800 1222·2022 ANNI

Università degli Studi di Padova

Dipartimento Matematica

Data Science
University of Padova

CHEMICAL BONDS

Master of Science in Data Science

Damiano Piovesan

Atomic theory - Dalton (1808)

DIPARTIMENTO MATEMATICA

- Matter is of **atoms**
- All atoms of the same **element** have the same chemical properties
- In **chemical reaction** atoms preserve their identity
- **Compounds** are made of a combination of two or more atom types
- A **molecule** is the combination of two or more bound atoms that act as a unit

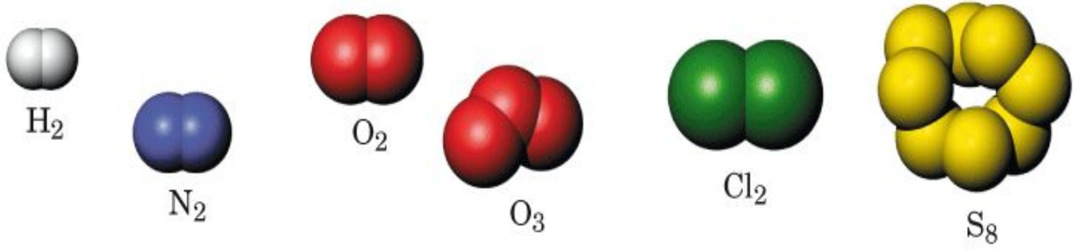
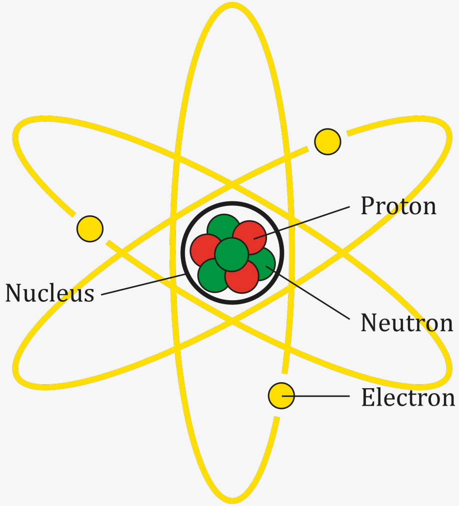


FIGURA 2.5 Alcuni elementi biatomicici, triatomici e poliatomici. Idrogeno, azoto, ossigeno e cloro sono elementi biatomici. L'ozono, O_3, è un elemento triatomico. Una forma dello zolfo, S_8, costituisce un elemento poliatomico.

Atoms abundance

	Human body (%) No. atoms	Human body (%) Mass	Earth (% crost mass)
H	63.0	10.0	0.9
O	25.4	64.8	49.3
C	9.4	18.0	0.08
N	1.4	3.1	0.03
Ca	0.31	1.8	3.4
P	0.22	1.4	0.12
K	0.06	0.4	2.4
S	0.05	0.3	0.06
Cl	0.03	0.2	0.2
Na	0.03	0.1	2.7
Mg	0.01	0.04	1.9
Si	—	—	25.8
Al	—	—	7.6
Fe	—	—	4.7
Altri	0.01	—	—

Subatomic particles



	Charge	Mass (g)	Mass (amu)	Mass (amu, rounded)
Proton	+1	1.6726×10^{-24}	1.0073	1
Electron	–1	9.1094×10^{-28}	5.4858×10^{-4}	0.0005
Neutron	0	1.6749×10^{-24}	1.0087	1

1 **Atomic Mass Unit** (amu) = 1 **Dalton**

1 / 12 of the mass of the carbon-12 atom

Periodic table - Mendeleev (1860)

Periods (rows)

