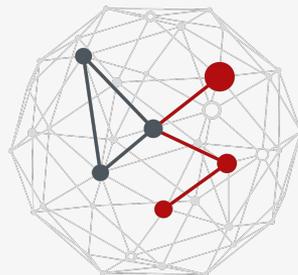


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UNIVERSITÀ
DEGLI STUDI
DI PADOVA

  DIPARTIMENTO
MATEMATICA



DATA SCIENCE
UNIVERSITY OF PADOVA

CHEMICAL BONDS

Master of Science in Data Science

Damiano Piovesan



What is chemistry

Matter → A substance that has mass and occupies space

Transformation → A process of change

Physical Transformation → The identity of the matter does not change

- Change of state (e.g., solid to liquid)
- Separation of a mixture (e.g., filtration or evaporation)
- Physical Properties: Density, color

Chemical Transformation → The change of matter from one form to another.

- Chemical reaction → A process where substances are converted into different substances with different properties



Atomic theory - Dalton (1808)

- 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

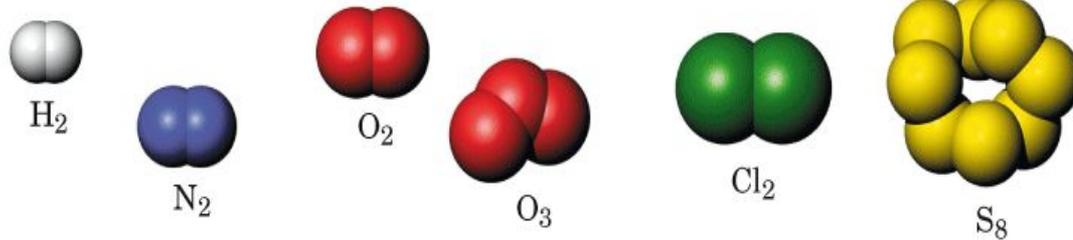
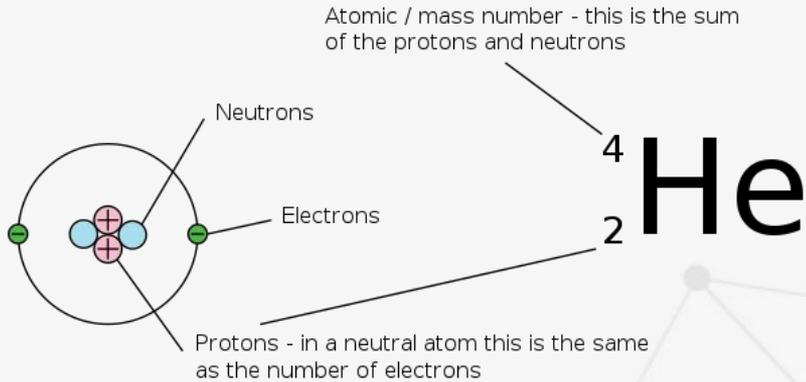


FIGURA 2.5 Alcuni elementi biatomici, triatomici e poliatomici. Idrogeno, azoto, ossigeno e cloro sono elementi biatomici. L'ozono, O_3 , è un elemento triatomico. Una forma dello zolfo, S_8 , costituisce un elemento poliatomico.

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



Atoms abundance

Human body (%) **Earth**
 No. atoms - Mass (% 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 | — | — |



Periodic table - Mendeleev (1860)

Periods (rows)

Groups (columns), similar properties

Main groups

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

| | 1A 1 | 2A 2 | | | | | | | | | | | 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 | 3B 3 | 4B 4 | 5B 5 | 6B 6 | 7B 7 | 8B 8 9 10 | | 1B 11 | 2B 12 | 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



Periodic table of the elements

| period | group 1* | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 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 Cn | 113 Nh | 114 Fl | 115 Mc | 116 Lv | 117 Ts | 118 Og |

| | | | | | | | | | | | | | | |
|---------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------|------------------|------------------|------------------|
| lanthanoid series 6 | 58 Ce | 59 Pr | 60 Nd | 61 Pm | 62 Sm | 63 Eu | 64 Gd | 65 Tb | 66 Dy | 67 Ho | 68 Er | 69 Tm | 70 Yb | 71 Lu |
| actinoid series 7 | 90 Th | 91 Pa | 92 U | 93 Np | 94 Pu | 95 Am | 96 Cm | 97 Bk | 98 Cf | 99 Es | 100 Fm | 101 Md | 102 No | 103 Lr |



