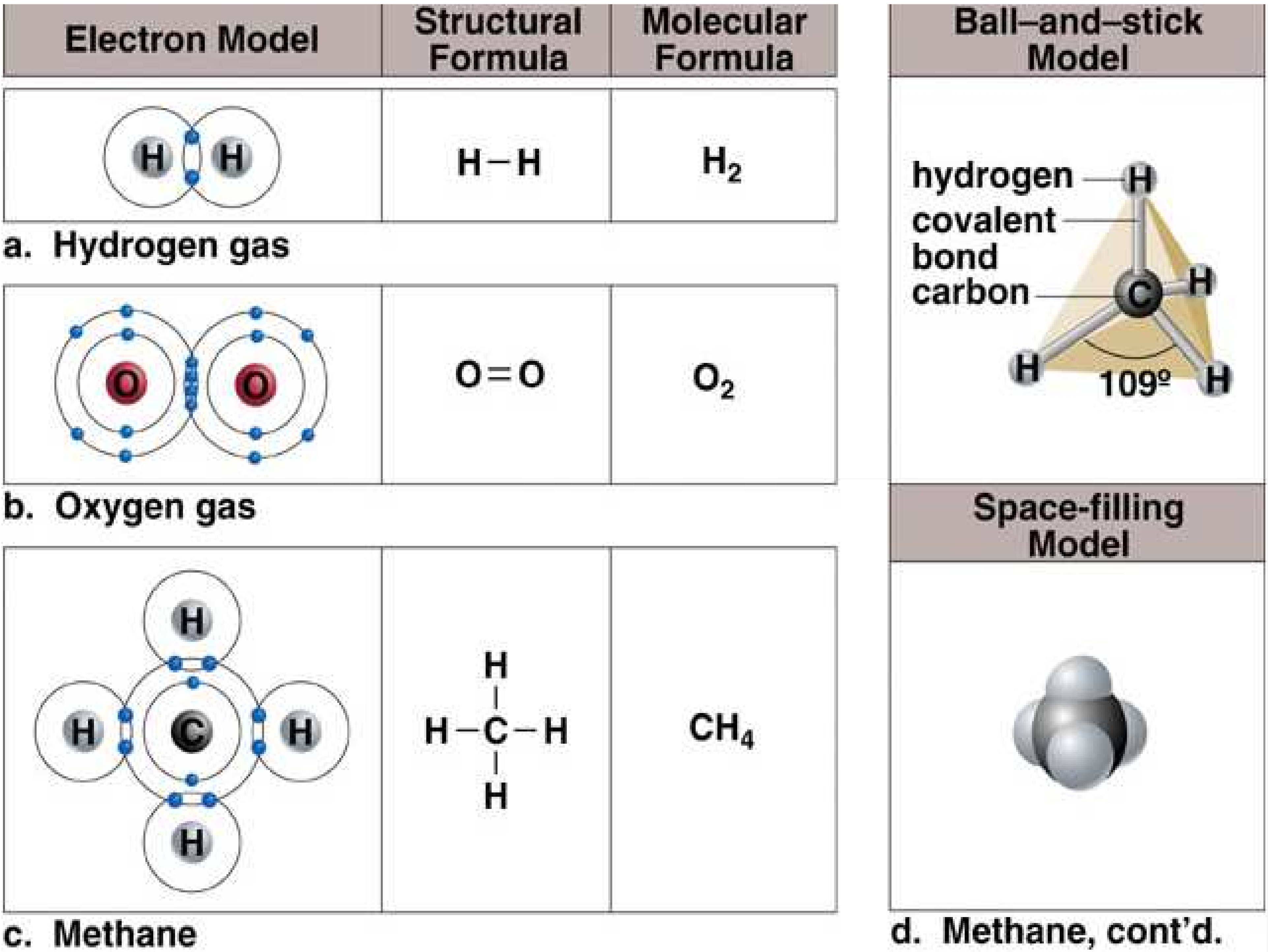
C



D

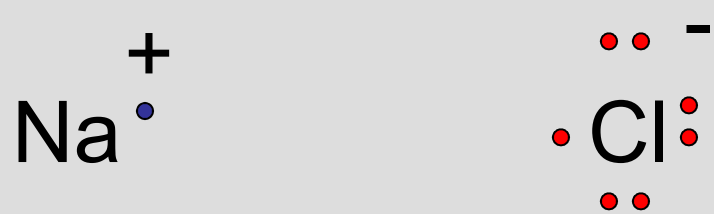


E


Electron Model
Structural Formula
Molecular Formula
H
H
H – H
H2
a. Hydrogen gas
O
O
O = O
O2
b. Oxygen gas
H
H
C
H
H
H
H – C – H
H
CH4
c. Methane
Ball–and–stick Model
hydrogen
covalent bond
carbon
H
C
H
H
H
109º
Space-filling Model
d. Methane, cont'd.