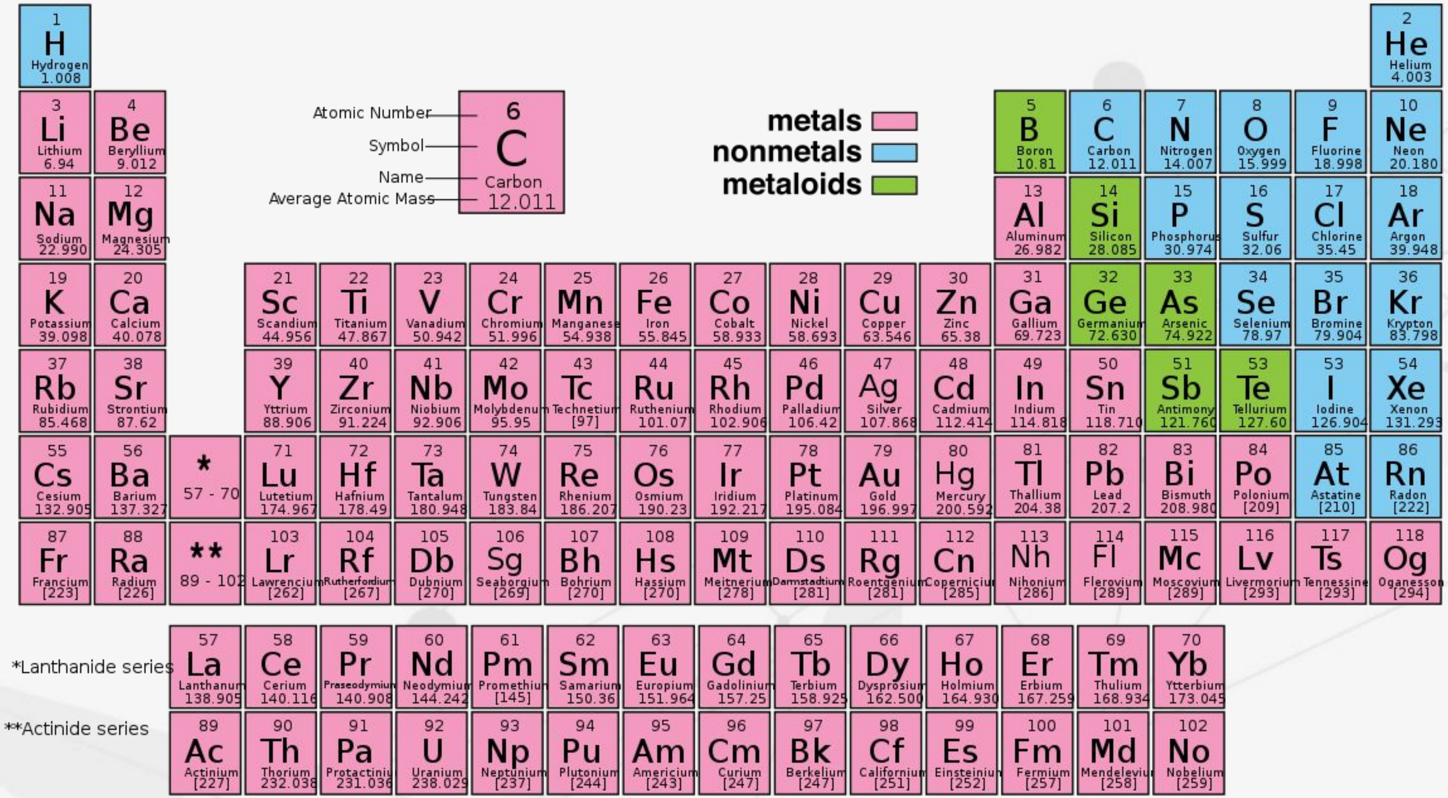
Groups (columns), similar properties

Main groups

- 1, 2, 13-18 (IUPAC)
- A (classic)

	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	8B 9	8B 10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116		

IUPAC = International Union of Pure and Applied Chemistry


Atomic Number
Symbol
Name
Average Atomic Mass
6 C Carbon 12.011
metals
nonmetals
metaloids
1 H Hydrogen 1.008
2 He Helium 4.003
3 Li Lithium 6.94
4 Be Beryllium 9.012
5 B Boron 10.81
6 C Carbon 12.011
7 N Nitrogen 14.007
8 O Oxygen 15.999
9 F Fluorine 18.998
10 Ne Neon 20.180
11 Na Sodium 22.990
12 Mg Magnesium 24.305
13 Al Aluminum 26.982
14 Si Silicon 28.085
15 P Phosphorus 30.974
16 S Sulfur 32.06
17 Cl Chlorine 35.45
18 Ar Argon 39.948
19 K Potassium 39.098
20 Ca Calcium 40.078
21 Sc Scandium 44.956
22 Ti Titanium 47.867
23 V Vanadium 50.942
24 Cr Chromium 51.996
25 Mn Manganese 54.938
26 Fe Iron 55.845
27 Co Cobalt 58.933
28 Ni Nickel 58.693
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.630
33 As Arsenic 74.922
34 Se Selenium 78.97
35 Br Bromine 79.904
36 Kr Krypton 83.798
37 Rb Rubidium 85.468
38 Sr Strontium 87.62
39 Y Yttrium 88.906
40 Zr Zirconium 91.224
41 Nb Niobium 92.906
42 Mo Molybdenum 95.95
43 Tc Technetium [97]
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.906
46 Pd Palladium 106.42
47 Ag Silver 107.868
48 Cd Cadmium 112.414
49 In Indium 114.818
50 Sn Tin 118.710
51 Sb Antimony 121.760
53 Te Tellurium 127.60
53 I Iodine 126.904
54 Xe Xenon 131.293
55 Cs Cesium 132.905
56 Ba Barium 137.327
* 57 - 70
71 Lu Lutetium 174.967
72 Hf Hafnium 178.49
73 Ta Tantalum 180.948
74 W Tungsten 183.84
75 Re Rhenium 186.207
76 Os Osmium 190.23
77 Ir Iridium 192.217
78 Pt Platinum 195.084
79 Au Gold 196.997
80 Hg Mercury 200.592
81 Tl Thallium 204.38
82 Pb Lead 207.2
83 Bi Bismuth 208.980
84 Po Polonium [209]
85 At Astatine [210]
86 Rn Radon [222]
87 Fr Francium [223]
88 Ra Radium [226]
** 89 - 102
103 Lr Lawrencium [262]
104 Rf Rutherfordium [267]
105 Db Dubnium [270]
106 Sg Seaborgium [269]
107 Bh Bohrium [270]
108 Hs Hassium [270]
109 Mt Meitnerium [278]
110 Ds Darmstadtium [281]
111 Rg Roentgenium [281]
112 Cn Copernicium [285]
113 Nh Nihonium [286]
114 Fl Flerovium [289]
115 Mc Moscovium [289]
116 Lv Livermorium [293]
117 Ts Tennessine [293]
118 Og Oganesson [294]
*Lanthanide series
57 La Lanthanum 138.905
58 Ce Cerium 140.116
59 Pr Praseodymium 140.908
60 Nd Neodymium 144.242
61 Pm Promethium [145]
62 Sm Samarium 150.36
63 Eu Europium 151.964
64 Gd Gadolinium 157.25
65 Tb Terbium 158.925
66 Dy Dysprosium 162.500
67 Ho Holmium 164.930
68 Er Erbium 167.259
69 Tm Thulium 168.934
70 Yb Ytterbium 173.045
**Actinide series
89 Ac Actinium [227]
90 Th Thorium 232.038
91 Pa Protactinium 231.036
92 U Uranium 238.029
93 Np Neptunium [237]
94 Pu Plutonium [244]
95 Am Americium [243]
96 Cm Curium [247]
97 Bk Berkelium [247]
98 Cf Californium [251]
99 Es Einsteinium [252]
100 Fm Fermium [257]
101 Md Mendelevium [258]
102 No Nobelium [259]