Groups

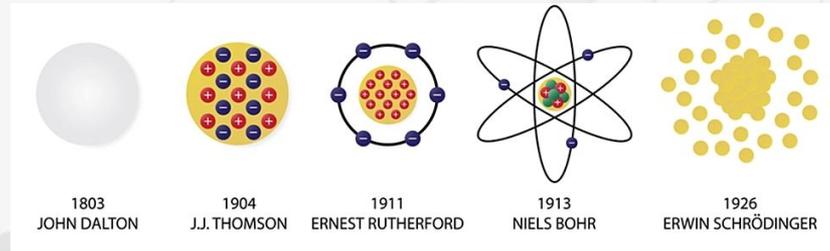
- **Metals**, solid at room temp. (except Mercury, Hg), lustrous, conduct electricity, react with halogens, group 7A ($\text{Zn} + \text{Cl} \rightarrow \text{ZnCl}$)
- **Non metals**, do not conduct electricity (except graphite), tend to accept electrons
 - **Halogens (group 7a)**, react with sodium NaX
 - **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
- Electrons are arranged into “shell” with growing energy
- The ground state corresponds to the minimum energy



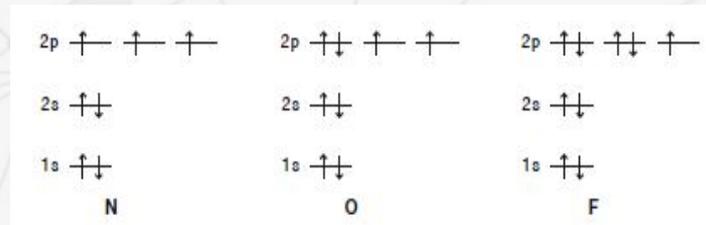
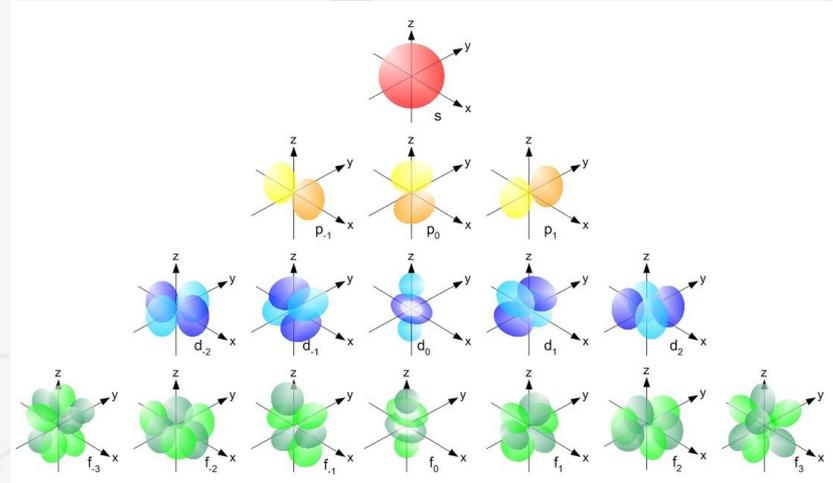
Quantum numbers

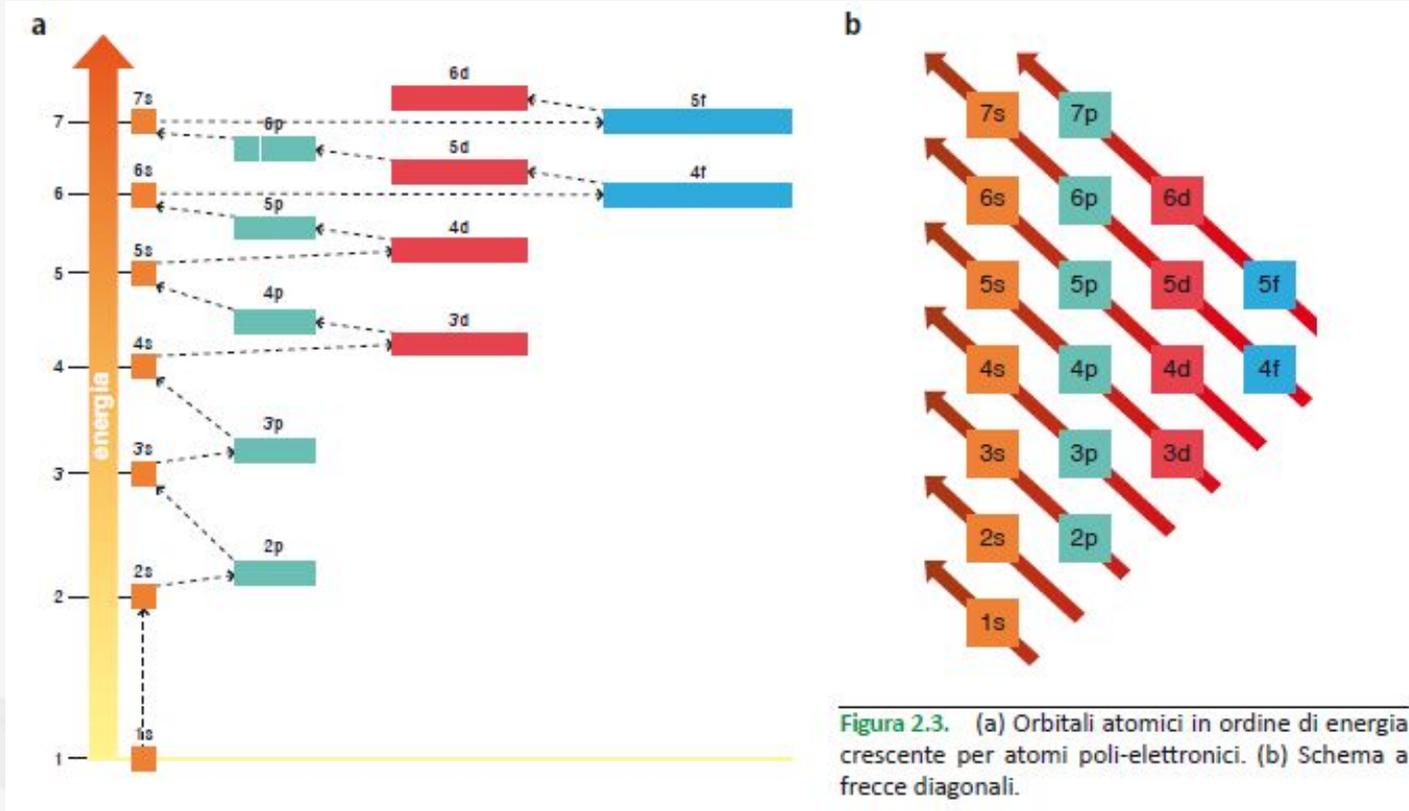
- **Shell - n** (1, 2, 3 ..., 7)
 - Main energetic level
 - Electron closer to the nucleus are attracted more strongly
- **Subshell - l** (s, p, d, f)
 - Energetic sublevel (same letter = same sublevel)
 - Contain the **orbitals**
 - Different types of subshells have different number of orbitals (s = 1, p = 3, d = 5, f = 7)
- **Orbital - m_l** (s = 0, p = -1 / 0 / +1, d = -2 / -1 / 0 / +1 / +2, ...)
 - Wave function of the electron density (Schrödinger equation)
 - Each orbital contains at most **two electrons** (Pauli's exclusion principle)
 - Electrons in the same orbital have opposite spin (spin number **m_s**)