Comparison between ionic and covalent bonds

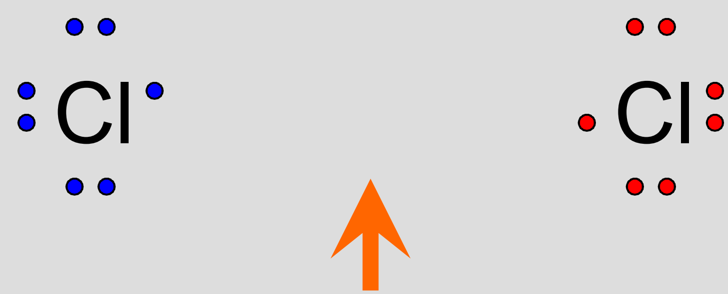
NaCl This is the formation of an ionic bond.



electron transfer

and the formation of ions

Cl_2 This is the formation of a covalent bond.



sharing of a pair of electrons

and the formation of molecules

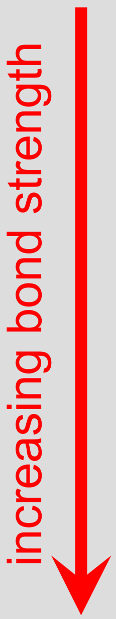
Bond Energy: energy required to form the bond or energy released when the bond is broken

X_2 + energy → X + X

F_2 single bond BE = 142 kJ/mole

O_2 double bond BE = 494

N_2 triple bond BE = 942



Types of Covalent

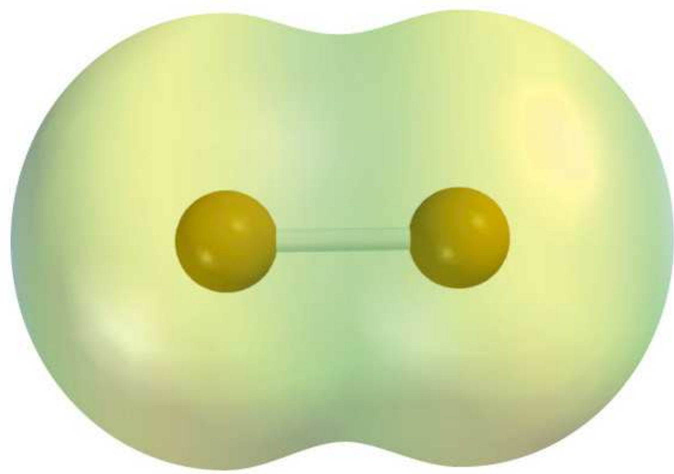
- **Non-Polar:** both atoms share electrons equally
- **Polar:** one atom has a stronger pull on the electron

Non-polar Covalent bond

- **Non-polar covalent bonds are formed:**
  - **When the sharing atoms have the same electronegativity**
  - **So the electrons are shared equally**
  - **Electron cloud is not displaced**

Cl:Cl

A nonpolar covalent bond

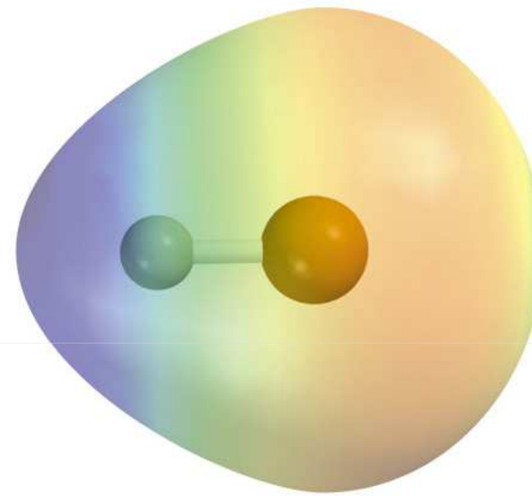


$^{\delta+}H — Cl^{\delta-}$

[H :Cl]

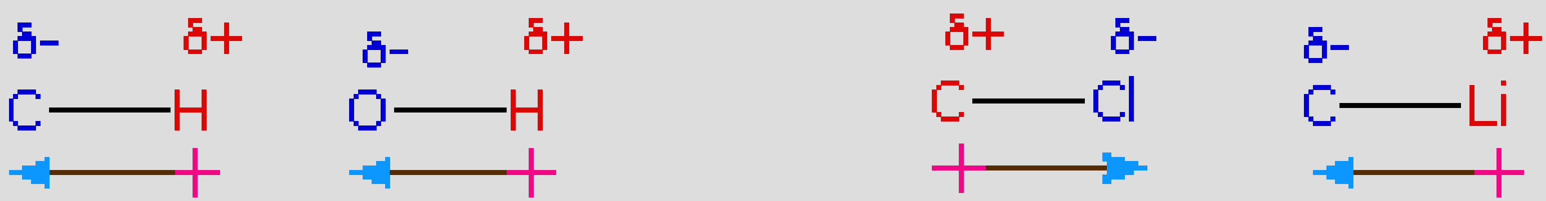
A polar covalent bond.

The bonding electrons are attracted more strongly by Cl than by H.