Groups

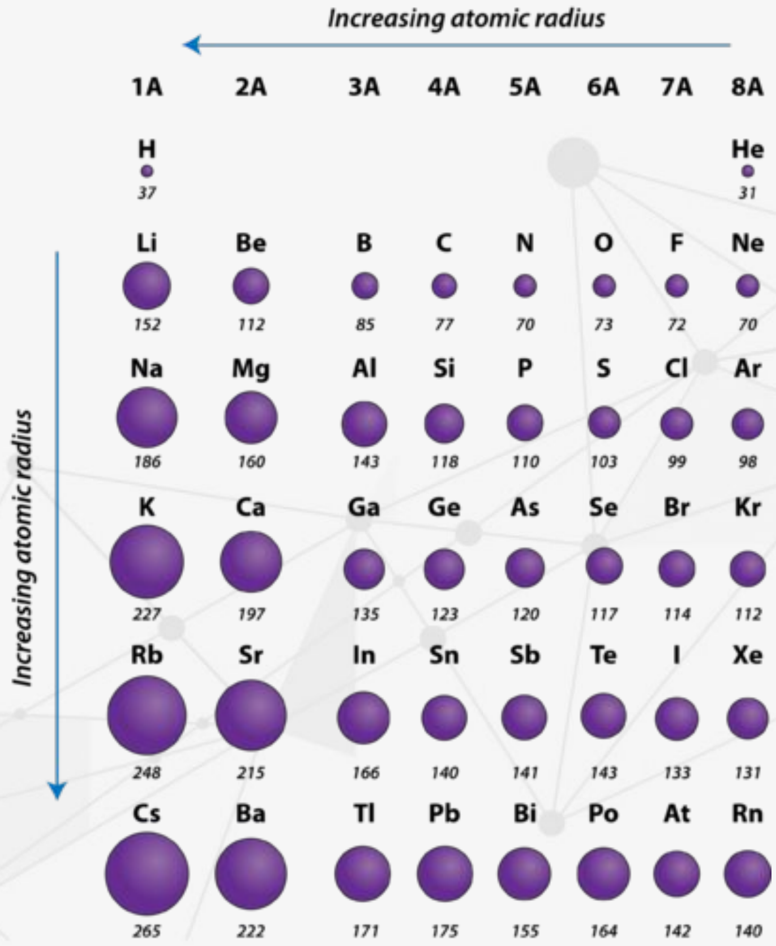
- **Metals**, solid at room temp. (except Mercury, Hg), lustrous, conduct electricity, react with halogens, group 7A (Zn + Cl → ZnCl)
- **Non metals**, do not coduct electricity (except graphite), tend to accept electrons
  - **Halogens (group 7a)**, react with sodium Na***X***
  - **Noble gas**, do not react
- **Metalloids (semimetals)**, B - Boron, Si - Silicon, Ge - Germanium, As - Arsenic, Sb - Antimony, Te - Tellurium

Electrons

Niels Bohr (1913)

- The energy of the electron is quantized
- The ground state corresponds is at minimum energy
- Electrons are arranged into “shell” with growing energy

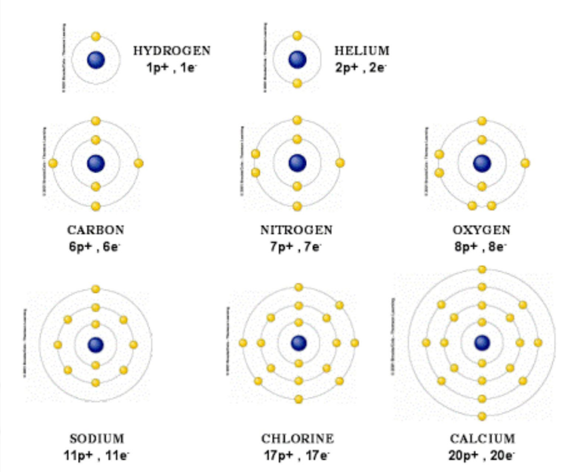
Atomic radius



Octet rule

The maximum atomic stability (lower pot. energy) is obtained taking/losing/sharing electrons with other atoms in order to reach **eighth electrons** in the **external (valence) shell**, irrespective of the number of protons (charge)

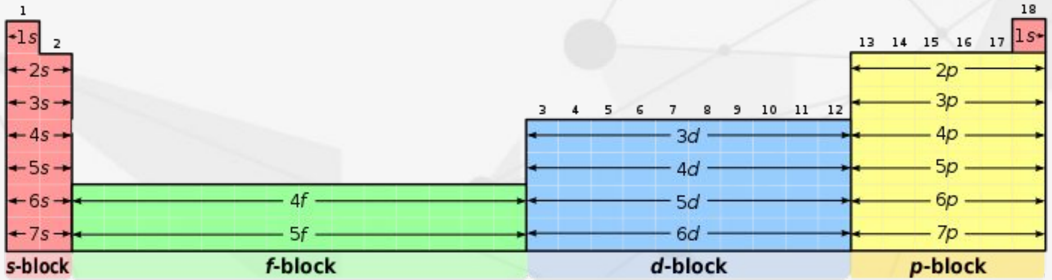
- Atoms tend to react to reach the electronic configuration of the closest **noble gas**
- The rules does not apply to transition metals
- Periods 1 and 2 do not form ions with charge >+2
- Atoms and the corresponding ions have completely different chemical properties

