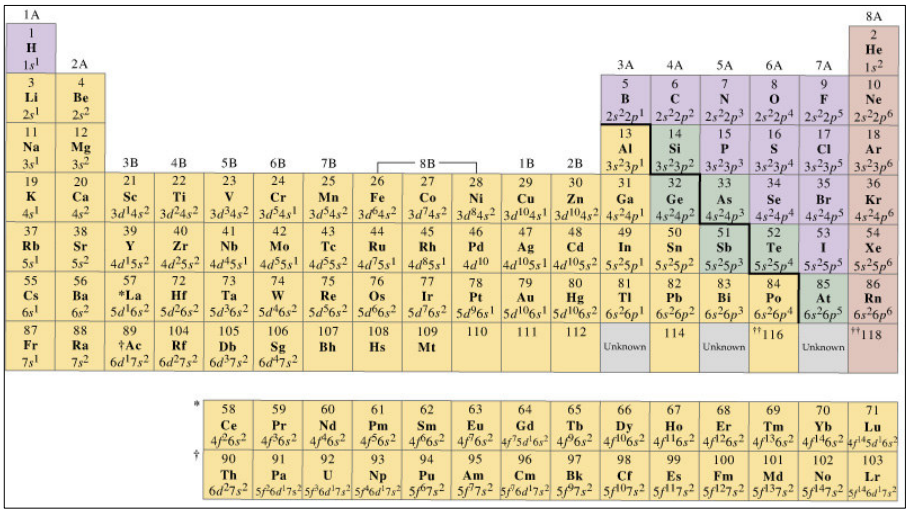
Lecture 4



1A												3A	4A	5A	6A	7A	8A
1 H $1s^1$	2A																2 He $1s^2$
3 Li $2s^1$	4 Be $2s^2$											5 B $2s^2 2p^1$	6 C $2s^2 2p^2$	7 N $2s^2 2p^3$	8 O $2s^2 2p^4$	9 F $2s^2 2p^5$	10 Ne $2s^2 2p^6$
11 Na $3s^1$	12 Mg $3s^2$	3B	4B	5B	6B	7B	8B		1B	2B		13 Al $3s^2 3p^1$	14 Si $3s^2 3p^2$	15 P $3s^2 3p^3$	16 S $3s^2 3p^4$	17 Cl $3s^2 3p^5$	18 Ar $3s^2 3p^6$
19 K $4s^1$	20 Ca $4s^2$	21 Sc $3d^1 4s^2$	22 Ti $3d^2 4s^2$	23 V $3d^3 4s^2$	24 Cr $3d^5 4s^1$	25 Mn $3d^5 4s^2$	26 Fe $3d^6 4s^2$	27 Co $3d^7 4s^2$	28 Ni $3d^8 4s^2$	29 Cu $3d^{10} 4s^1$	30 Zn $3d^{10} 4s^2$	31 Ga $4s^2 4p^1$	32 Ge $4s^2 4p^2$	33 As $4s^2 4p^3$	34 Se $4s^2 4p^4$	35 Br $4s^2 4p^5$	36 Kr $4s^2 4p^6$
37 Rb $5s^1$	38 Sr $5s^2$	39 Y $4d^1 5s^2$	40 Zr $4d^2 5s^2$	41 Nb $4d^4 5s^1$	42 Mo $4d^5 5s^1$	43 Tc $4d^5 5s^2$	44 Ru $4d^7 5s^1$	45 Rh $4d^8 5s^1$	46 Pd $4d^{10}$	47 Ag $4d^{10} 5s^1$	48 Cd $4d^{10} 5s^2$	49 In $5s^2 5p^1$	50 Sn $5s^2 5p^2$	51 Sb $5s^2 5p^3$	52 Te $5s^2 5p^4$	53 I $5s^2 5p^5$	54 Xe $5s^2 5p^6$
55 Cs $6s^1$	56 Ba $6s^2$	57 *La $5d^1 6s^2$	72 Hf $5d^2 6s^2$	73 Ta $5d^3 6s^2$	74 W $5d^4 6s^2$	75 Re $5d^5 6s^2$	76 Os $5d^6 6s^2$	77 Ir $5d^7 6s^2$	78 Pt $5d^9 6s^1$	79 Au $5d^{10} 6s^1$	80 Hg $5d^{10} 6s^2$	81 Tl $6s^2 6p^1$	82 Pb $6s^2 6p^2$	83 Bi $6s^2 6p^3$	84 Po $6s^2 6p^4$	85 At $6s^2 6p^5$	86 Rn $6s^2 6p^6$
87 Fr $7s^1$	88 Ra $7s^2$	89 †Ac $6d^1 7s^2$	104 Rf $6d^2 7s^2$	105 Db $6d^3 7s^2$	106 Sg $6d^4 7s^2$	107 Bh	108 Hs	109 Mt	110	111	112	Unknown	114	Unknown	††116	Unknown	††118