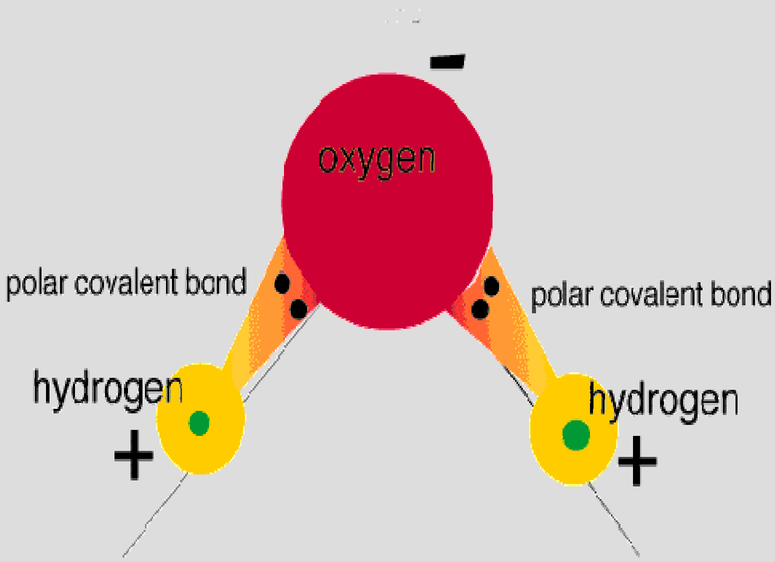
Polar covalent bonds

- When two different atoms are bonded covalently, the shared electrons are attracted to the more electronegative atom of the bond, resulting in a shift of electron density toward the more electronegative atom.
- Such a covalent bond is **polar**, and will have a **dipole** (one end is positive and the other end negative).
- The degree of polarity and the magnitude of the bond dipole will be proportional to the difference in electronegativity of the bonded atoms.
  - Thus a O–H bond is more polar than a C–H bond, with the hydrogen atom of the former being more positive than the hydrogen bonded to carbon.
  - Likewise, C–Cl and C–Li bonds are both polar, but the carbon end is positive in the former and negative in the latter.
- The dipolar nature of these bonds is often indicated by a partial charge notation (δ+/–) or by an arrow pointing to the negative end of the bond.
- Although there is a small electronegativity difference between carbon and hydrogen, the C–H bond is regarded as weakly polar at best, and hydrocarbons in general are considered to be non-polar compounds.