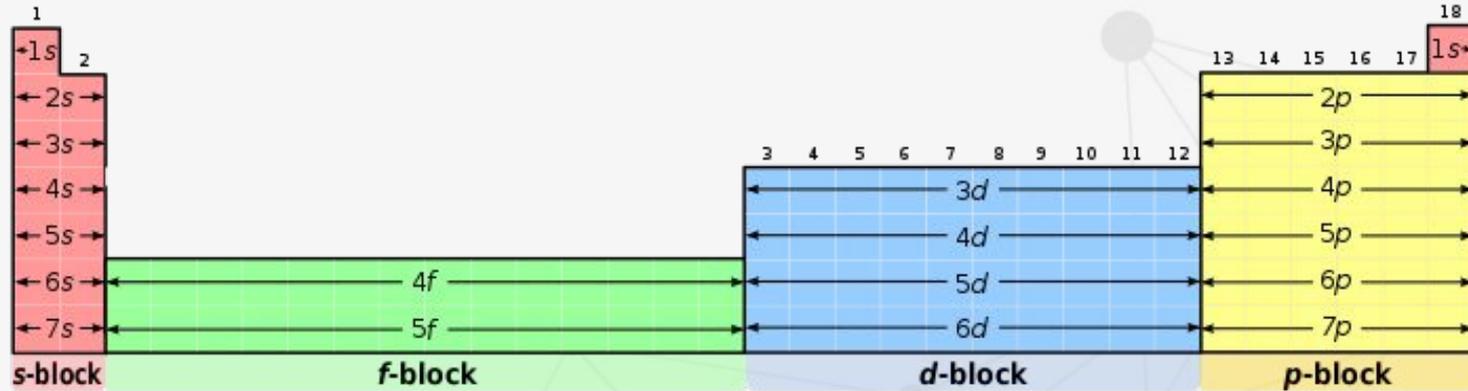
Orbitals

- Each orbital can be populated by at most 2 electrons (**Pauli's exclusion principle**)
- Electrons fill subshells of the lowest available energy (**Aufbau principle**)
- Isoenergetic orbitals are initially filled with electrons with the same spin and after the other electrons are added (**Hund's rule**)
- Organic compounds (H, C, S, N, O, P) use only 1s, 2s, 2p, 3s, 3p





Electronic configurations



| 1 | 2 | ... | 13 | 14 | 15 | 16 | 17 | 18 |
|----|----|-----|----|----|----|----|----|----|
| H | | | | | | | | He |
| Li | Be | B | C | N | O | F | Ne | |
| Na | Mg | Al | Si | P | S | Cl | Ar | |



Exercises



1. Identify the element $^{194}_{78}\text{X}$ and indicate its

- a. Atomic number
- b. Mass number
- c. Number of protons
- d. Number of electrons
- e. Number of neutrons