*	58 Ce $4f^2 6s^2$	59 Pr $4f^3 6s^2$	60 Nd $4f^4 6s^2$	61 Pm $4f^5 6s^2$	62 Sm $4f^6 6s^2$	63 Eu $4f^7 6s^2$	64 Gd $4f^7 5d^1 6s^2$	65 Tb $4f^9 6s^2$	66 Dy $4f^{10} 6s^2$	67 Ho $4f^{11} 6s^2$	68 Er $4f^{12} 6s^2$	69 Tm $4f^{13} 6s^2$	70 Yb $4f^{14} 6s^2$	71 Lu $4f^{14} 5d^1 6s^2$
†	90 Th $6d^2 7s^2$	91 Pa $5f^2 6d^1 7s^2$	92 U $5f^3 6d^1 7s^2$	93 Np $5f^4 6d^1 7s^2$	94 Pu $5f^6 7s^2$	95 Am $5f^7 7s^2$	96 Cm $5f^7 6d^1 7s^2$	97 Bk $5f^9 7s^2$	98 Cf $5f^{10} 7s^2$	99 Es $5f^{11} 7s^2$	100 Fm $5f^{12} 7s^2$	101 Md $5f^{13} 7s^2$	102 No $5f^{14} 7s^2$	103 Lr $5f^{14} 6d^1 7s^2$

http://www.tcd.ie/Chemistry/teaching/chemistry/jf/intro/intro.php

Lecture 4

Chemical Bonding

Outline

4.1 Law of conversation of mass

4.2 Law of definite composition

4.3 Bonding in chemical substances

Ionic, covalent and metallic bonding

4.4 Electronegativity

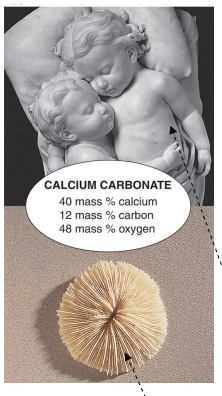
Law of Conservation of Mass:

The total mass of substances does not change during a chemical reaction.

reactant 1 + reactant 2 → product

total mass = total mass

calcium oxide	**+**	**carbon dioxide**	**→**	**calcium carbonate**
CaO	**+**	**CO_2**	**→**	**$CaCO_3$**
56.08g	**+**	**44.00g**	**→**	**100.08g**



Law of Definite (or Constant) Composition:

No matter what its source, a particular chemical compound is composed of the same elements in the same parts (fractions) by mass.

$CaCO_3$

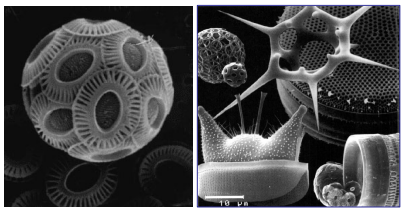
1 atom of Ca	**40.08 amu**
1 atom of C	**12.00 amu**
3 atoms of O	**3 x 16.00 amu**
	100.08 amu

$$\frac{40.08\ amu}{100.08\ amu} = 0.401\ parts\ Ca$$

$$\frac{12.00\ amu}{100.08\ amu} = 0.120\ parts\ C$$

$$\frac{48.00\ amu}{100.08\ amu} = 0.480\ parts\ O$$

Biominerals

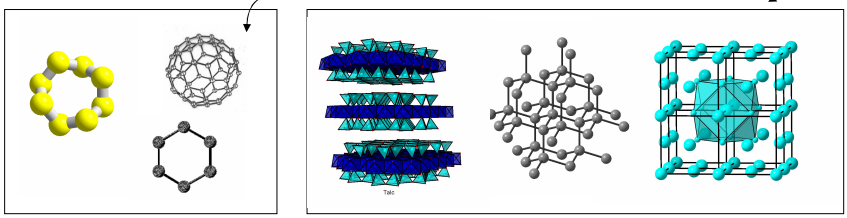


Bonding in chemical substances

Compounds: → Inter-atomic interactions lead to aggregation

A) "Infinite" assemblies of atoms → e.g. metals, extended ionic or covalent compounds

