COURSE – MINT CHEMISTRY

Topic 3
Molecules, Ions and Bonds

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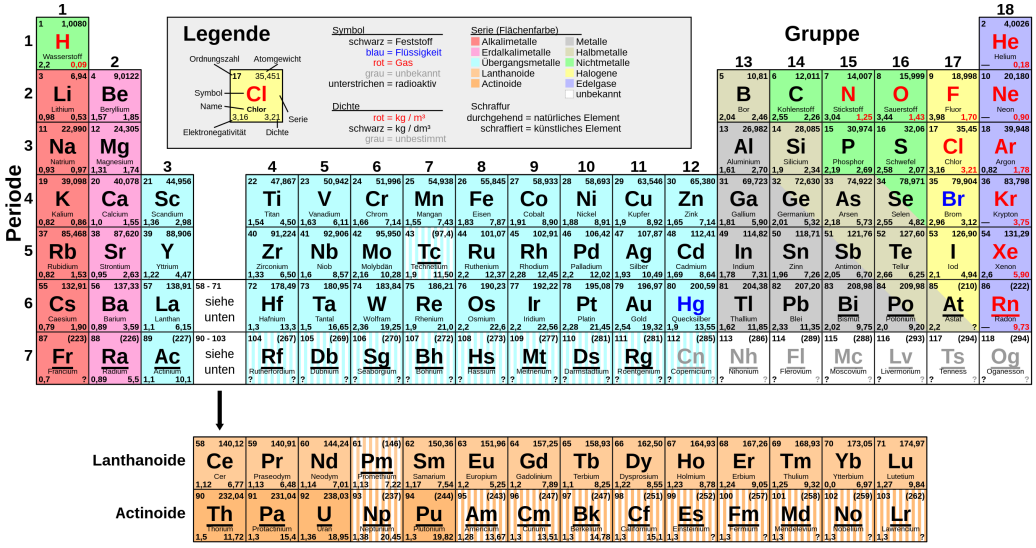
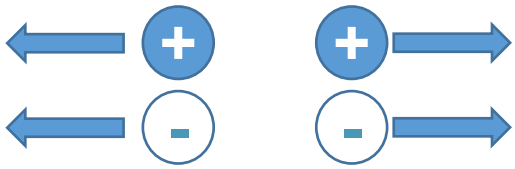
Atoms ➡ Ions, Molecules



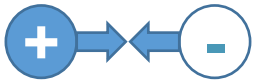
Basics of Chemical Compounds

1) Coulombic interraction

Like charges repel each other

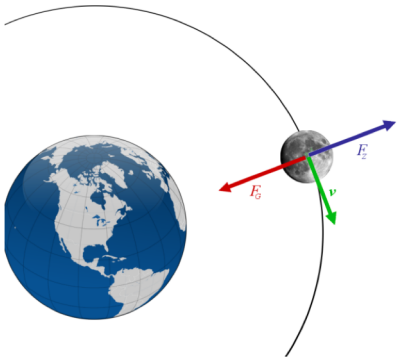


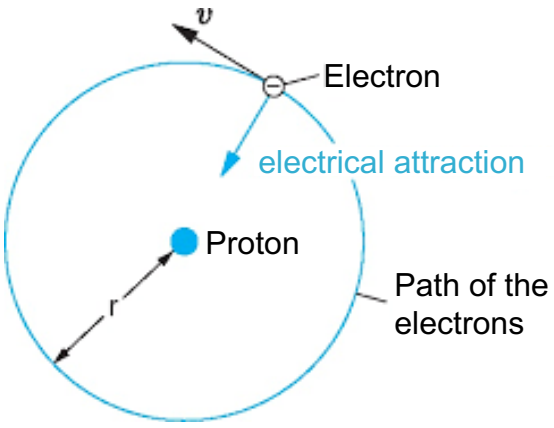
Opposite charges attract each other



Basics of Chemical Compounds

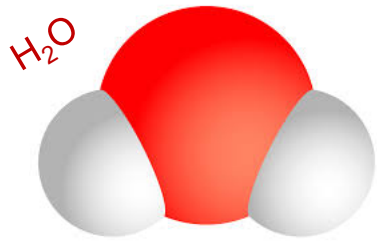
2) Systems look for the state with minimum energy

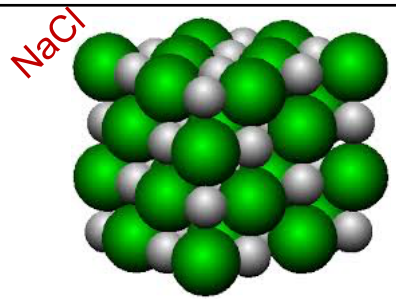




From Elements to Chemical Compounds

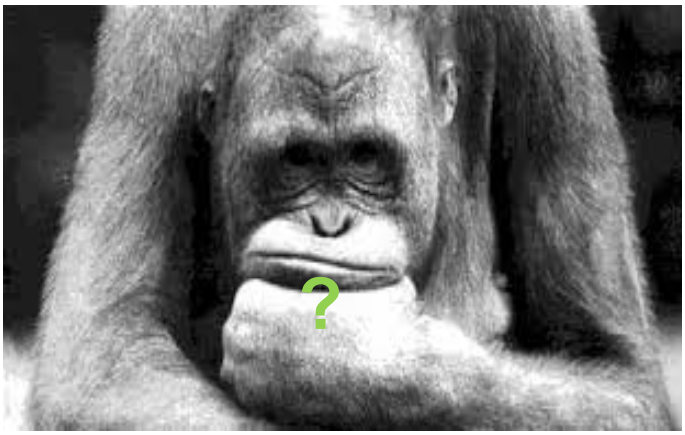
A chemical compound is a substance made up of two or more atoms (of a different kind) that are in a fixed ratio to each other.





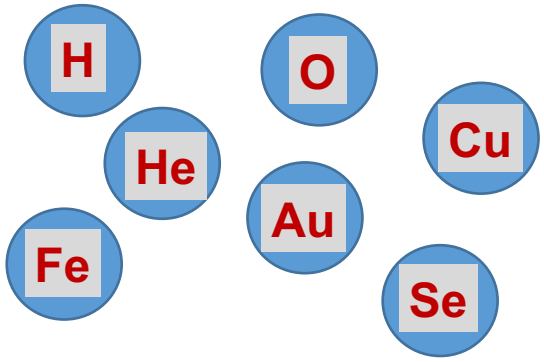
The composition is indicated by a chemical formula.