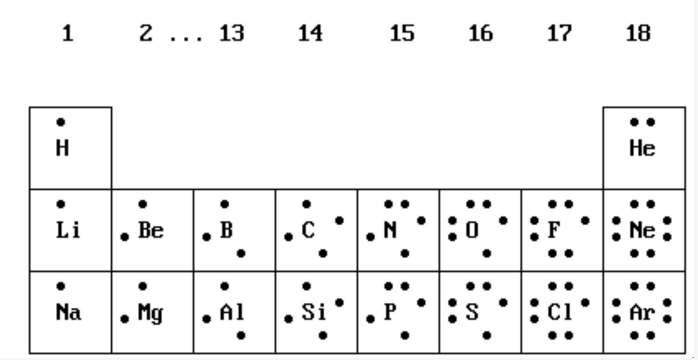


Noble Gas	Electron Configuration
He	$1s^2$
Ne	$[He]2s^2\,2p^6$
Ar	$[Ne]3s^2\,3p^6$
Kr	$[Ar]4s^2\,4p^6\,3d^{10}$
Xe	$[Kr]5s^2\,5p^6\,4d^{10}$

Stable configurations

- The **first period** (first energetic level) can accommodate **2 electrons**
- The **other levels** can accomodate **8 electrons**
- Each level has a **S** and **P sublevels** of 2 and 6 electrons, respectively
- **H** and **He** don't have P level
- Also other atoms can have only S when considering the external (valence) shell





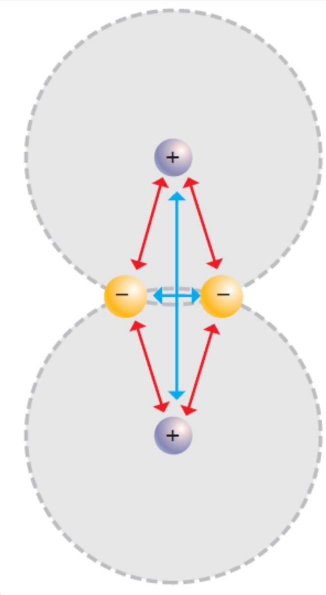
Valence electrons

- The most external shell
- Participate to bond formation
- Provide chemical properties of an atom

He:	$1s^2$
:Ne:	$1s^2 2s^2 2p^6$
:Ar:	$1s^2 2s^2 2p^6 3s^2 3p^6$
:Kr:	$[Ar]4s^2 3d^{10} 4p^6$
:Xe:	$[Kr]5s^2 4d^{10} 5p^6$
:Rn:	$[Xe]6s^2 4f^{14} 5d^{10} 6p^6$

Bonds

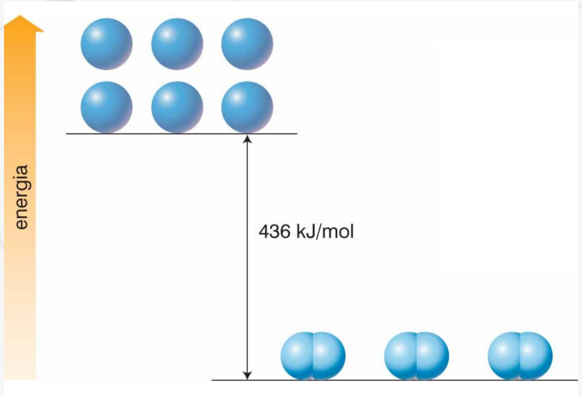
Bond formation and energy transfers



- **Chemical bonds** are forces that hold atoms together to make compounds or molecules
- Nuclei and electrons inside a molecule feel attraction and repulsion because they are **charged**
- When two atoms form a **bond** the resulting molecule (or ion) has a **lower potential energy**

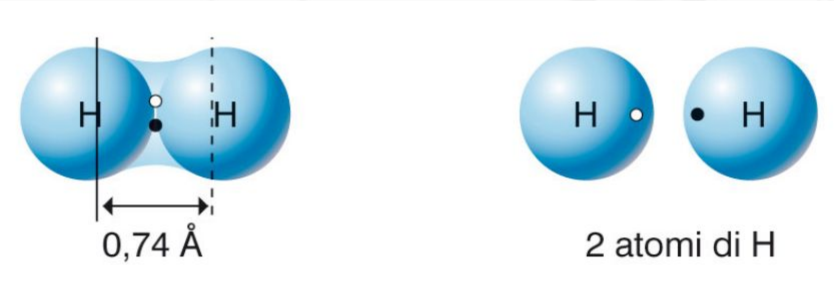
Bond energy

- Not all atomic combinations (molecules) are possible
- The potential energy of the molecule has to be lower than isolated atoms
- A molecule forms only if binding atoms release potential energy
- The bond energy (kJ/mol) is the energy necessary to break all atoms bonds of a mole of compound
- Higher the energy, higher the bond strength



Bond length

- The bond length is the distance between two atomic nuclei
- Increase with atom size and with the opposite of the bonding force