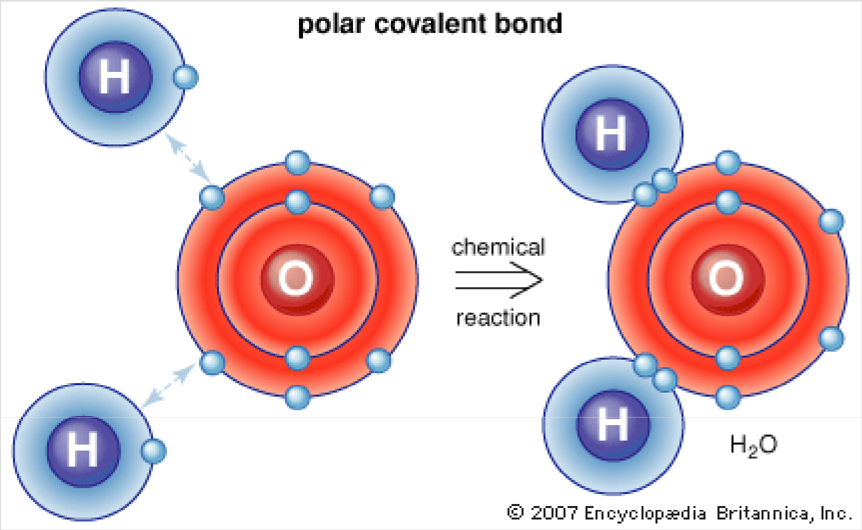


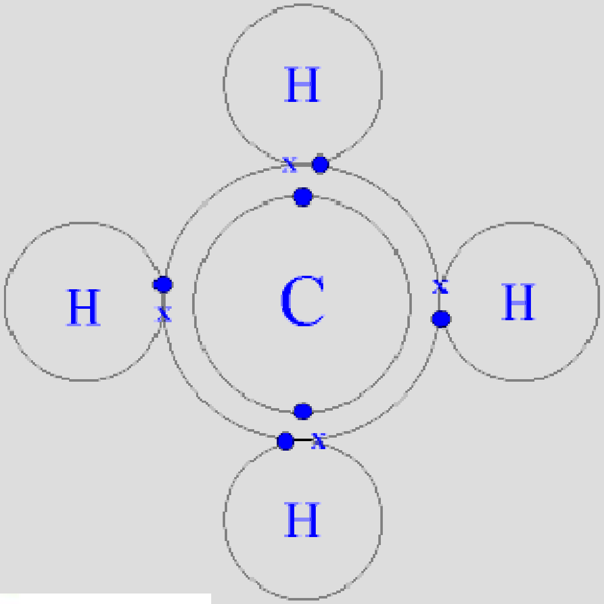
Polar Covalent Bonds

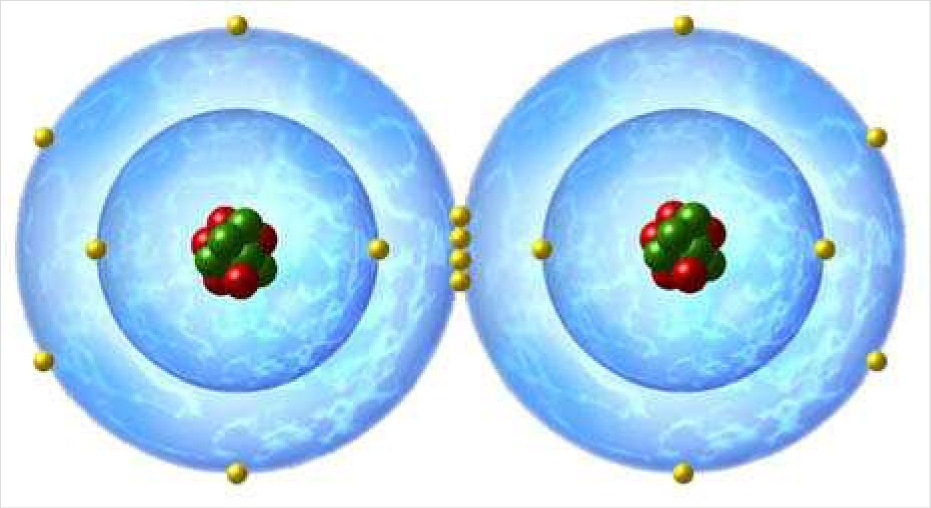
- Polar covalent bonds are a particular type of covalent.
- In a polar covalent bond, the electrons shared by the atoms spend a greater amount of time, on the average, closer to the Oxygen nucleus than the Hydrogen nucleus. This is because of the geometry of the molecule and the great electronegativity difference between the Hydrogen atom and the Oxygen atom.
- The result of this pattern of unequal electron association is a charge separation in the molecule, where one part of the molecule, the Oxygen, has a parital negative charge and the Hydrogens have a partial positive charge.
- Tis molecule is not an ion because there is no excess of proton or electrons, but there is a simple charge separation in this electrically neutral molecule.
- Water is not the only molecule that can have polor covalent bonds. Examples of other molecules that have polar covalent bonds are Peptide bonds and amines .
- The biological consequence of polar covalent bonds is that these kinds of bonds can lead to the formation of a weak bond called a Hydrogen bond.