2. Identify the highest energy subshell occupied in the atoms of the following elements

- a. Iodine
- b. Scandium
- c. Arsenic
- d. Aluminum



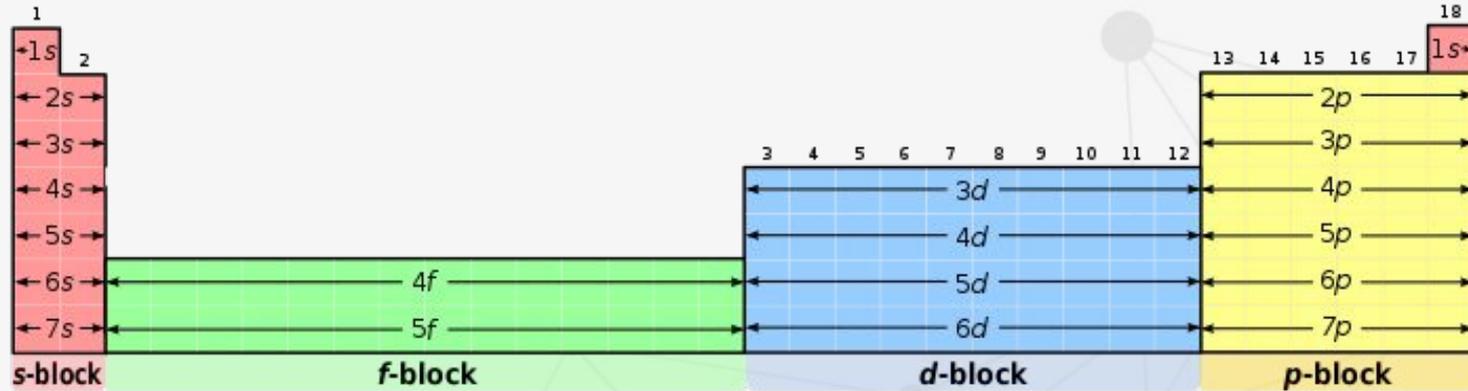
3. An unidentified element has an electronic configuration, from the lowest to the highest level, equal to 2, 8, 18, 8, 2
- To which group and period does this element belong?
 - Is it a metal or a non-metal?
 - How many protons does it have?
 - What is its name?
 - Write its Lewis dot symbol
4. Determine the only possible $2+$ ion for which the total ionic charge is one-tenth of the nuclear charge.



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



Electronic configurations



| 1 | 2 | ... | 13 | 14 | 15 | 16 | 17 | 18 |
|---------|----------|----------|----------|----------|-----------|------------|------------|----------|
| • H | | | | | | | | •• He |
| • Li | •• Be | •• B | •• C | ••• N | •••• O | •••• F | •••• Ne | |
| • Na | •• Mg | •• Al | •• Si | ••• P | •••• S | •••• Cl | •••• Ar | |



Bonds



Electronegativity

- 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

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------------------|------------------|------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|------|--|--|--|--|--|--|--|--|--|--|--|--|--|--|--|--|--|
| 1 H 2.20 | | | | | | | | | | | | | | | | | 2 He no data | | | | | | | | | | | | | | | | | | |
| 3 Li 0.98 | 4 Be 1.57 | | | | | | | | | | | 5 B 2.04 | 6 C 2.55 | 7 N 3.04 | 8 O 3.44 | 9 F 3.98 | 10 Ne no data | | | | | | | | | | | | | | | | | | |
| 11 Na 0.93 | 12 Mg 1.31 | | | | | | | | | | | 13 Al 1.61 | 14 Si 1.90 | 15 P 2.19 | 16 S 2.58 | 17 Cl 3.16 | 18 Ar no data | | | | | | | | | | | | | | | | | | |
| 19 K 0.82 | 20 Ca 1.00 | 21 Sc 1.36 | 22 Ti 1.54 | 23 V 1.63 | 24 Cr 1.66 | 25 Mn 1.55 | 26 Fe 1.83 | 27 Co 1.88 | 28 Ni 1.91 | 29 Cu 1.90 | 30 Zn 1.65 | 31 Ga 1.81 | 32 Ge 2.01 | 33 As 2.18 | 34 Se 2.55 | 35 Br 2.96 | 36 Kr 3.00 | | | | | | | | | | | | | | | | | | |
| 37 Rb 0.82 | 38 Sr 0.95 | 39 Y 1.22 | 40 Zr 1.33 | 41 Nb 1.6 | 42 Mo 2.16 | 43 Tc 1.9 | 44 Ru 2.2 | 45 Rh 2.28 | 46 Pd 2.20 | 47 Ag 1.93 | 48 Cd 1.69 | 49 In 1.78 | 50 Sn 1.96 | 51 Sb 2.05 | 52 Te 2.1 | 53 I 2.66 | 54 Xe 2.6 | | | | | | | | | | | | | | | | | | |
| 55 Cs 0.79 | 56 Ba 0.89 | 57-71 | 72 Hf 1.3 | 73 Ta 1.5 | 74 W 2.36 | 75 Re 1.9 | 76 Os 2.2 | 77 Ir 2.2 | 78 Pt 2.28 | 79 Au 2.54 | 80 Hg 2.00 | 81 Tl 1.62 | 82 Pb 2.33 | 83 Bi 2.02 | 84 Po 2.0 | 85 At 2.2 | 86 Rn no data | | | | | | | | | | | | | | | | | | |
| 87 Fr 0.7 | 88 Ra 0.89 | 89-103 | 104 Rf no data | 105 Db no data | 106 Sg no data | 107 Bh no data | 108 Hs no data | 109 Mt no data | 110 Ds no data | 111 Rg no data | 112 Cn no data | 113 Nh no data | 114 Fl no data | 115 Mc no data | 116 Lv no data | 117 Ts no data | 118 Og no data | | | | | | | | | | | | | | | | | | |
| Low | | | | | | | | | | | | | | | | | | High | | | | | | | | | | | | | | | | | |