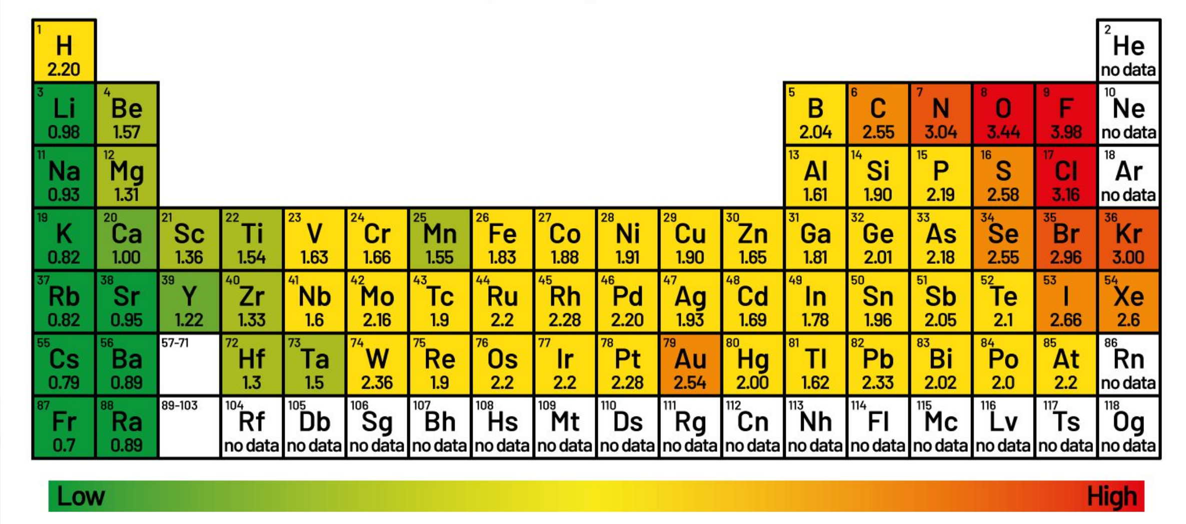
Bond types

- **Ionic**, two ions with **opposite charge**, metal + nonmetal (Δelettronegativity > 1.9)
- **Covalent**, two atoms that share one or more **electron pairs**, two nonmetals or nonmetal + metalloid
  - **Pure (non polar)**, Δelettronegativity < 0.5
  - **Polar**, 0.5 < Δelettronegativity < 1.9
  - **Dative**, the shared electron pair come from a single atom

Electronegativity

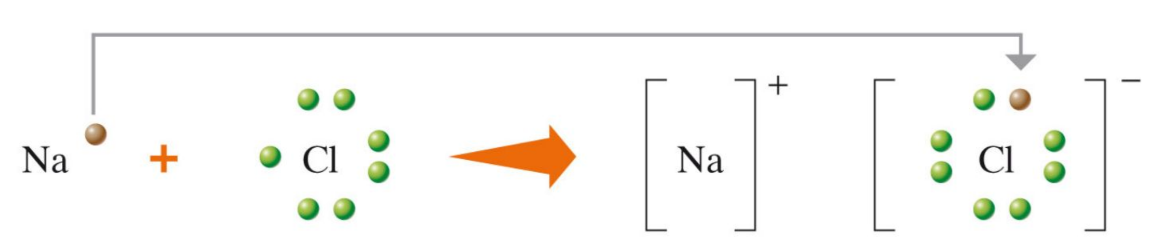
DIPARTIMENTO MATEMATICA

- Tendency of an atom to **attract** a shared **pair of electrons** (of a bonded atom)
- Affected by atomic number (**group**) and the distance (atom radius) of valence electrons (**period**) from the charged nucleus



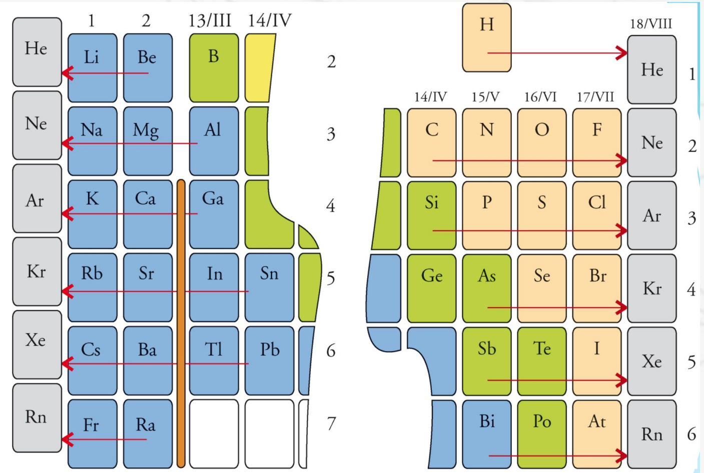
Ionic bond

- **Transfer** of one or more **electrons** from the valence shell of the atom with the lower electronegativity the other atom
- **Electrostatic force** between ions of opposite charge. The total charge is zero
- Ionic compounds are **not molecules** but have a precise stoichiometry



