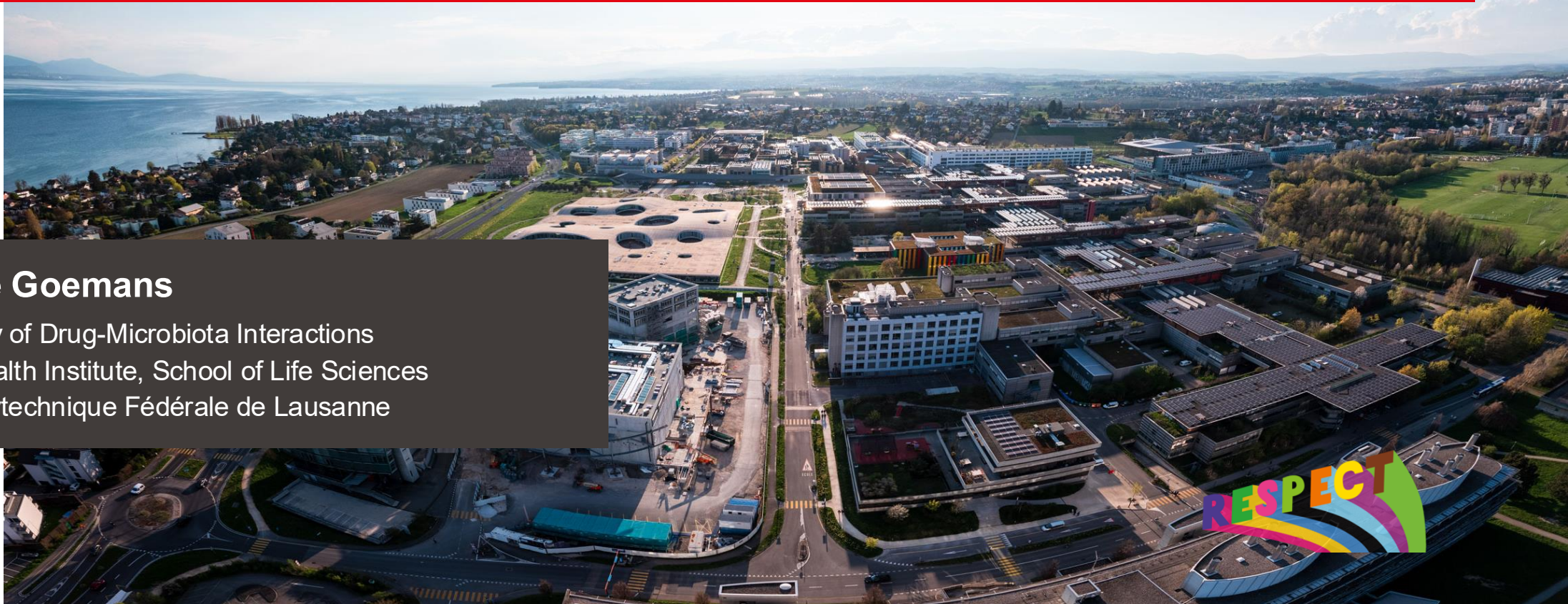


# General Chemistry - Lecture 4

## Bonds between atoms

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# Questions from last week

- **What defines how a wave behaves after passing through a slit (double slit experiment)**
  - **Diffraction** is the bending and spreading of waves when they encounter an obstacle or pass through a narrow opening.
  - Occurs with all types of waves – sound, water, light, and even matter waves (like electrons).
  - More noticeable when the obstacle or opening is comparable in size to the wavelength of the wave.
  - **Results in wave spreading** instead of continuing in a straight line.

# Questions from last week

- **Are electrons particles that move on waves?**
  - Electrons are not particles *on* waves — they are **quantum objects** that can be described as both a localized particle *and* a spread-out wave of probability.
  - Electrons do **not** literally wiggle or travel like a water wave. Instead:
    - The **wave** in quantum mechanics is the **wavefunction** ( $\Psi$ ).
    - This wavefunction is not a physical wave of matter, but a **mathematical description** of where the electron is likely to be.
    - The square of the wavefunction's amplitude  $|\Psi|^2$  gives the **probability density** — i.e. the chance of finding the electron at a certain position if you measure it.

# Questions from last week

- Can you clarify the uncertainty principle?

- You cannot know everything about a particle at once with perfect accuracy.