Covalent Bonds

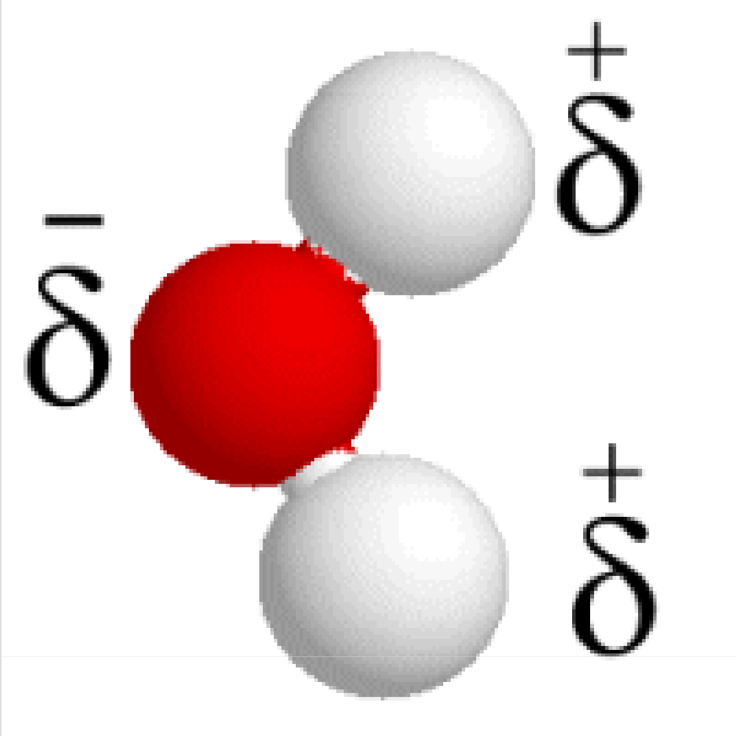


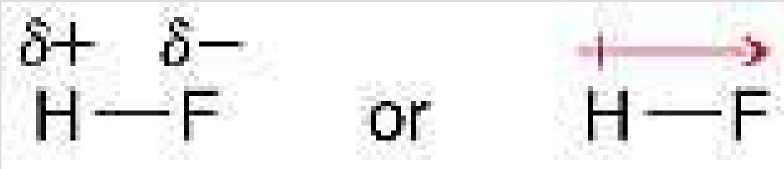




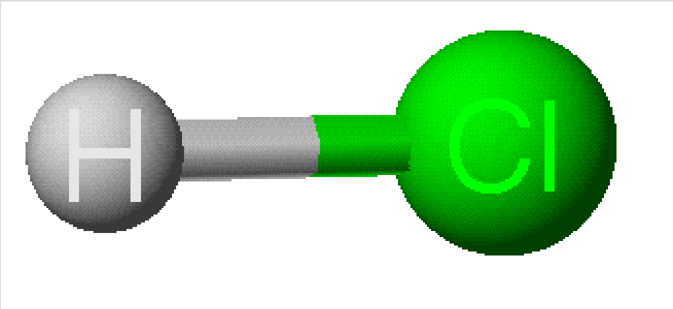
Polar Bonds

- The lower case Greek letter delta shows that atoms involved in the covalent bond acquire only partial charges, much less than 1+ or 1-
- The polarity of a bond may also be represented with an arrow pointing to the more electronegative atom

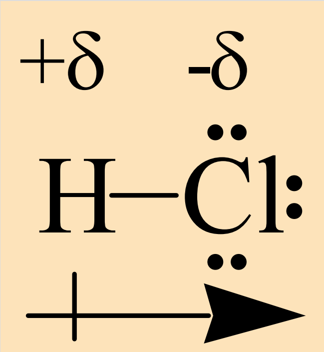




Bond Polarity



HCl is POLAR because it has a positive end and a negative end. (difference in electronegativity)



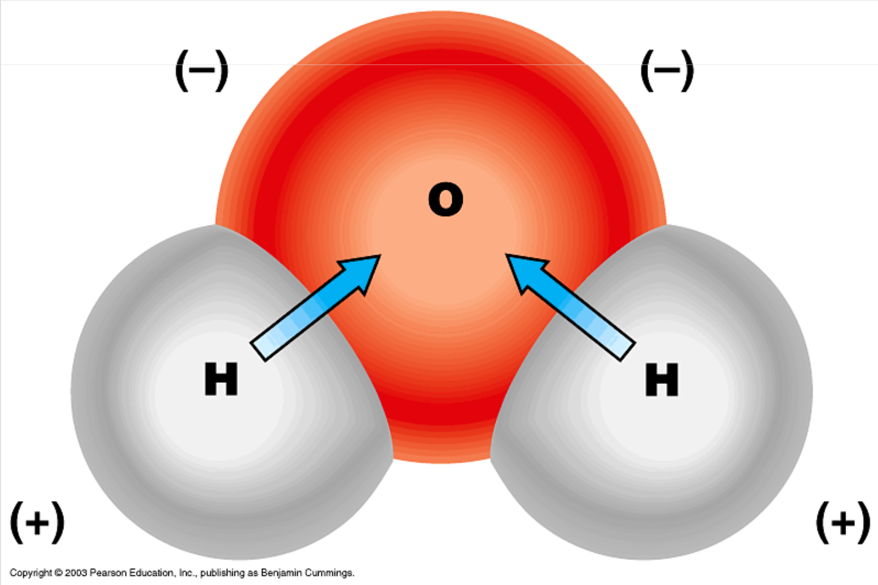
Cl has a greater share in bonding electrons than does H.