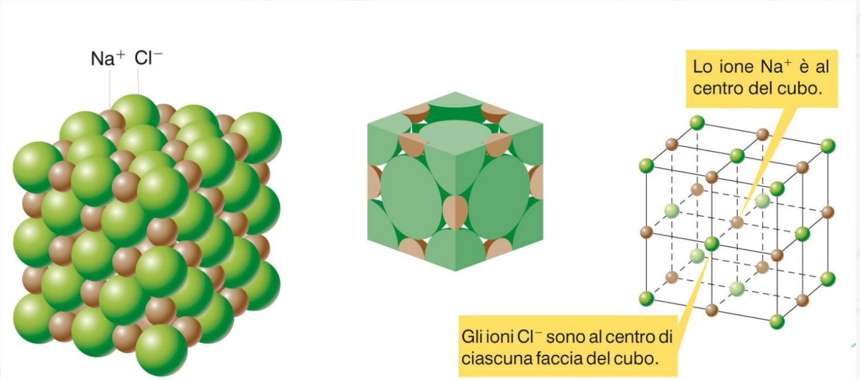
Ionic bond

- **Negative ions** get the configuration of the following noble gas
- **Positive ions** get the configuration of the preceding noble gas
- Ionic bonds have the **longest range effect**
- The force has **radial direction**
- **High energy** 170 - 1500 kJ/mol

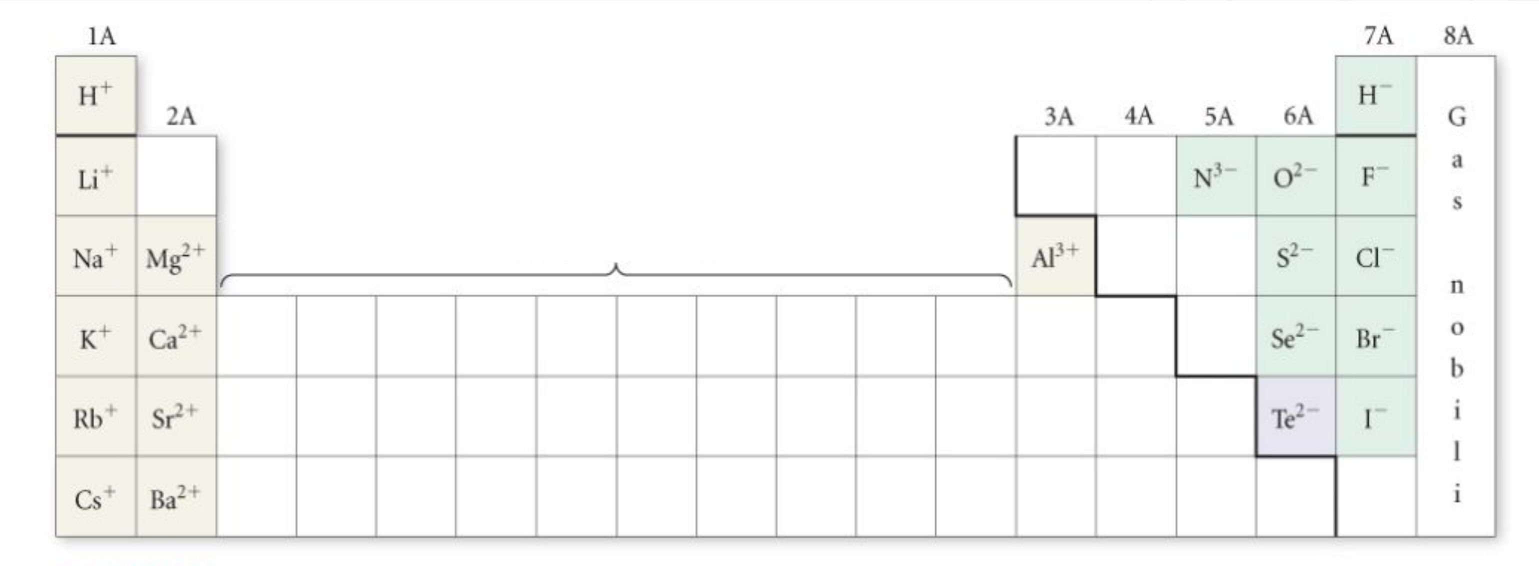


Ionic bond

- Ions are well ordered in the compound so that they form **crystals**
- Ionic compounds melt at high temperature, are **solid** at room temperature and are **good conductors**



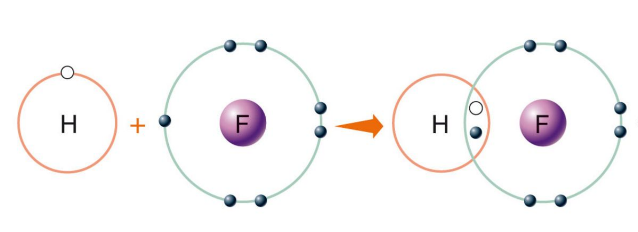
Ions with a predictable charge



Covalent bond

DIPARTIMENTO MATEMATICA

- Two atoms **share** one or more **electron pairs**
- Electrons are used to reach the octet and belong to both atoms at the same time
- Bond energy is around 50 - 110 Kj/mol
  - **Pure (non polar)**, Δelettronegativity < 0.5
  - **Polar**, 0.5 < Δelettronegativity < 1.9
  - **Dative**, the shared electron pair come from a single atom