Atoms - Molecules



Atoms - Molecules

- Atoms are the smallest unit of a chemical element



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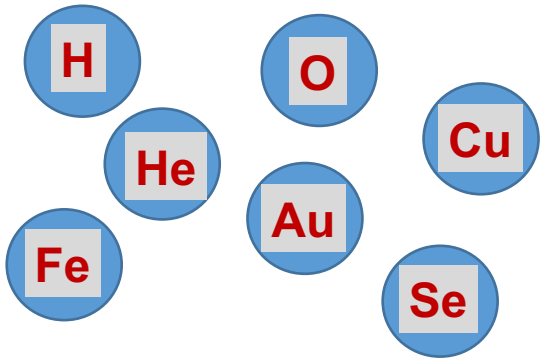
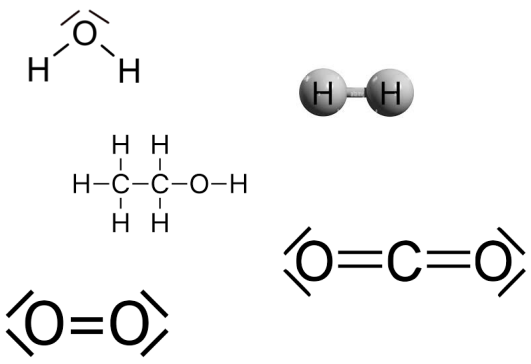


- Molecules are made up of two or more atoms



Molecules

- a specific **electrically neutral group of bonded atoms**
  charged molecules are **molecular ions**
- the smallest particle of a compound that possesses the chemical properties of that compound
- can be solid, liquid or gaseous at room temperature.
- cohesion (bonding) is a consequence of coulombic interactions

Molecules of chemical elements

Certin elements exist as **2-atom (diatomic) molecules**:

H_2 N_2 O_2 Cl_2

Some elements form **larger molecules**: S_8

Molecules of chemical elements

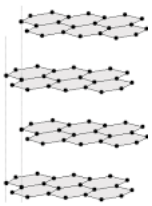
Certin elements exist as **2-atom (diatomic) molecules**:

H_2 N_2 O_2 Cl_2

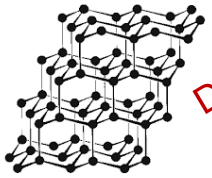
Some elements form **larger molecules**: S_8

Some elements form 3-dimensional structures (crystals) as solids, but they are pure elements and the smallest self-contained building block remains the **atom**:

e.g. Carbon (C)

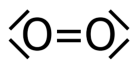


GRAPHITE
C

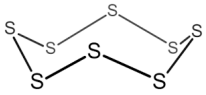


DIAMOND
C

Molecules of Compounds

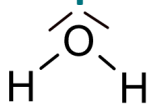


Oxygen (O_2)

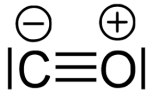


Sulphur (S_8)

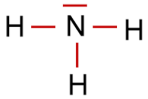
Phosphorus (P_4) (white)



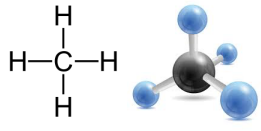
Water (H_2O)



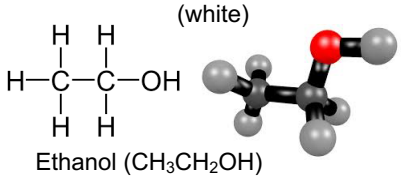
Carbon monoxide (CO)



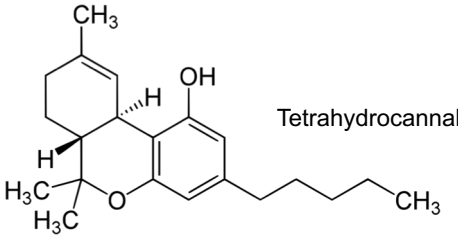
Ammonia (NH_3)



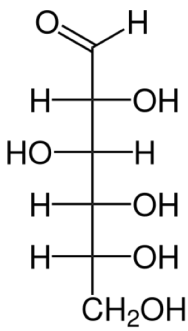
Methane (CH_4)



Ethanol (CH_3CH_2OH)



Tetrahydrocannabinol



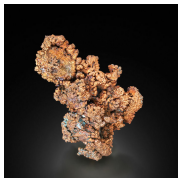
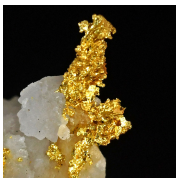
Glucose ($C_6H_{12}O_6$)

Metals

Metals also form 3-dimensional structures (crystals) as solids, but they are the pure element and the smallest self-contained building block remains the **atom**:

e.g. Iron (Fe) Copper (Cu) Gold (Au)



Chemical Bonding in Molecules (Overview)

$NaCl$, $Mg(NO_3)_2$	**Ionic bond** Forces of attraction between anions and cations
H_2O, CH_4, SiO_2, H_2, C	**Covalent bond** Attractive forces of nuclei and electrons: Atoms share a pair of electrons
Fe, Mg, Cu	**Metal bond** Forces of attraction between metal ions and free electrons in a metal lattice
$[Cu(NH_3)_4]^{2+}$; $Al(OH)_4^-$	**Coordinative bond** Attraction of the nucleus of the central atom to the lone pairs of electrons of the ligands: Lone pairs of electrons from ligands bind into the d-orbitals of transition elements. (they form complexes)

The Chemical Bond

- Compounds with ionic bonds are solid at normal temperatures and pressures. (e.g. Sodium chloride and silver sulphate)

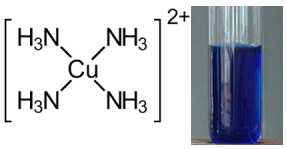

- Substances with covalent bonds are:

  a) molecular solids, liquids or gases (glucose, water and ammonia)
  b) solids composed of extended structures of connected atoms (diamond, boron nitride, quarz)

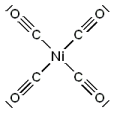

The Chemical Bond

- Metals are solids (except Hg: liquid)


- Complexes are molecules that are stable in solution or in the gaseous phase (uncharged molecule) or form salt-like compounds (solid) as molecular ions in combination with a cation or anion.