Specifically, you can't know both:

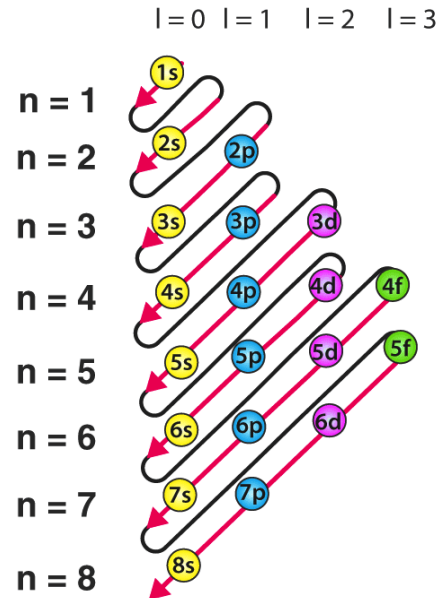
- **where it is** (position), and
    - **how fast it's moving / in what direction** (momentum).
    - The more precisely you measure one, the fuzzier the other becomes.
  - Imagine trying to take a photo of a racing car at night:
    - If you use a very **short exposure**, you get a sharp picture of *where* the car is — but it looks frozen, so you can't tell how fast it was going.
    - If you use a **long exposure**, you see the streak (showing speed/direction) — but now you've lost the precise position.
    - That's basically the uncertainty principle!

# Information on Exam

- It will last ?h
- You can bring a **pen, eraser** and **simple calculator**
- You will have **12 multiple choice questions** (each 2.5 points, no negative points) and **3 open questions** (each 10 points) --> total of **60** points
- In the last weeks of the semester, we will provide a **mock exam** for you to test yourselves but in general, the best preparation is to be able to do the **exercise series!**

# Orbitals – filling and ion formation

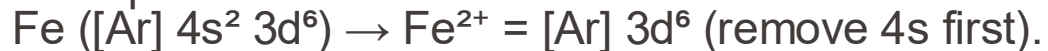
- When we fill orbitals, we follow the energy level – this tells us how many electrons are in each orbital.
- When we write the electron configuration, we can either follow the energy level (Br<sup>-</sup> : [Ar] 4s<sup>2</sup> 3d<sup>10</sup> 4p<sup>6</sup>) or the principal quantum number (Br<sup>-</sup> : [Ar] 3d<sup>10</sup> 4s<sup>2</sup>4p<sup>6</sup>) – both are **correct**



# Orbitals – filling and ion formation

- When we add or remove electrons to form ions:
  - For main-group elements (s- and p-block):
    - When forming **cations**, electrons are removed from the orbital with the **highest principal quantum number (n)** first (the outermost shell).
    - When forming **anions**, electrons are **added** to the orbital with the **lowest available energy** (usually the lowest empty p orbital in that shell).
  - For transition metals (d-block):
    - This is the tricky part: although the 3d orbitals fill after 4s, when forming cations we remove electrons from the **4s (n=4) orbital before 3d (n=3)**, because 4s is higher in energy once the d orbitals have electrons.

Example:



# Orbitals – filling and ion formation

## So the general rule:

- 👉 Electrons are removed first from the orbital with the highest principal quantum number ( $n$ ).
- 👉 If two orbitals have the same  $n$ , the one with the higher azimuthal quantum number ( $l$ ) is removed first (so  $p$  before  $s$ ,  $d$  before  $p$ , etc.).

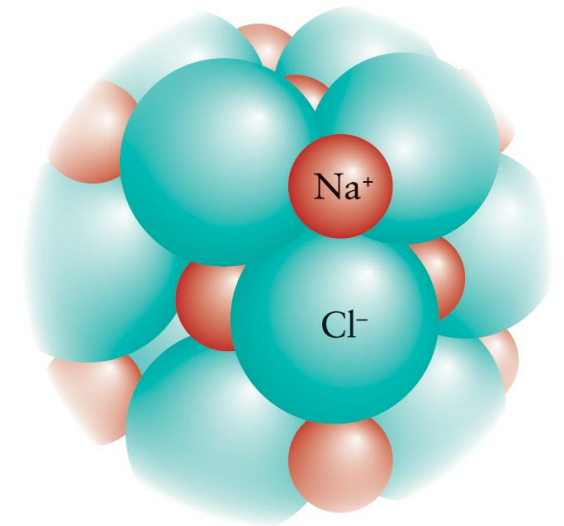
- **Introduction**
  - What is a chemical bond
  - What are the different types of bonds
- Lewis representation
  - Octet rule
  - Examples
  - Limitations
- Geometric representation (VSEPR)
- Quantum approach