B) Clearly defined assemblies → molecules



Chemical Formula:

Element symbols of the atoms involved in the compound

Composition given by the indices (bottom right of the element symbol)

Bonding in chemical substances

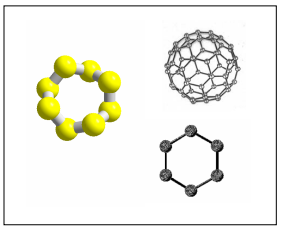
Molecules

H_2: Molecule of two atoms of hydrogen

→ Molecule of the element hydrogen

S_8: Molecule of eight sulphur atoms

→ Molecule of the element sulphur



HCl: Molecule built from one atom of hydrogen and one atom of chlorine

→ Molecule of the compound hydrogenchloride

H_2O: Molecule built from two atoms of hydrogen and one atom of oxygen

→ H_2O: Molecule of the compound water

Bonding in chemical substances

A ***molecular formula*** shows the exact number of atoms of each element in the smallest unit of a substance.

An ***empirical formula*** shows the simplest whole-number ratio of the atoms in a substance.

Molecular formula in inorganic chemistry:

- No information how the atoms are connected (constitution)
- No information about the 3D arrangement (structure)

molecular	**empirical**
H_2O	H_2O
N_2H_4	NH_2

Bonding in chemical substances

Chemical Bonds - Forces that hold the atoms together in the compound:

1) Inter-atomic electrostatic interactions

2) Formation of stable compounds if the attractive forces between positive protons and negative electrons over-compensate the proton-proton and electron-electron repulsion.

- **Covalent Compounds** — Electrons are shared between atoms of different elements to form covalent compounds

Ionic Compounds — Electrons are transferred from one atom to another to form ionic compounds.

Bonding in chemical substances

Important Rule: Octet rule (Lewis, 1916)

Compounds of building units with noble gas configuration are especially stable (8 valence electrons for 2nd period)

→ can also be extended to 18 electrons

Bonding in chemical substances

Different types of bonding:

Ionic bond ……(e.g. NaCl, CsI; MgO)

Covalent bond ……..(H_2, HF, O_2, S_8) → strong

Metallic bond …… ….(e.g. Ag, Cu_3Au; Pb)

Hydrogen bonds ……(H_2O) → weak

van der Waals bonding …(organic compounds, hydrocarbons)

Bonding in chemical substances

Bond energy: Is the energy that is released when a bond is formed

Dissociation energy: Is the energy necessary to break a bond

Bond Type	Bond Energy	Examples
Ionic bonds	400-700KJ/mol	NaCl, CsF, MgO (salts)
Covalent	100-400KJ/mol	H_2, HF, O_2, S_8 (molecules)
Metallic	100-400KJ/mol	Ag, Cu_3Au, Pb (metals)

Ionic Bonding

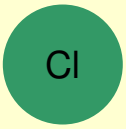
An ***ion*** is an atom, or group of atoms, that has a net positive or negative charge.

cation – ion with a positive charge. If a neutral atom **loses** one or more electrons it becomes a cation.