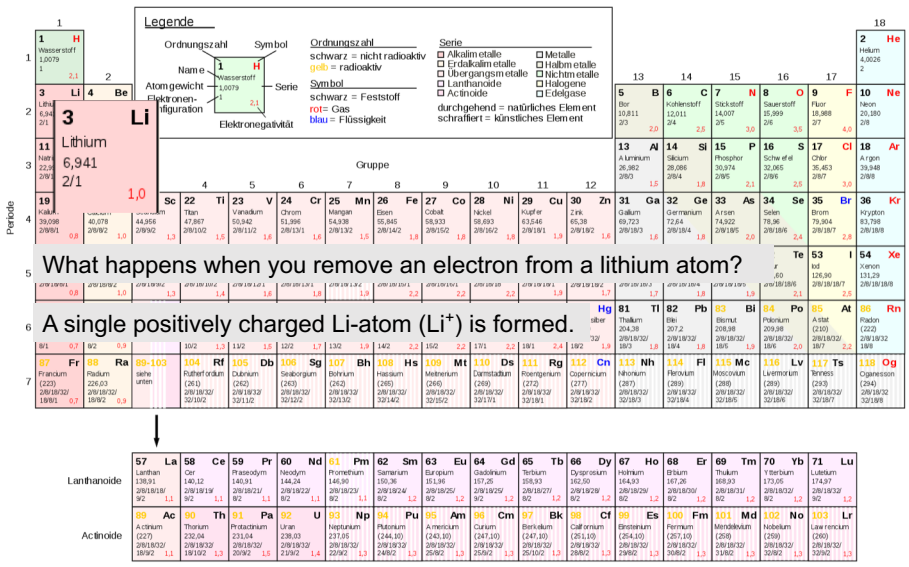
$Cu(NH_3)_4^{2+}$
copper tetraammine complex



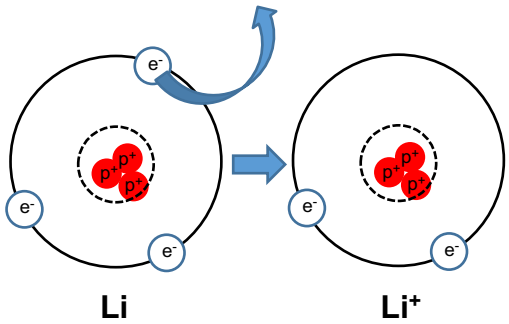
$Ni(CO)_4$
tetracarbonylnickel

$K_3[Fe(CN)_6]$
Potassium hexacyanoferrate(III)

FROM ATOMS TO IONS

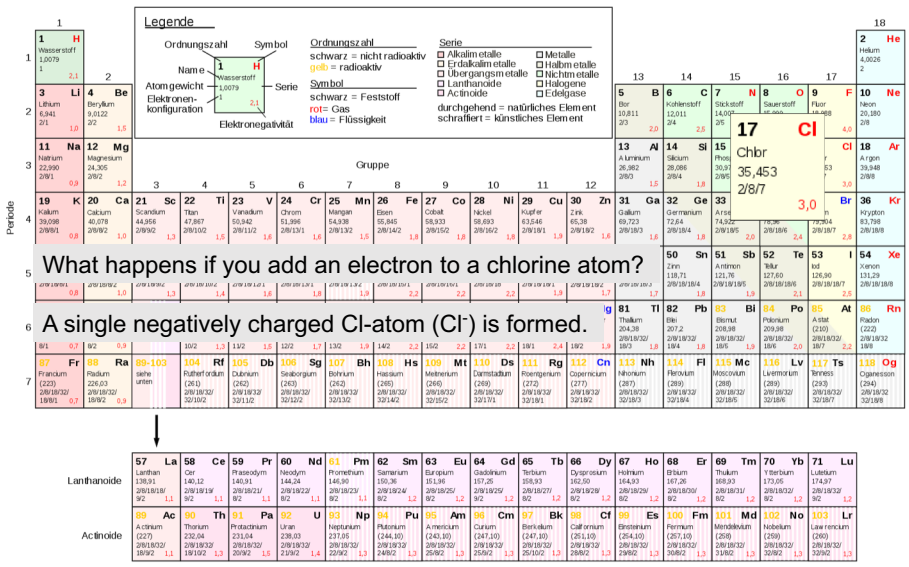


Ions



What happens when you remove an electron from a Li atom?

IONS



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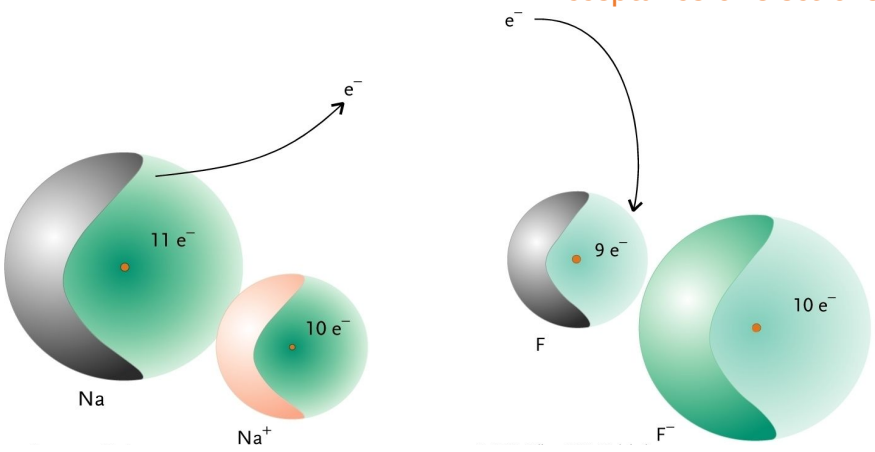
Formation of Ions

Formation of cations
Release of electrons

Formation of anions
Acceptance of electrons



Why are cations smaller and anions larger than their atoms?

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IONS

Ion = positively or negatively charged particle

Atom = (Atomic) ion
Group of atoms = Molecular ion

Atomic ions: Li^+, Na^+, Ca^{2+}; F^-, Cl^-, S^{2-}
Molecular ions: NH_4^+; H_3O^+; OH^-; NO_3^-; SO_4^{2-}

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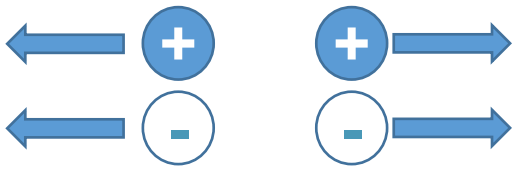
Positively charged ions are referred to as CATIONS

Negatively charged ions are referred to as ANIONS

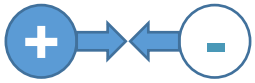
Basics of Chemical Compounds

Coulombic interraction

Like charges repel each other



Opposite charges attract each other



What happens when a cation and an anion "come together"?