Valence

- Valence electrons are those located in the outermost shell
- They are the only electrons involved in the formation of chemical bonds
- They are represented as dots in Lewis structures

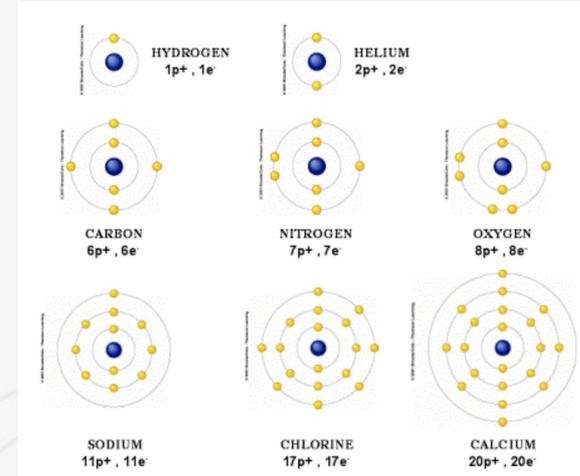
| 1A | 2A | 3A | 4A | 5A | 6A | 7A | 8A |
|-----|-----|-----|------|-----|-----|------|------|
| H· | | | | | | | He· |
| Li· | Be· | B· | ·C· | ·N· | ·O· | ·F· | ·Ne· |
| Na· | Mg· | Al· | ·Si· | ·P· | ·S· | ·Cl· | ·Ar· |



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 rule 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

1s²

Ne

[He]2s² 2p⁶

Ar

[Ne]3s² 3p⁶

Kr

[Ar]4s² 4p⁶ 3d¹⁰

Xe

[Kr]5s² 5p⁶ 4d¹⁰

Chemical bonds

- **Covalent bond**
- **Electrostatic bond**
 - Ionic (chemical bond)
 - Ion-dipole, hydrogen, Van der Waals (secondary interactions)
- **Metallic bond**



Bond types

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



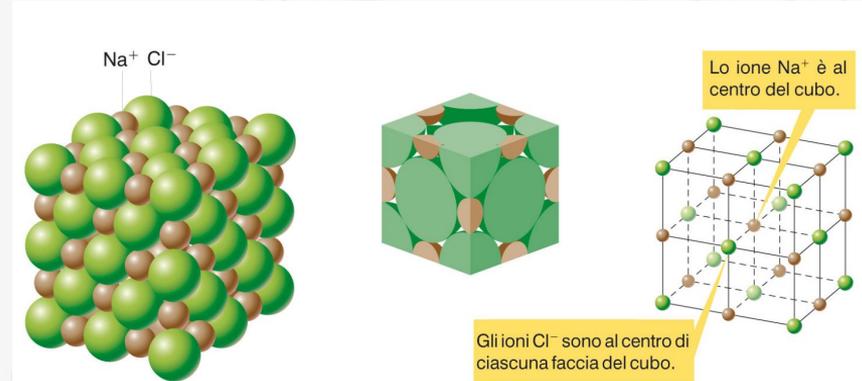
Ionic bond

- **Transfer** of one or more **electrons** from the valence shell of the atom with the lower electronegativity to 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