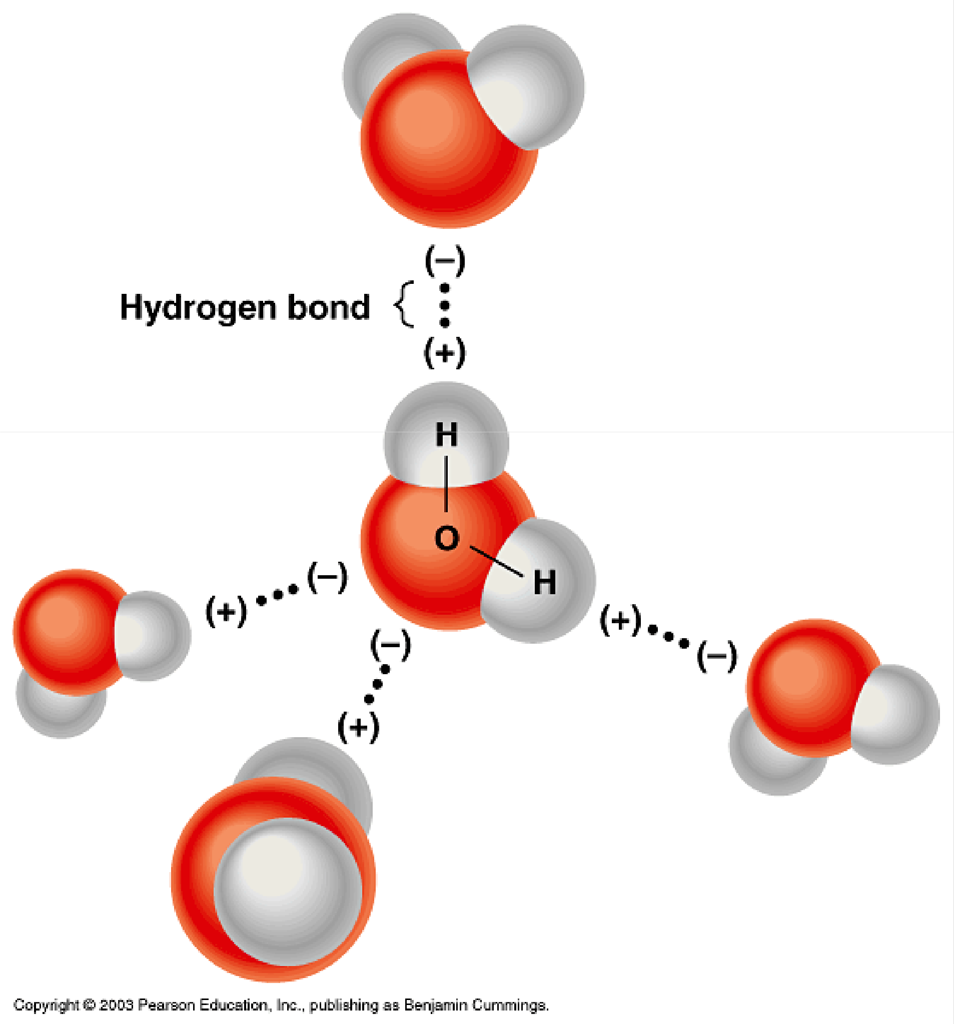
Cl has slight negative charge (-δ) and H has slight positive charge (+ δ)

Bonding

Covalent bonding

<u>Polar covalent bond</u>





Polar Molecules

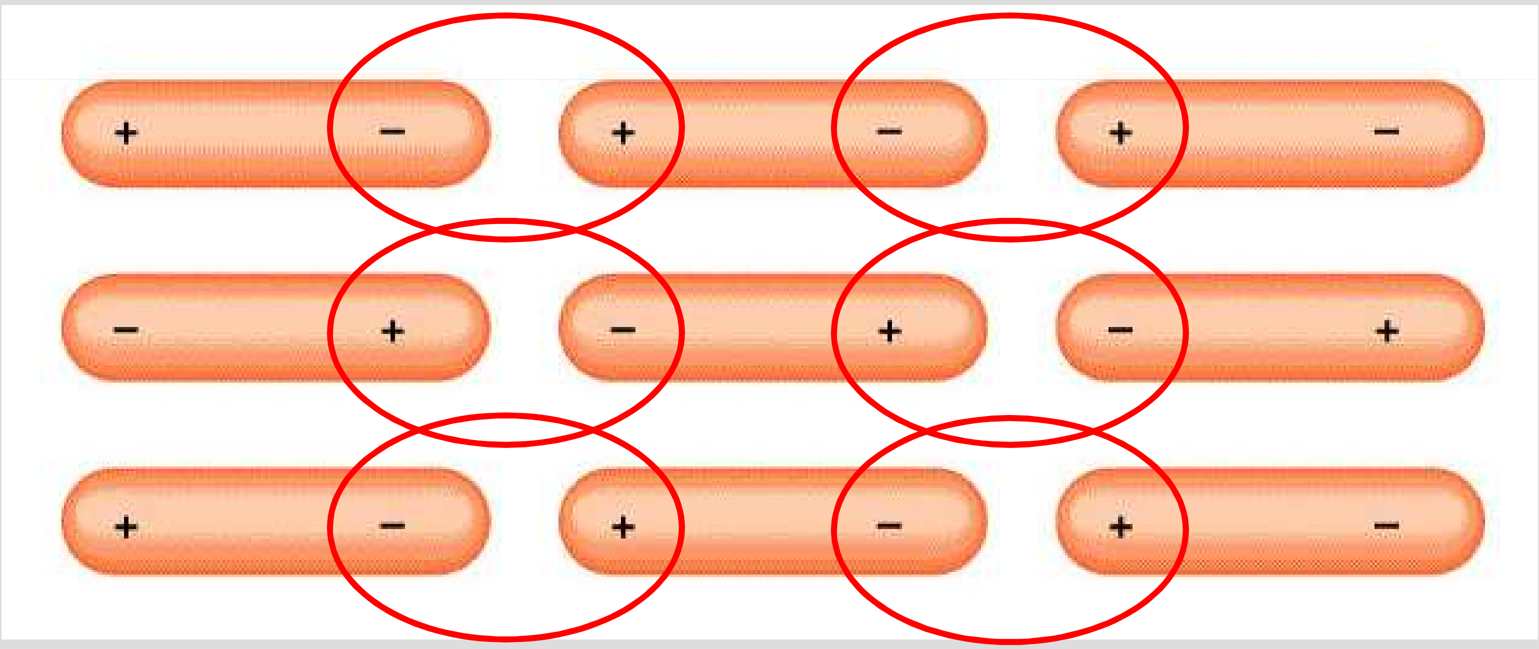
- In a polar molecule, one end of the molecule is slightly negative and the other end is slightly positive.
- The electrically charged regions are called poles.
- A molecule that has two poles is called a dipolar molecule or dipole.
- The effect of polar bonds on the polarity of a molecule depends on its shape.
  - CO_2
  - H_2O