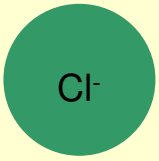
11 protons
11 electrons

11 protons
10 electrons

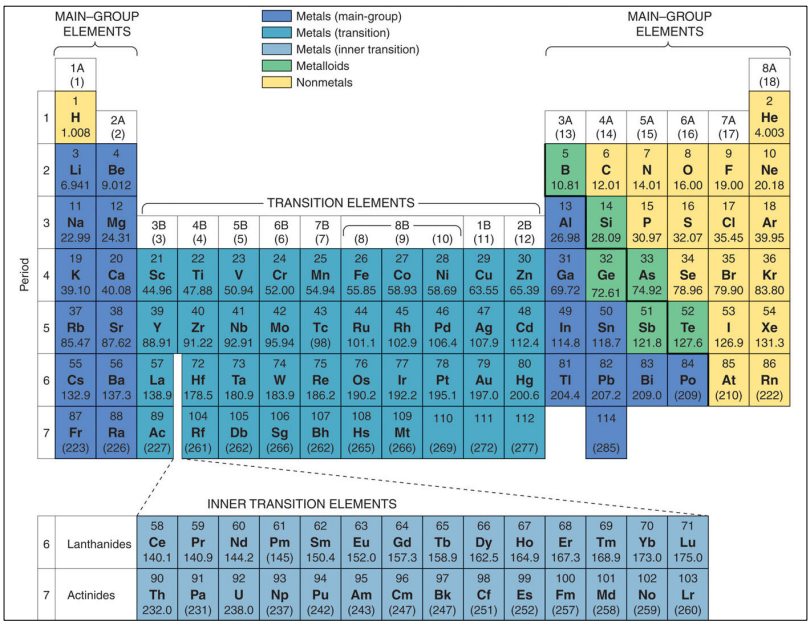
anion – ion with a negative charge. If a neutral atom **gains** one or more electrons it becomes an anion.



17 protons
17 electrons



17 protons
18 electrons



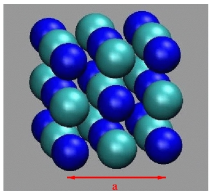
Ionic Bonding

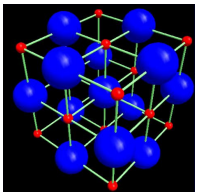
ionic compounds

- consist of a combination of cations and anions
- the formula is usually the same as the empirical formula
- the sum of the charges on the cation(s) and anion(s) in each formula unit must equal zero

Ionic Bonding

- Formed between elements with a high difference of their electronegativity
- Strong bond; the bonding is not directed in space (electrostatic bonding)
- This type of bonding results in "infinite" aggregates built from cations and anions
- The compounds form ionic lattices
- Substances with ionic lattices are called "salts"

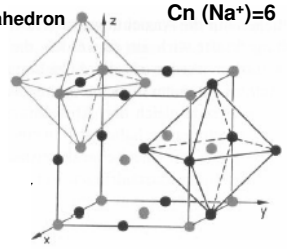




Unit Cell

$NaCl_6$ octahedron

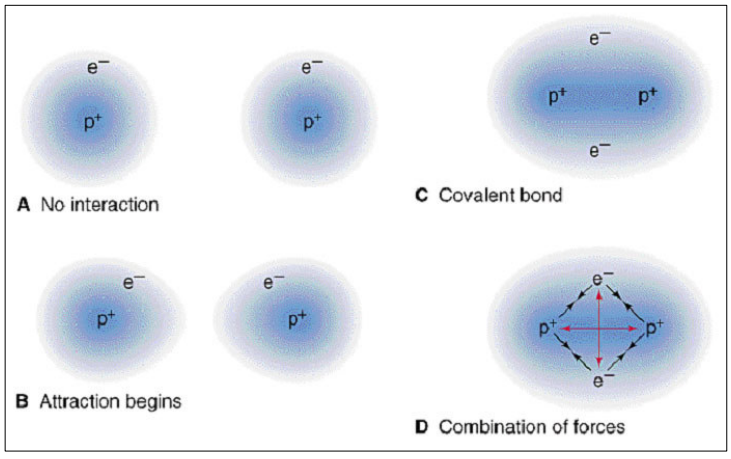
Cn (Na^+)=6



$ClNa_6$ octahedron

Cn (Cl^-)=6

Formation of a Covalent Bond between Two H Atoms



Bonding in chemical substances

Characteristics - Covalent Bonding:

2 or more valence electrons belong at the same time to the electron shell of different atoms.

High probability that the bonding electrons are located between the two bonding partners.

Different models to describe covalent bonds:

a) Lewis formula (Element symbols, dots, lines)

b) Valence bond model (orbitals, dots)

c) Molecular orbital model (Energy level diagrams, arrows)

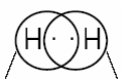
Bonding in chemical substances

Covalent Bonding

Lewis Formula

- According to Lewis: At least two electrons are shared between two atoms. These atoms reach noble gas configuration.
- The electrons are symbolised by dots or a line (bond = 2 electrons) between the elements.
- Further valence electrons which do not contribute to the bond remain as non-bonding "free" electrons next to the element symbol.