Ions and Ionic Compounds

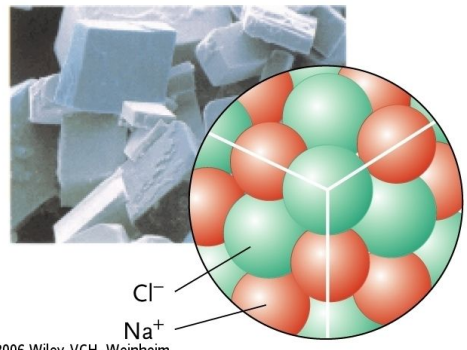
Ionic compounds (salts):

Consist of positively and negatively charged ions that attract each other electrostatically.

The ratio of the ions results from the fact that the same number of positive and negative charges are given in the smallest integer ratio.

The ionic crystal is overall UNCHARGED

Salts form 3 dimensional CRYSTALS



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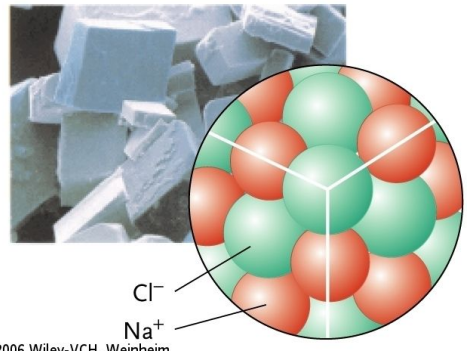
The ionic crystal is overall UNCHARGED

Salts form 3 dimensional CRYSTALS

Na^+/Cl^-	1 : 1	NaCl
Ca^{2+}/Cl^-	1 : 2	$CaCl_2$
K^+/SO_4^{2-}	2 : 1	K_2SO_4



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Some common anions and cations

LEARN!!!

Positive ions (cations)	Negative ions (anions)
Ammonium (NH_4^+)	Acetate ($C_2H_3O_2^-$)
Potassium (K^+)	Bromide (Br^-)
Copper(I) (Cu^+)	Chloride (Cl^-)
Sodium (Na^+)	Chlorate (ClO_3^-)
Silver (Ag^+)	Cyanide (CN^-)
Hydrogen (H^+)	Fluoride (F^-)
	Hydride (H^-)
Barium (Ba^{2+})	Hydrogen carbonate (HCO_3^-)
Lead(II) (Pb^{2+})	or bicarbonate
Calcium (Ca^{2+})	Hydrogen sulphate (HSO_4^+)
Chromium(II) (Cr^{2+})	Hydroxide (OH^-)
Cobalt(II) (Co^{2+})	Iodide (I^-)
Iron(II) (Fe^{2+})	Nitrate (NO_3^-)
Copper(II) (Cu^{2+})	Perchlorate (ClO_4^-)
Magnesium(II) (Mg^{2+})	Permanganate (MnO_4^-)
Manganese(II) (Mn^{2+})	
Mercury(II) (Hg^{2+})	Carbonate (CO_3^{2-})
Zinc (Zn^{2+})	Chromate (CrO_4^{2-})
Tin(II) (Sn^{2+})	Oxide (O^{2-})
	Peroxide (O_2^{2-})
Aluminium (Al^{3+})	Sulphate (SO_4^{2-})
Iron(III) (Fe^{3+})	Sulphide (S^{2-})
Chromium(III) (Cr^{3+})	Sulphite (SO_3^{2-})
	Phosphate (PO_4^{3-})

Chemical Nomenclature

If a type of ion occurs more than once, their number is indicated with Greek numerals:

1 = mono; 2 = di; 3 = tri; 4 = tetra; 5 = penta; 6 = hexa; 7 = hepta; 8 = octa; 9 = nona; 10 = deca; 11 = undeca; 12 = dodeca

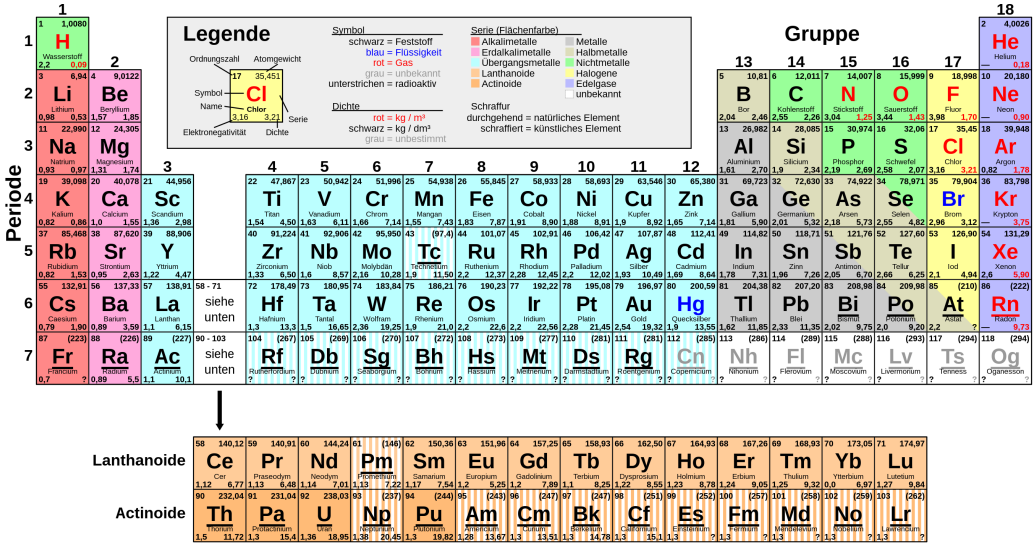
Chemical Nomenclature - Cations

Systematic names for cations:

For metal ions, the charge of the cation is given in Roman numerals in brackets.

- e. g.: Cu^{2+} - Cu(II)-ion,
  Fe^{3+} - Fe(III)-ion

Observaton: which elements (rather) form atomic cations?