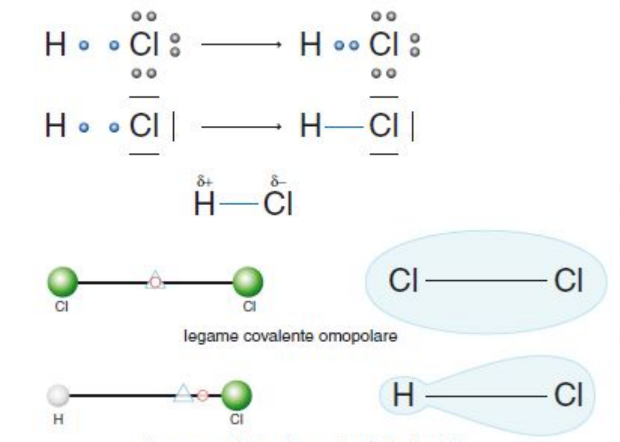


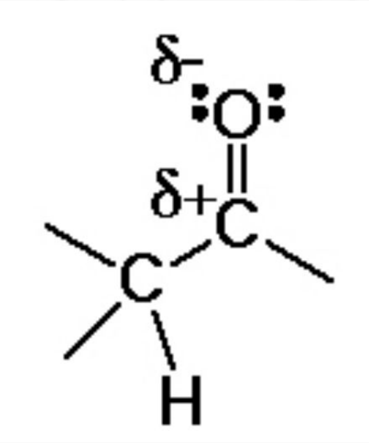
Covalent bond types

- Single, only one pair of electrons is shared
- Double, two pairs
- Triple, three pairs

Polar covalent bond

- Oxygen, nitrogen and sulfur **electrons** are usually displaced when they bind a hydrogen
- Groups **-OH, -NH, -SH** polarize surrounding regions
- **C=O** is also polar



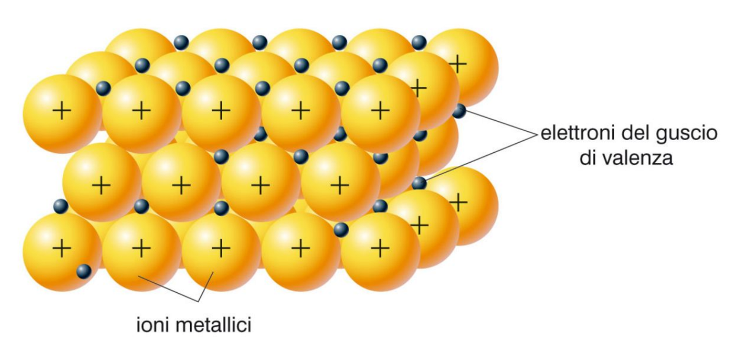


Polar covalent and ionic bonds

- Higher the **electronegativity difference** between bound atoms higher the polar tendency of the bond
- With **Δ-electronegativity > 1.9** the atom rip off the electron from the binding partner and form an **ionic bond**

Metal bond

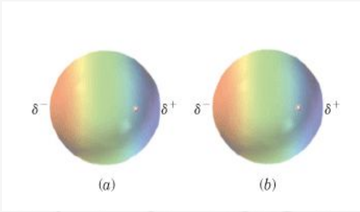
- Valence electrons are shared between multiple nuclei
- Higher the strength, higher the number of shared electrons
- Mobility of external electrons defines the properties
  - shineness
  - electric/thermal conduction
  - malleability
  - ductility

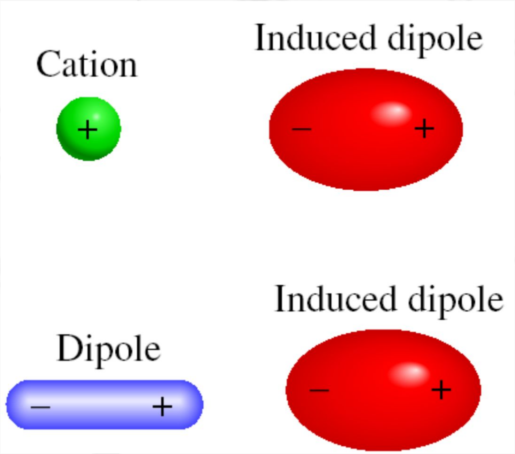


Weak interactions (non-covalent)

Van der Waals

- Instantaneous or induced dipoles
- Attractive at long range
- Repulsive at short range
- Depending on fluctuations they can be
  - Temporary dipoles (London)
  - Dipole-dipole induced (Debye)
  - Permanent dipoles (Keesom)



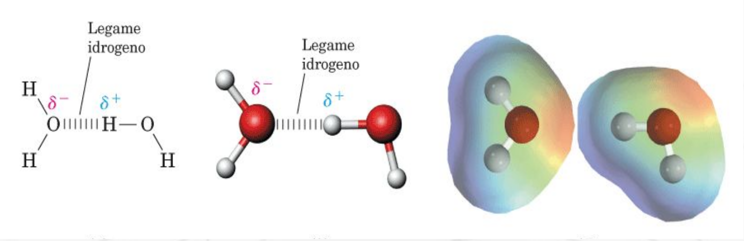


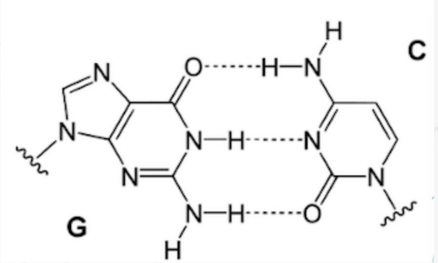
Van der Waals

- Very weak forces (**1 kj/mol**)
- Thanks to London dispersion forces all compounds can become liquid (Neon -246 ° C)
- Geckos use toe-pads consisting of millions of thin-hairs to increase the number of VdW interactions

Hydrogen bond

- Special case of dipole-dipole but more energetic
- H get slightly positive when bound to an O, N, F. Then it can interact with another O, N, F
- How many H-bonds a molecule of H_2O can have?
- How many ligands are bound to O?