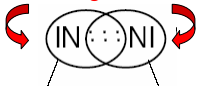
bonding electrons



Helium Configuration

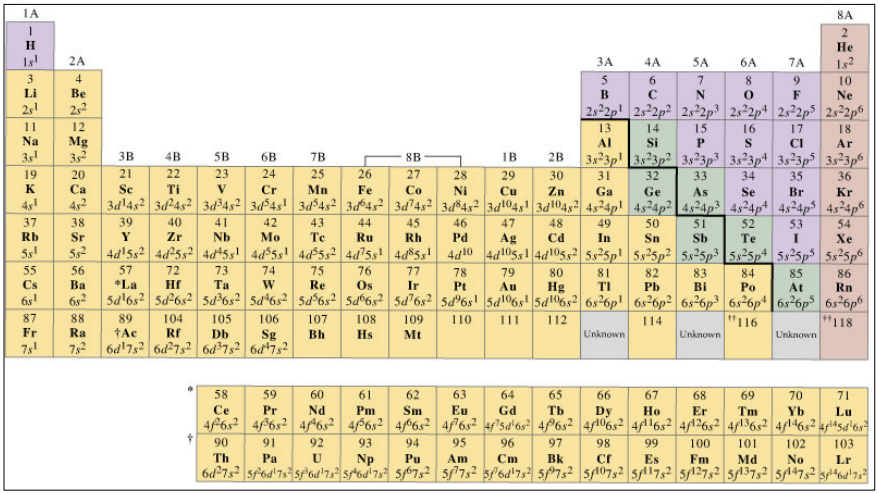
$(1s^2)$

Non-bonding electrons



Neon Configuration

$(1s^2)(2s^2)(2p^6)$



Bonding in chemical substances Covalent Bonding

Lewis formula		No. of Bonds	Electron Pairs *bonding*	*not bonding*
H · · H	H — H	Single Bond	1	0
O : : O	O = O	Double Bond	2	4
IN : : : NI	IN ≡ NI	Triple Bond	3	2

Atoms from the 2nd period of the Periodic Table can form a maximum of 4 covalent bonds.

8-n bonds: CH_4 (8-4), NH_3 (8-5), H_2O (8-6), HF (8-7)

main group of periodic table ..... all neutral

Bonding in chemical substances

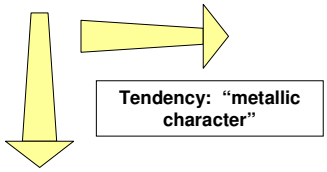
Metallic Bonding: ➡ Formed by atoms with a low ionisation energy;

Characteristics: “Infinite” aggregates with highly flexible/moveable electrons delocalised over the whole metallic aggregate

➡ “electron gas”

Bonding: electrostatic attraction between electron gas and positively charged atom nuclei.

Properties: High electrical and thermal conductivity as a result of the highly moveable electrons.



Electronegativity (EN)

Related to the chemical bond:

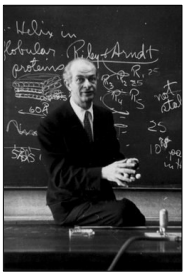
➡ ability of an atom or molecule to attract electrons

If the difference of EN between atoms is very high, the electron will be transferred to one atom and an ionic bond will form. In a covalent bond, if one atom pulls slightly “harder” than the other, a polar covalent bond will form.

➡ Most important: Pauling scale (1932):

The most electronegative chemical element (fluorine) is given an electronegativity value of 3.98 (or in text books 4.0); Francium is the most electropositive atom and has a value of 0.7. The other elements have values in between. Hydrogen is arbitrarily assigned a value of 2.1 or 2.2.

Electronegativity (EN)



Linus Pauling (1901–1994)

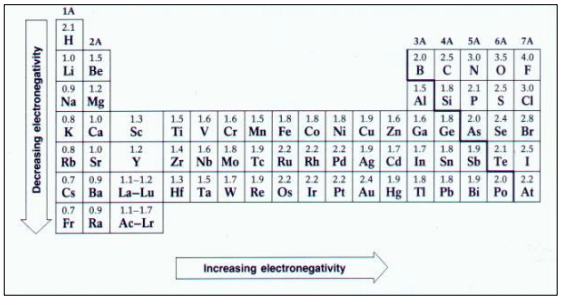
ΔEN is the difference in electronegativity between two atoms or elements.