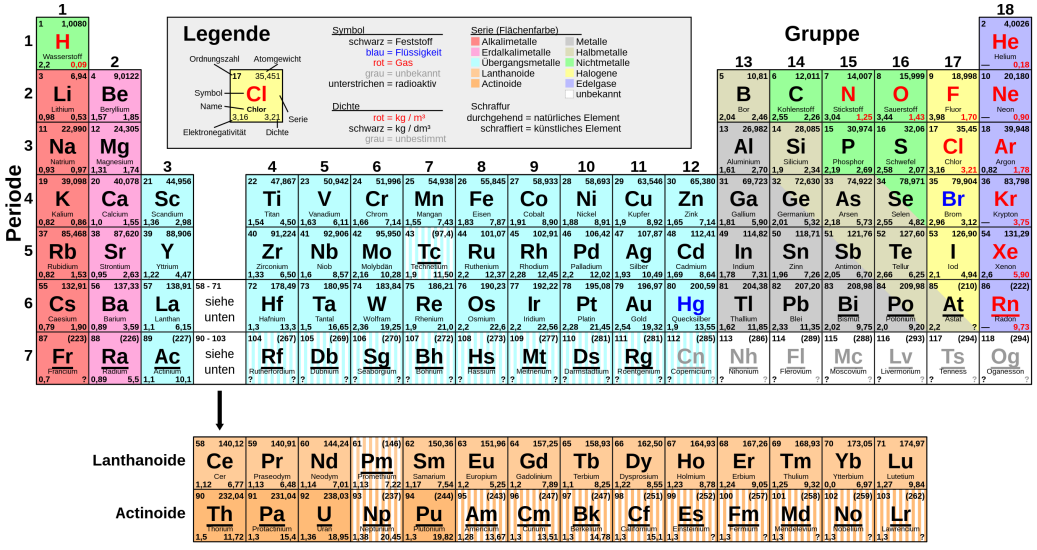


Chemical Nomenclature - Anions

Latin root + suffix -ide

Fluorine	F^-	- Fluoride
Chlorine	Cl^-	- Chloride
Bromine	Br^-	- Bromide
Iodine	I^-	- Iodide
Carbon	C_2^{2-}; C_3^{4-}; C^{4-} (z.B.: CaC_2)	- Carbide
Silicon	Si^{4-}	- Silicide
Nitrogen	N^{3-}	- Nitride
Phosphor	P^{3-}	- Phosphide
Sulphur	S^{2-}	- Sulphide
Oxygen	O^{2-}	- Oxide

Observaton: which elements (rather) form atomic anions?



Chemical Nomenclature – Molecular anions

Systematic names for molecular anions with oxygen :

Maximum number of oxygens: latin root + suffix -ate

Carbon	CO_3^{2-}	- Carbonate
Nitrogen	NO_3^-	- Nitrate
Phosphorus	PO_4^{3-}	- Phosphate
Sulphur	SO_4^{2-}	- Sulphate

Chemical Nomenclature – Molecular anions

Systematic names for molecular anions with oxygen :

Maximum number of oxygens: latin root + suffix -ate

One oxygen atom fewer: latin root + suffix -ite

Carbon	CO_3^{2-}	- Carbonate
Nitrogen	NO_3^-	- Nitrate
	NO_2^-	- Nitrite
Phosphorus	PO_4^{3-}	- Phosphate
Sulphur	SO_4^{2-}	- Sulphate
	SO_3^{2-}	- Sulphite

Chemical Nomenclature – Molecular anions

Molecular anions of halogens with oxygen:

Perhalogenate:	Perchlorate, Perbromate, Periodate	ClO_4^- BrO_4^- IO_4^-
Halogenate:	Chlorate, Bromate, Iodate	ClO_3^- BrO_3^- IO_3^-
Halogenite:	Chlorite, Bromite, Iodite	ClO_2^- BrO_2^- IO_2^-
Hypohalogenite:	Hypochlorite, Hypobromite, Hypoiodite	ClO^- BrO^- IO^-
Halogenide:	Chloride, Bromide, Iodide	Cl^- Br^- I^-

Chemical Nomenclature – Molecular anions

Oxoanions with hydrogen :

Sulfate, SO_4^{2-} ➡ Hydrogensulphate, HSO_4^-

Phosphate, PO_4^{3-} ➡ Hydrogenphosphate, HPO_4^{2-}

Dihydrogenphosphate, $H_2PO_4^-$

Oxide, O^{2-} ➡ Hyroxide, OH^-

Hydrate

Solid, inorganic compounds containing water molecules (water of hydration).

This is bound in the crystal lattice (stoichiometrically).

$Cu_2SO_4 \times 5H_2O \rightleftharpoons Cu_2SO_4 + 5H_2O$

e.g.:
Blue copper(II) sulphate pentahydrate loses water above 150 °C and becomes a white powder

When water is added, the colour reappears

Lattice Enthalpy

The lattice enthalpy $\Delta H^0_{lattice}$ is a measure of the strength of the ionic bond in an ionic solid.

Lattice enthalpy is released when distant positive and negative ions, which are in the gaseous state, combine to form a crystal:

$$M^+(g) + X^-(g) \rightleftharpoons MX(s) \qquad \Delta H^0_{lattice} < 0 \ *$$

- When an ionic bond is broken down into a gas composed of ions, the supply of this energy is required
- The stronger the bond in the solid, the greater the amount of energy required to break the bond and form the gas

* Here, we follow the definition from Mortimer

Lattice Enthalpy

A strong bond in solids:

- leads to high lattice enthalpies
- causes high melting and boiling points

Salt	- $\Delta H^0_{lattice}$ Lattice enthalpy kJ/mol	Melting point °C	Boiling point °C
NaCl	780	801	1413
LiF	1039	842	1676
$MgCl_2$	2502	708	1412
MgO	3925	2800	3600
Al_2O_3	13000	2015	2980

Interactions Between Ions

The strength of the interaction between ions

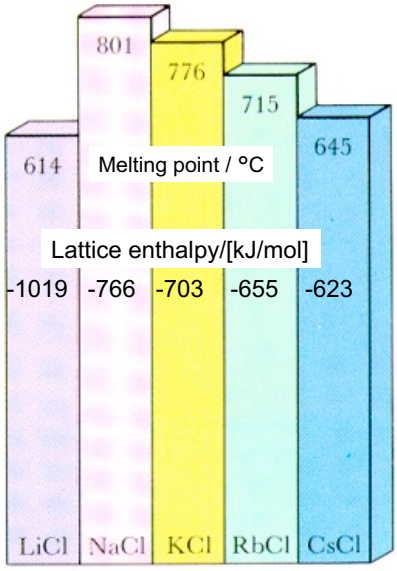
- decreases with the size of the ions
- increases with the value of the charge