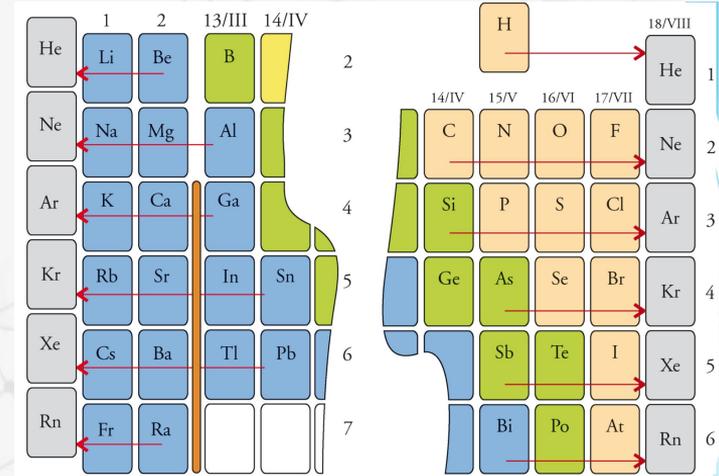
Ionic bond

- 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**



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

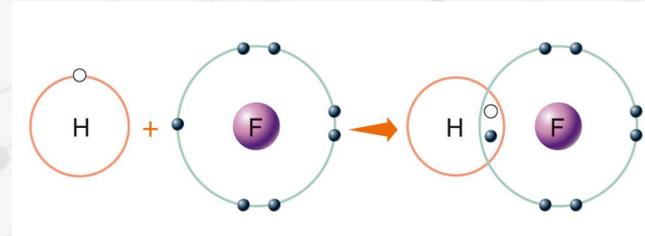


| | 1 | 2 | 13/III | 14/IV | | | 18/VIII |
|----|----|----|--------|-------|---|----|---------|
| He | Li | Be | B | | 2 | H | He |
| Ne | Na | Mg | Al | | 3 | C | Ne |
| Ar | K | Ca | Ga | | 4 | Si | Ar |
| Kr | Rb | Sr | In | Sn | 5 | Ge | Kr |
| Xe | Cs | Ba | Tl | Pb | 6 | Sb | Xe |
| Rn | Fr | Ra | | | 7 | Bi | Rn |



Covalent bond (VB valence-bond theory)

- **Two atoms share** one or more **electron pairs** (1 pair = 1 single bond) that fill the valence shell of both atoms
- Formation of a **molecular orbital (MO)**
- Bond energy is around 50 - 110 KJ/mol
 - **Pure (non polar)**, $\Delta\text{elettronegativity} < 0.5$
 - **Polar**, $0.5 < \Delta\text{elettronegativity} < 1.9$
 - **Dative**, the shared electron pair come from a single atom



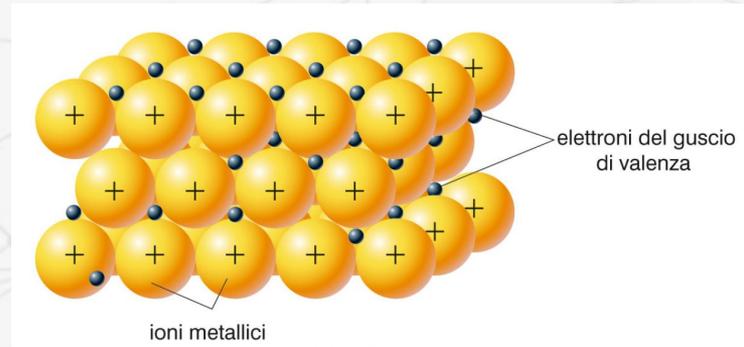
Covalent bond types

- Single (σ), only one pair of electrons is shared
- Double (π), two pairs
- Triple (π , 2x), three pairs

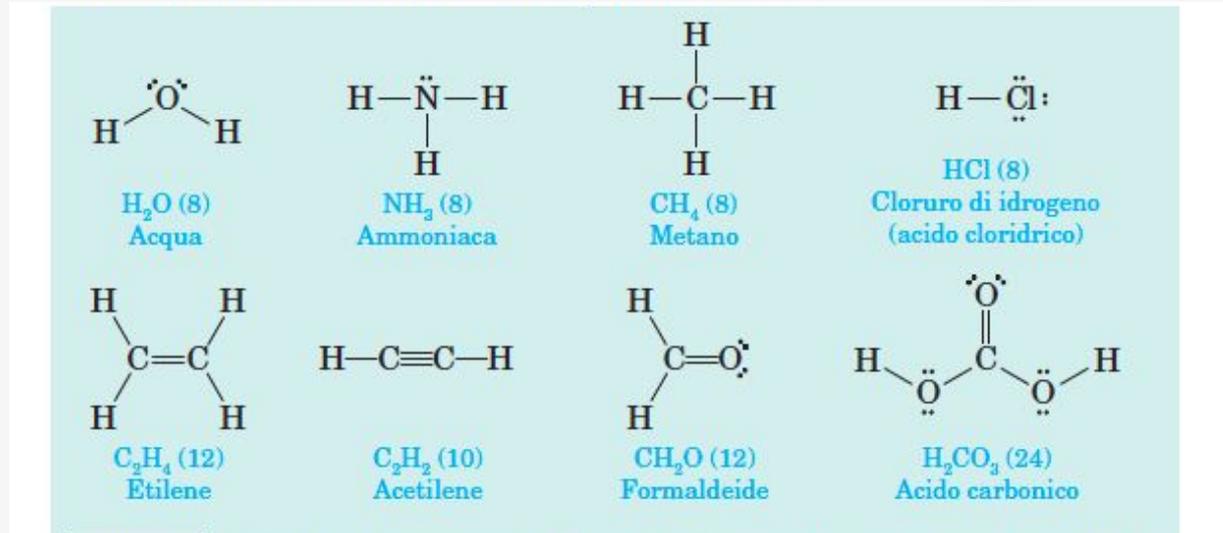


Metal bond

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



Lewis structures



Water, ammonia, methane, hydrochloric acid
 Ethylene, acetylene, formaldehyde, carbonic acid