Interaction forces

Kcal / mol

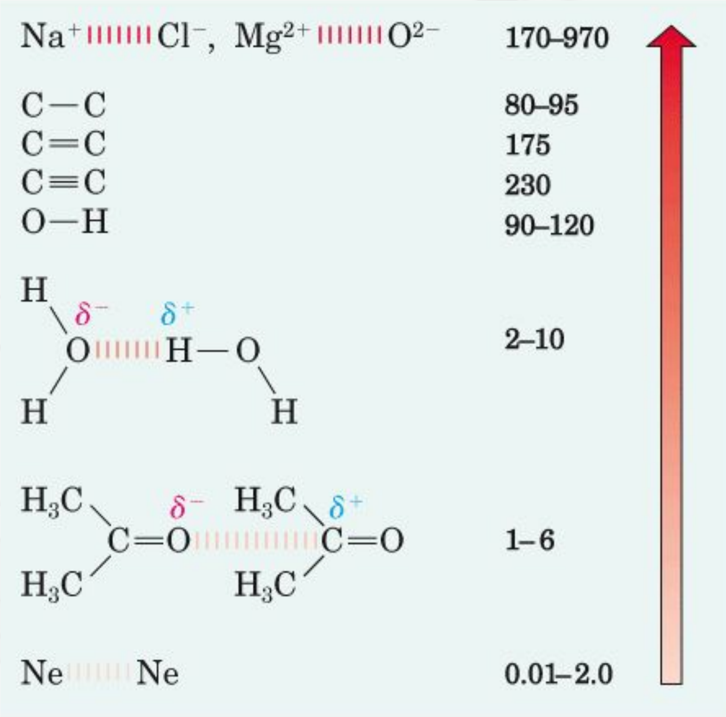
Ionic bonds

Covalent bonds

Hydrogen bonds

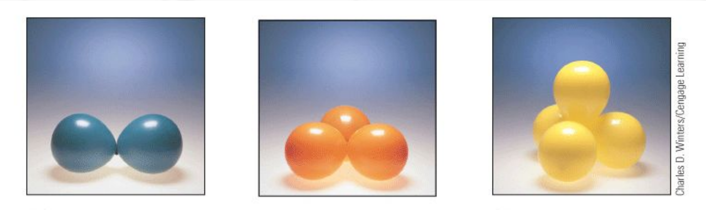
Dipole-dipole interactions

London dispersion forces



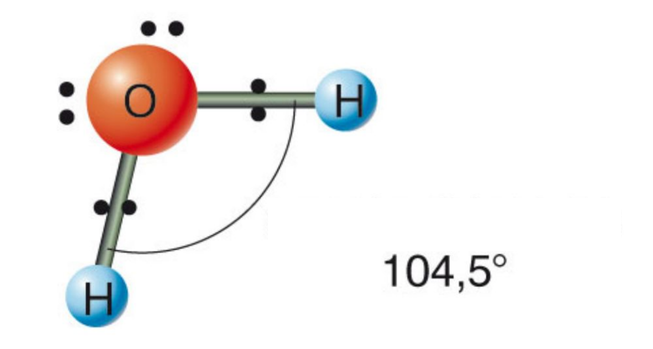
Molecular shape

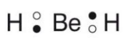
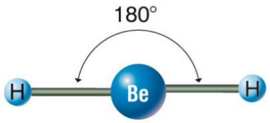
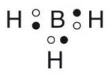
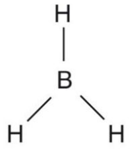
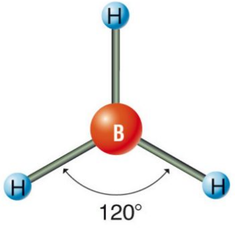
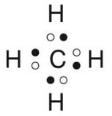
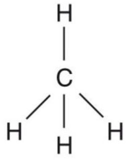
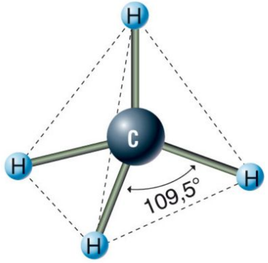
- Molecular geometry is given by bond angles
- Valence Shell Electron-Pair Repulsion theory (**VSEPR**)
- Electron density is distributed to maximize the distance between bonds (or electron pairs)
- Depending on the number of pairs in the central nucleus
  - Two pairs → linear, 180°
  - Three pairs → equilateral triangle, 120°
  - Four pairs → tetrahedron, 109.5°

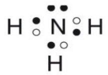
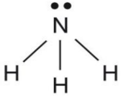
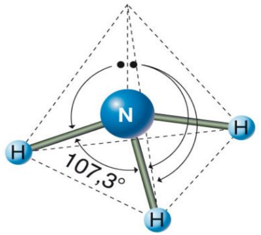
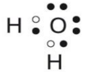
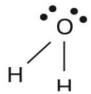
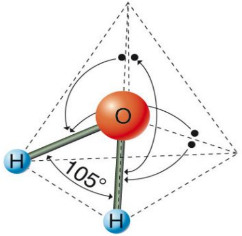
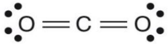
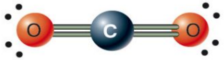
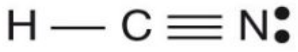


VSEPR - Free electrons pairs

- Free electron pairs have a stronger repulsion in comparison with shared pairs (occupy more space)
- Double and triple covalent bonds have same geometry of single bonds



Beryllium hydride	BeH_2	2		H — Be — H	180°	
Trihydridoboron (borane)	BH_3	3			120°	
Methane	CH_4	4			109,5°	

Ammonia	NH_3	4			107,3°	
	H_2O	4			105°	
	CO_2	2			180°	
Hydrogen cyanide	HCN	2			180°