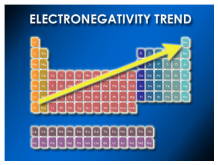
But many exceptions !!!!

ΔEN ≥ 1.7: often considered to be ionic bonds

ΔEN = 1.7–0.4: often considered as polar covalent

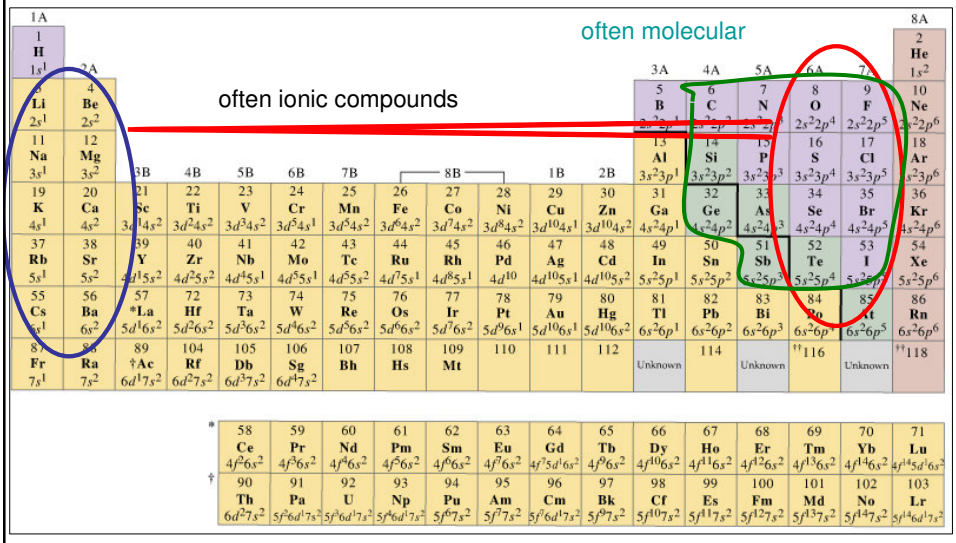
below 0.4–0: are considered as non-polar bonds





Tendencies

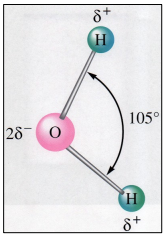
Electronegativity (EN)

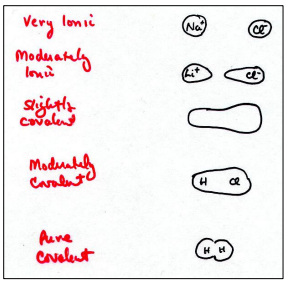


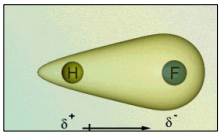
Electronegativity (EN)

Polar Bonds:

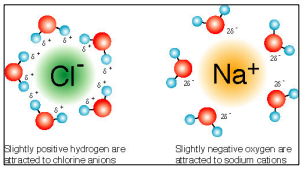
$H \rightarrow Cl$ $\quad$ $H \blacktriangleleft Cl$

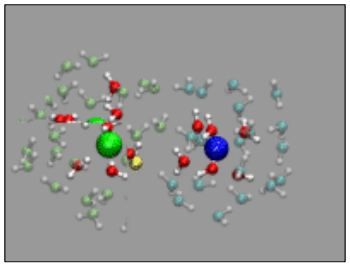


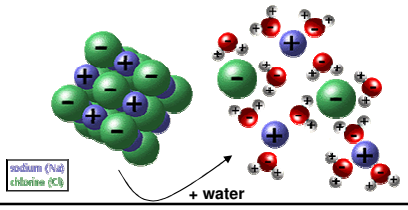




Hydration:



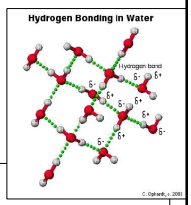




Bonding in chemical substances

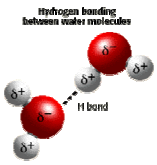
Weaker Bonds

Type	Bond Energy (KJ/mol)	Example
Hydrogen bonding	< 30	HF; H_2O; NH_3; CH_3CO_2H
van der Waals	< 3	He, Ne, hydrocarbons



➡ Interactions between positively and negatively polarised centres

Permanent dipoles (H-bond)



➡ Interactions between temporary positively and negatively polarised centres

Induced dipoles (van der Waals bond)