Name	Formula	Ionic radius of monovalent alkali metal cations X^+ in pm	- $\Delta H^0_{lattice}$ Lattice enthalpy in kJ per mol
Lithium fluoride	LiF	74	1039
Natrium fluoride	NaF	102	920
Kalium fluoride	KF	138	816
Rubidium fluoride	RbF	149	780
Caesium fluoride	CsF	170	749

Melting Points of Alkali Metal Halides

General trend:
with increasing size of the ions ⇨ lower melting points

Example:
falling melting points of the alkali metal chlorides: from 801 °C for NaCl to 645 °C for CsCl.



Interactions Between Ions

Compounds do not always follow trends.

Example:

- Lithium chloride: small, highly charged ion with an unusually low melting point

- Oxides of aluminum and magnesium:
  Solid with the smaller cation (Al_2O_3) has the lower melting point, 2015 °C < 2800 °C

The more highly-charged, small cation polarizes the neighbouring anion

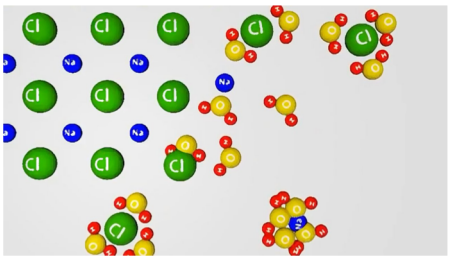
⇨ bond becomes more covalent in character,

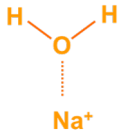
⇨ melting point of the solid is therefore lowered

SALTS in AQUEOUS SOLUTIONS

- Salts dissolve in water with the formation of ions

$$NaCl \rightleftharpoons Na^+ + Cl^-$$
$$NaCl \rightleftharpoons Na^+ + Cl^-$$
$$CaCl_2 \rightleftharpoons Ca^{2+} + 2Cl^-$$
$$K_2SO_4 \rightleftharpoons 2K^+ + SO_4^{2-}$$





A hydration shell forms

SALTS in AQUEOUS SOLUTIONS

- Salts dissolve in water with the formation of ions

$$NaCl \rightleftharpoons Na^+ + Cl^-$$
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$$CaCl_2 \rightleftharpoons Ca^{2+} + 2Cl^-$$
$$K_2SO_4 \rightleftharpoons 2K^+ + SO_4^{2-}$$

- Some salts dissolve well (e.g.: NaCl – 358 g/L),
  some salts dissolve little (e.g.: AgCl – 1.88 mg/L)

Rule of thumb: If less than 0.01 mol of the salt dissolves in 1 litre of water, it is referred to as a SLIGHTLY SOLUBLE salt. ($c = 10^{-2}$ mol/L)

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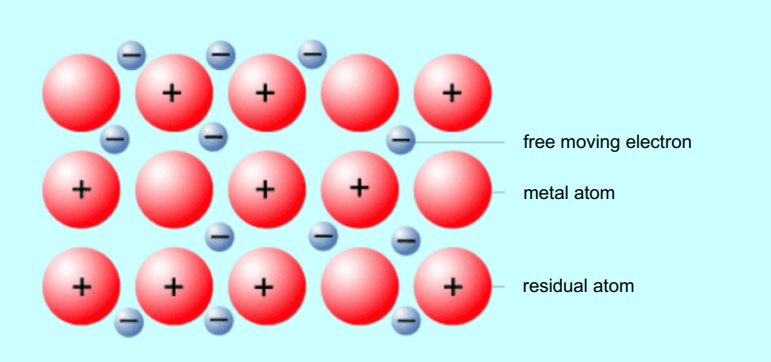
Metal Bond

- In the metal crystal: cations are fixed at the lattice positions while the electrons are free to move.
- These freely moving electrons hold the cations together



Metal Bond

- In the metal crystal: cations are fixed at the lattice positions while the electrons are free to move.
- These freely moving electrons hold the cations together
- Metal atoms have relatively low ionization energies
- Donate electrons easily

Atomium: an iron crystal

Copper nugget

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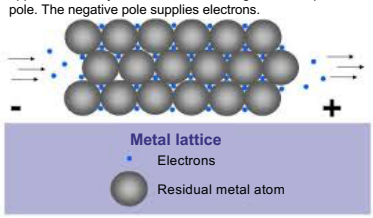
Metal Bond

Properties of Metals

- **Electric conductivity** (moveable electrons)

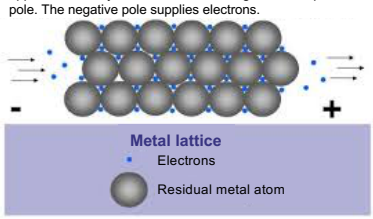
Fig.: Electrical conductivity of metals: When a voltage is applied, the freely movable electrons migrate to the positive pole. The negative pole supplies electrons.



Properties of Metals

- **Electric conductivity** (moveable electrons)
- **Metallic shine** (excitation of the electrons in the band)

Fig.: Electrical conductivity of metals: When a voltage is applied, the freely movable electrons migrate to the positive pole. The negative pole supplies electrons.



Properties of Metals

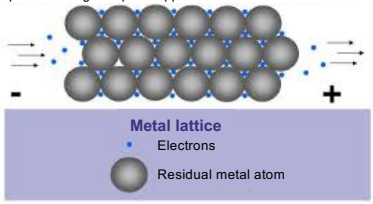
- When light shines on a metal, an electron within the band is promoted to a higher energy level.
- Since there are many energy levels, almost any amount of energy can be used.
- When falling back to a lower level, a light quantum (photon) is released => **metalic shine of metals**




Properties of Metals

- **Electric conductivity** (moveable electrons)
- **Metallic shine** (excitation of the electrons in the band)
- **Good thermal conductivity** (rapid mobility of the electrons)

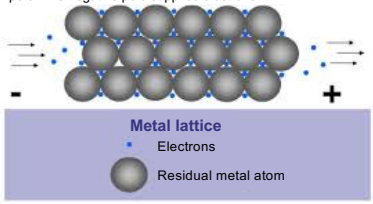
Fig.: Electrical conductivity of metals: When a voltage is applied, the freely movable electrons migrate to the positive pole. The negative pole supplies electrons.