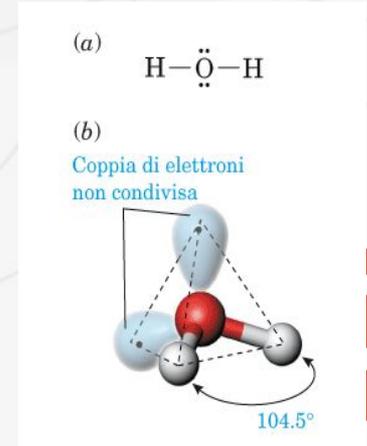
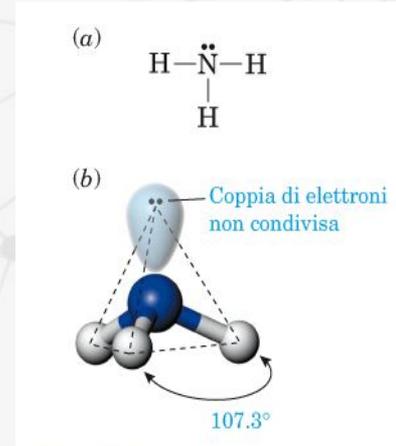
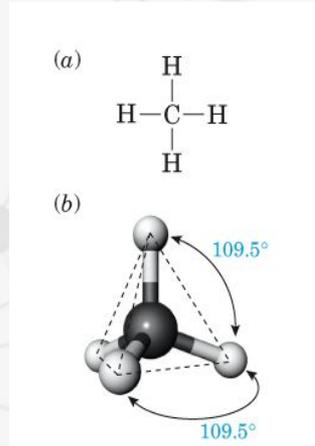
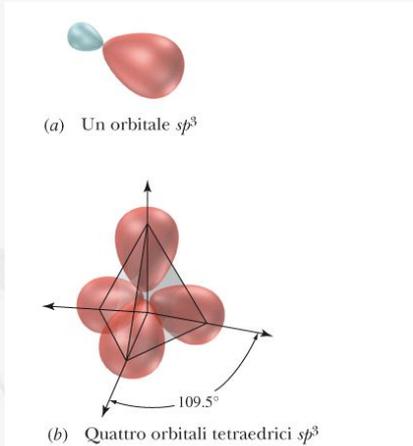
Orbital hybridization

- Diatomic molecules are all **linear**; to understand the geometry of molecules with more than 2 atoms, the concept of hybridization must be introduced
- **VB theory** → The bond is formed by the **overlap of partially occupied orbitals**, giving rise to a **molecular orbital** in which the electrons from the two atomic orbitals pair up (bonding pair)
- In the carbon **$1s^2 2s^2 2p^2$** configuration, only two bonds could be formed (2 partially occupied p orbitals). In this case, the four orbitals of the same main energy level mix to form **hybrid orbitals**
 - **$2s^2 2p^2$** → **sp^3** → 4 hybrid orbitals
 - **$2s^2 2p^2$** → **sp^2** → 3 hybrid orbitals + 1 unchanged p orbital (pz)
 - **$2s^2 2p^2$** → **sp** → 2 hybrid orbitals + 2 unchanged p orbitals



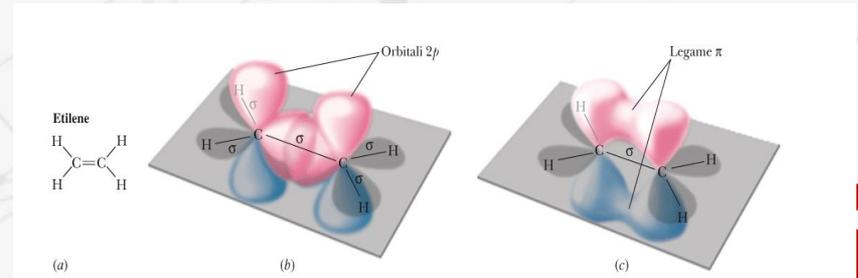
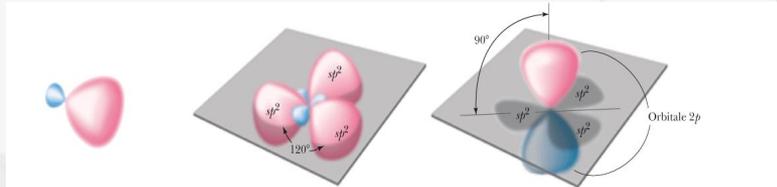
sp^3 hybridization

- 4 sp^3 orbitals directed towards the vertices of a tetrahedron
- 109.5°
- 4 sigma bonds (single bonds)
- C of **diamond**, saturated organic molecules