Types of Intermolecular Forces

3. Dipole-Dipole Forces

Attractive forces between **polar molecules**

Orientation of Polar Molecules in a Solid



Is the sharing of electrons in molecules always equal?

non-polar bond

X : Y $\quad \Delta EN = 0$

Which element is more electronegative?

X : Y $\quad \Delta EN = 0.3$

X : Y $\quad \Delta EN = 0.6$

$EN_Y > EN_X$

polar bond

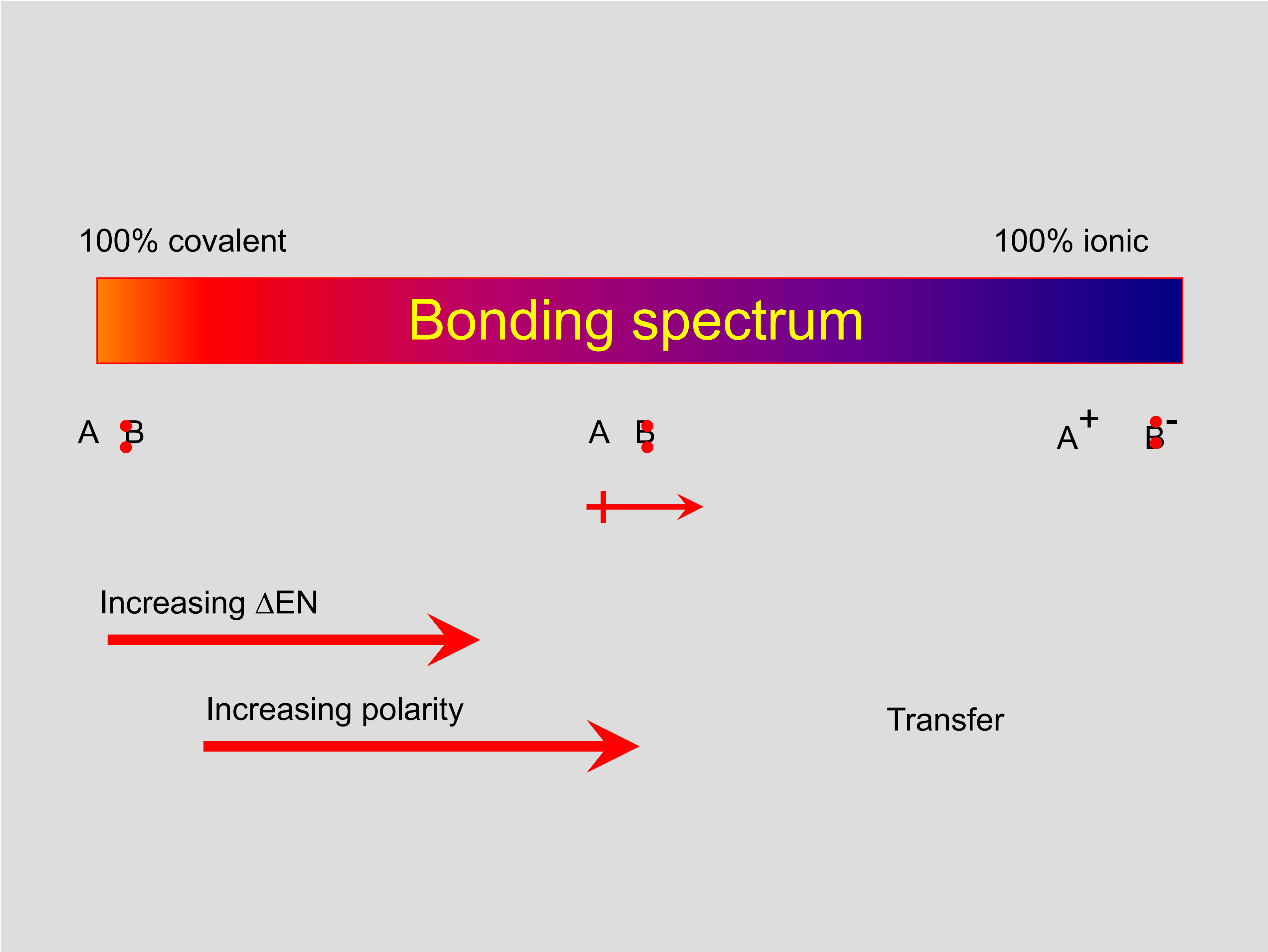
X : Y $\quad \Delta EN = 0.9$

$0 < EN < 1.7$

X ⟶ : Y $\quad \Delta EN = 1.2$

Direction of electron migration

increasing polarity of bond


100% covalent
100% ionic
Bonding spectrum
A B
A B
A+ B-
Increasing ΔEN
Increasing polarity
Transfer

Metallic bonds

- The valence electrons are dilocalised (not attached to a particular atom) known as a sea of electrons , are free to move throughout the metal .
- A metallic bond is the attraction between the positive ions and the mobile valence electrons .