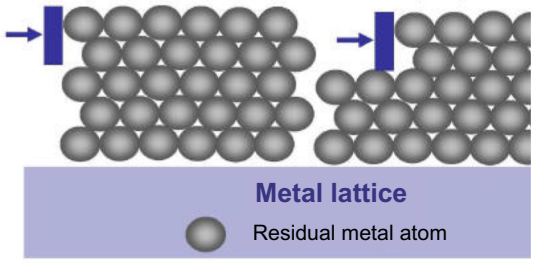


Properties of Metals

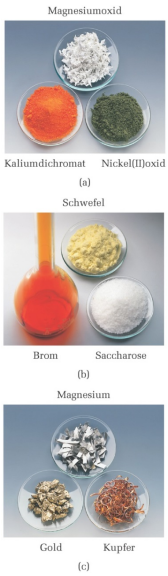
- **Electric conductivity** (moveable electrons)
- **Metallic shine** (excitation of the electrons in the band)
- **Good thermal conductivity** (rapid mobility of the electrons)
- **Ductility** (mobility of the cations)

Fig.: Electrical conductivity of metals: When a voltage is applied, the freely movable electrons migrate to the positive pole. The negative pole supplies electrons.



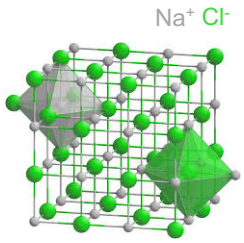


The Chemical Bond



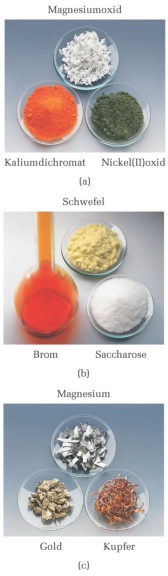
Ionic bond

Forces of attraction between anions and cations



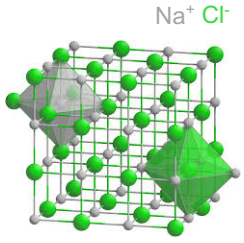
NaCl

The Chemical Bond



Ionic bond

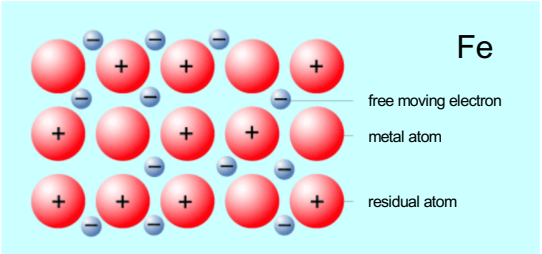
Forces of attraction between anions and cations



NaCl

Metal bond

electrostatic forces of attraction between metal ions and free electrons in a metal lattice



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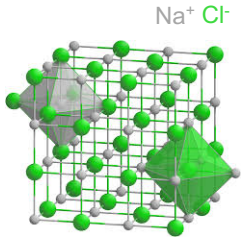
The Chemical Bond

Ionic bond

Forces of attraction between anions and cations

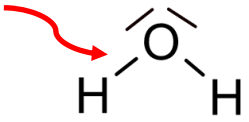


NaCl

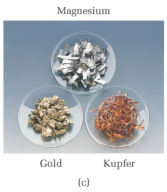
Covalent bond

Atoms share a pair of electrons

binding electron pair

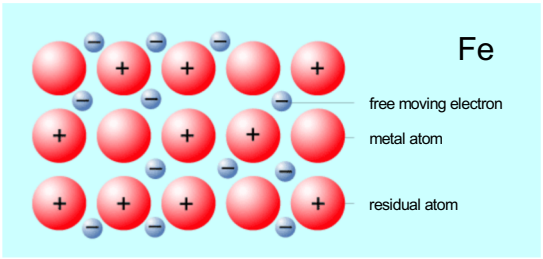


H_2O



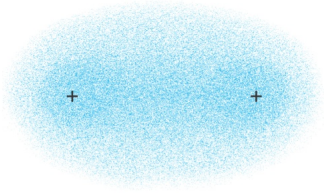
Metal bond

electrostatic forces of attraction between metal ions and free electrons in a metal lattice

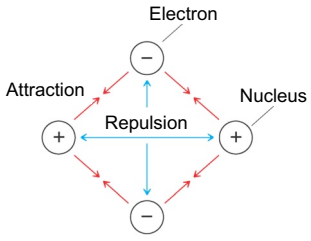


The Electron Bond Pair

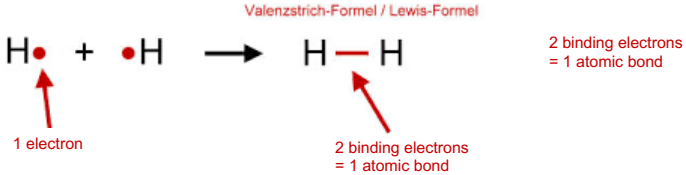
A covalent bond consists of a pair of electrons shared between two atoms.



(b)

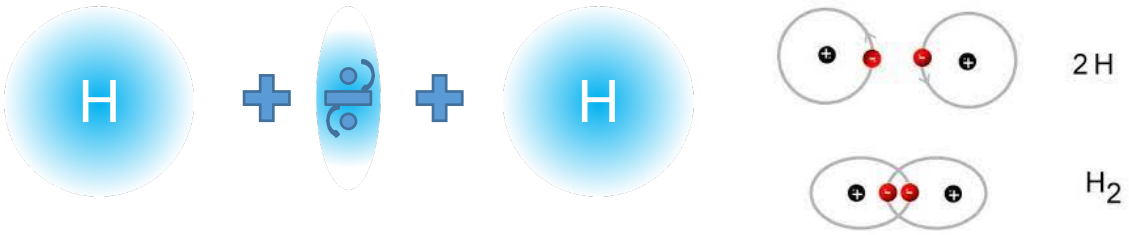


(a)