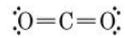
sp^2 hybridization

- 3 sp^2 orbitals in the same plane + 1 perpendicular $2p$ orbital
- 120°
- Double bond \rightarrow 1 sigma bond + 1 π bond
- C of **graphite**. The pure p orbitals are all parallel and perpendicular to the xy plane, each with 1 electron forming a delocalized cloud \rightarrow Conductivity, black color, lubricant



sp hybridization

Biossido di carbonio



Vista laterale



Vista dall'estremità

Acetilene



Vista laterale



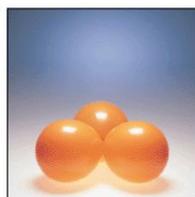
Vista dall'estremità

FIGURA 3.10 Forme dell'anidride carbonica, CO_2 , e dell'acetilene, C_2H_2 .



Molecular shape

- **Valence Shell Electron-Pair Repulsion (VSEPR) model**
- Electron density is distributed to **maximize the distance between bonds** (or electron pairs)
- **Electron pairs fill more space** than a bond



Charles D. Wilentz / Computer Learning



Intermolecular forces

(Non-covalent interactions)



Intermolecular Forces

Van der Waals Forces

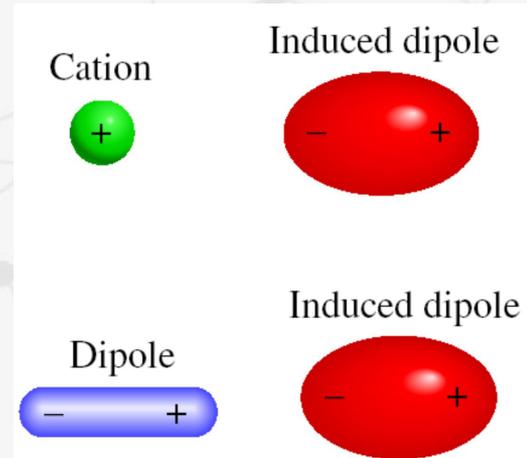
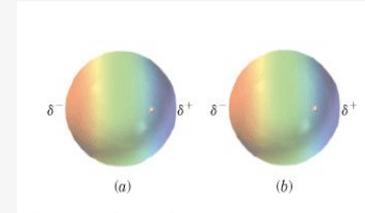
- Permanent dipole–permanent dipole (**Keesom forces**)
- Permanent dipole–induced dipole (**Debye forces**)
- Instantaneous dipole–induced dipole (**London dispersion forces**)

Hydrogen bond



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)



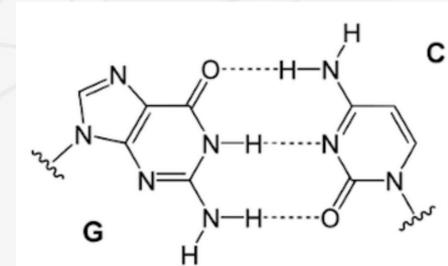
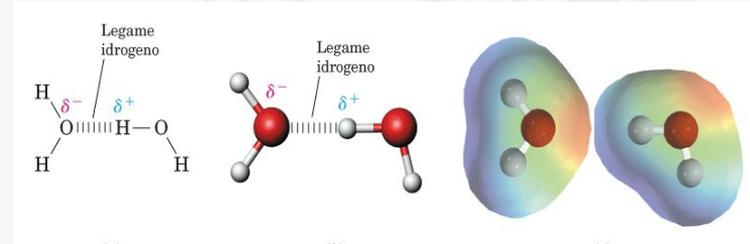
London dispersion forces

- Very weak forces (**1 kJ/mol**)
- Thanks to London dispersion forces all compounds can become liquid (Neon $-246\text{ }^{\circ}\text{C}$)
- Geckos use toe-pads consisting of millions of thin-hairs to increase the number of VdW interactions

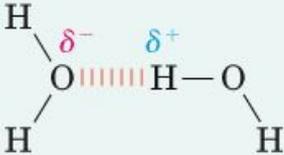
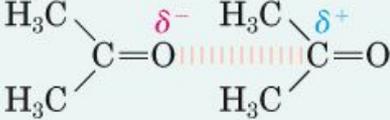


Hydrogen bond

- 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 H₂O can have?



Interaction forces

| | | Kcal / mol |
|----------------------------|--|--|
| Ionic bonds | $\text{Na}^+ \text{-----} \text{Cl}^-$, $\text{Mg}^{2+} \text{-----} \text{O}^{2-}$ | 170-970 |
| Covalent bonds | $\text{C}-\text{C}$ | 80-95 |
| | $\text{C}=\text{C}$ | 175 |
| | $\text{C}\equiv\text{C}$ | 230 |
| | $\text{O}-\text{H}$ | 90-120 |
| | Hydrogen bonds |  |
| Dipole-dipole interactions |  | 1-6 |
| London dispersion forces | $\text{Ne} \text{-----} \text{Ne}$ | 0.01-2.0 |