Metallic Bonds

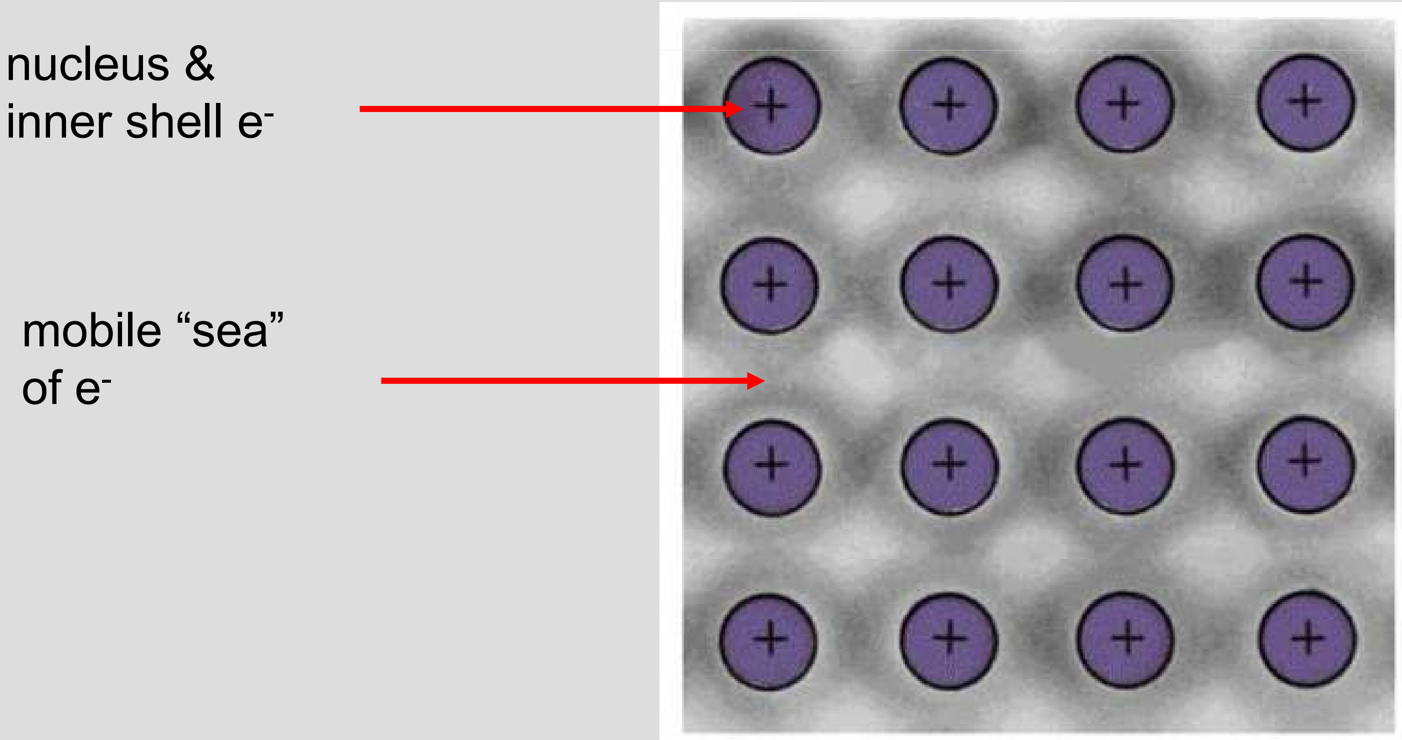
- In metallic bonding instead of sharing electrons between two atoms the electrons in the outer shells are shared amongst all the atoms in a lattice with all the atoms positively charge. These atoms are attracted to the negatively charged 'cloud' of electrons.
- The movement of the free electrons means that metallic bonded materials have good thermal and electrical conduction.

Types of Crystals

<u>Metallic Crystals</u> – Typically weaker than covalent, but can be in the low end of covalent

- Lattice points occupied by metal atoms
- Held together by metallic bonds
- Soft to hard, low to high melting point
- Good conductors of heat and electricity

Cross Section of a Metallic Crystal



Intermolecular bonding: Non-covalent bonds

- Molecules often link together by weak interactions that do not require large amounts of energy and can be broken easily. These bonds are non-covalent in nature.
- There are four common non-covalent interactions:
  - hydrogen bonds,
  - ionic bonds,
  - van der Waals forces, and
  - hydrophobic interactions.

Inter and Intramolecular bonds

Intermolecular: between molecules (not a bond)

Intramolecular: bonds within molecules (stronger)