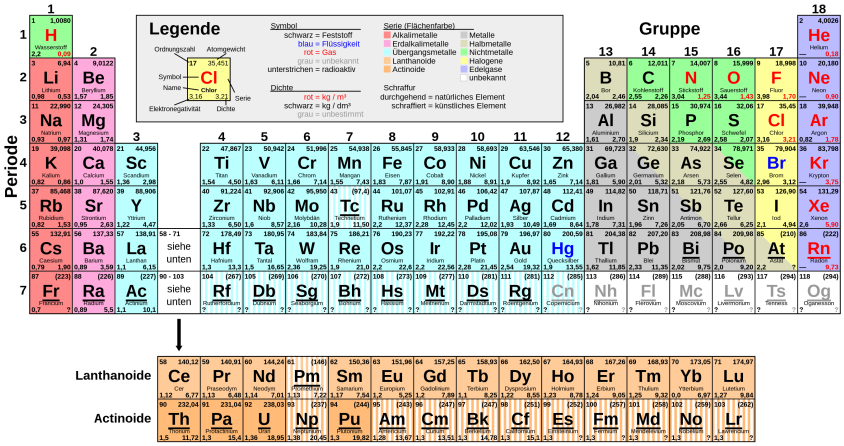


Covalent Bond

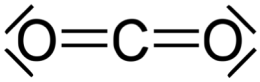
- When two hydrogen atoms come together:
  - The atomic orbitals overlap and the electron density between the nuclei becomes denser
  - This increased negative charge density attracts the two positively charged nuclei
  - The same applies to the shared electrons in this electron cloud: both electrons have opposite spins (Pauli principle)

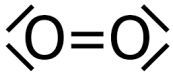


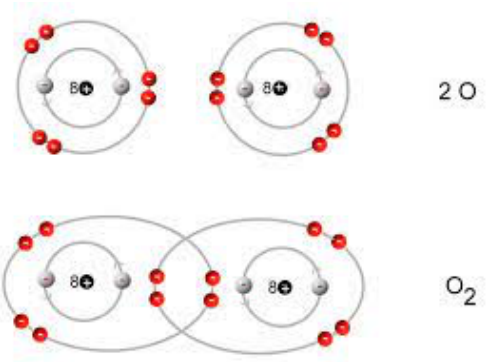
The Principle of the "Valence Electrons"



Multiple Bonds







Chemical Formulas

There are different ways to describe the composition or structure of chemical compoundshreiben:

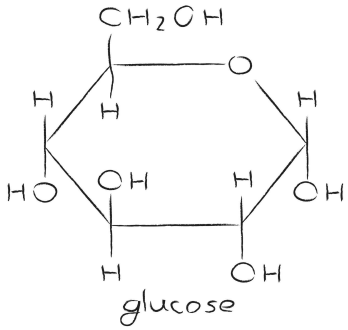
- The empirical formula (= ratio formula)
- The molecular formula (= chemical formula)
- The structural formula

Molecular Formulas

A molecular formula shows the actual number of atoms in a molecule.

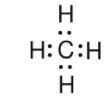
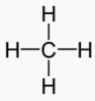
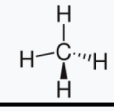
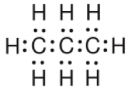
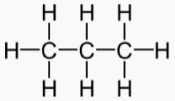
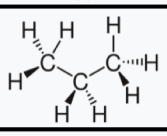
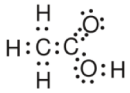
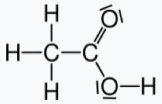
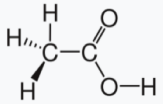
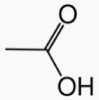
Examples are molecular formulas of

Water:	H_2O
Methane:	CH_4
Carbondioxide:	CO_2
Ammonia:	NH_3
Ethanol:	C_2H_6O
Glucose:	$C_6H_{12}O_6$



Structural Formula

A structural formula is used to represent atoms in molecules and illustrates the structure of the molecules

	Condensed Structural Formula	Lewis Structure	Valence Structural Formula	Wedge & dash projection	Skeletal Formula
Methane (CH_4)	CH_4				Does not exist
Propane (C_3H_8)	$CH_3CH_2CH_3$				
Acetic acid ($C_2H_4O_2$)	CH_3COOH				
Water (H_2O)	H_2O				Does not exist

Chemical Nomenclature

Generally:
Names are formed as if the compound were made up of ions

Advantage: Simplicity ☺

Disadvantage: one does not know whether compound really consists of ions or not ☹

Examples: Sulphur dioxide (SO_2) – covalent bond
Calcium oxide (CaO) – ionic bond

Examples of Nomenclature for Simple Compounds
(Nomenclature in Organic Chemistry: Chemistry 2 VU)

1. In the case of binary compounds, the metal name is given first (NH4+ means ammonium), then the designation of the (non-metal) anion.

2. In the case of binary covalent compounds, the element with the positive oxidation number is named first (electropositive component).

3. The suffix nonmetal atom or ion of binary compounds with a negative oxidation number ends in -ide.

4. The ending -ide is also used for anions such as B. CN^- = cyanide; OH^- = hydroxide; O_2^{2-} = -peroxide; NH_2^- = -amide or N_3^- = -azide.

5. If a cation (metal) exists in different oxidation states, the oxidation number is placed after the cation designation as a Roman numeral. The alkaline-(I) and alkaline earth metals(II) as well as B(III), Al(III), Zn(II) and Cd(II) have only one oxidation number.

6. If several elements of one type occur in covalent compounds, their number is indicated with Greek numerals: 1 = mono; 2 = di; 3 = tri; 4 = tetra; 5 = penta; 6 = hexa; 7 = hepta; 8 = octa; 9 = nona; 10 = deca; 11 = undeca; 12 = dodeca

Examples of Nomenclature for Simple Compounds
(Nomenclature in Organic Chemistry: Chemistry 2 VU)

CO_2
SO_3
N_2O
Al_2S_3
IF_5

Dihydrogen monoxide

- Dihydrogen monoxide poses the following dangers, among others:
- As a so-called 'hydroxy acid', it is a main component of acid rain
- It contributes to soil erosion
- It contributes to the greenhouse effect
- It accelerates corrosion and the failure of electrical systems and devices
- Excessive intake can lead to unpleasant consequences
- Prolonged contact with DHMO in the solid state causes severe tissue damage
- Inhalation, even in small amounts, can be fatal
- Its gaseous state can cause severe burns
- It was detected in the tumours of end-stage cancer patients
- For addicts, withdrawal leads to certain death within 168 hours

- **Despite these grave dangers, the government and corporations still maintain widespread use.**