# Bonds between atoms

- Each atom is unique due to their differing sizes, electron affinities, and ionization energies
- Atoms minimize these imbalances by forming bonds
- Atoms strive to fill their outer shell with electrons just like a noble gas does
- In a generalized way, atoms can achieve satisfaction by forming three types of bonds
  - **Ionic bonds** are formed by *gaining & losing* electrons.
  - **Covalent bonds** are formed by *sharing* electrons.
  - **Metallic bonds**

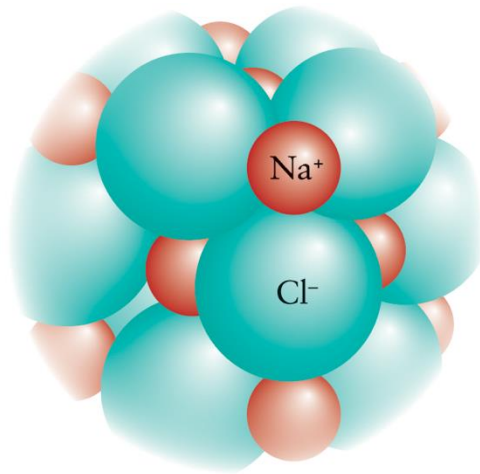
# Ionic bonding

- **Ionic bonds** form when one element loses electrons and the other atom gains electrons, until both atoms reach a *noble-gas configuration*
- This typically happens in metal-nonmetal bond where the electrons of the metal go to the nonmetal
- Ionic bond is a bond between ions of opposite charge (+ and -)
- The entire compound is held together by electrostatic attractions between all the ions.
- This happens when there is a large electronegativity difference between the atoms ( $>1.7$ )
- The new ionic partnership is lower in energy than the separate atoms.



# Properties of ionic compounds

- Cations and anions stack into alternating, oppositely charged ions that line up in three dimensions, to form an ionic crystalline solid
- Bonding energy is high and fusion points are also high
- Soluble in water but not in organic solvents
- Conduct electricity in water solution



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(d)

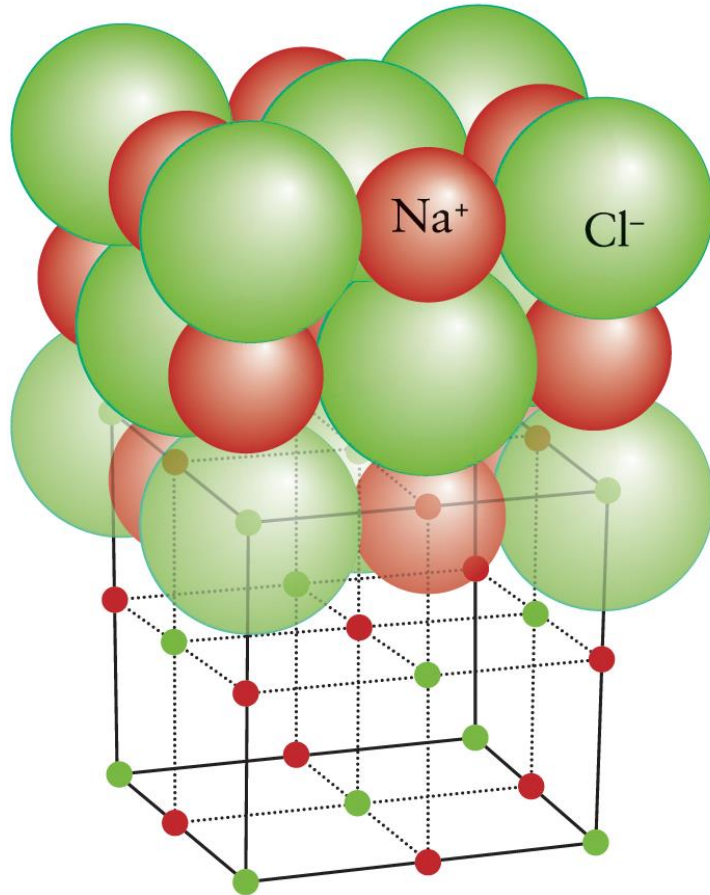


(e)

Parts (d) and (e) Paul Silverman/Fundamental Photographs.  
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# Ion crystal formation

Large numbers of oppositely charged ions combine, releasing large amounts of energy.



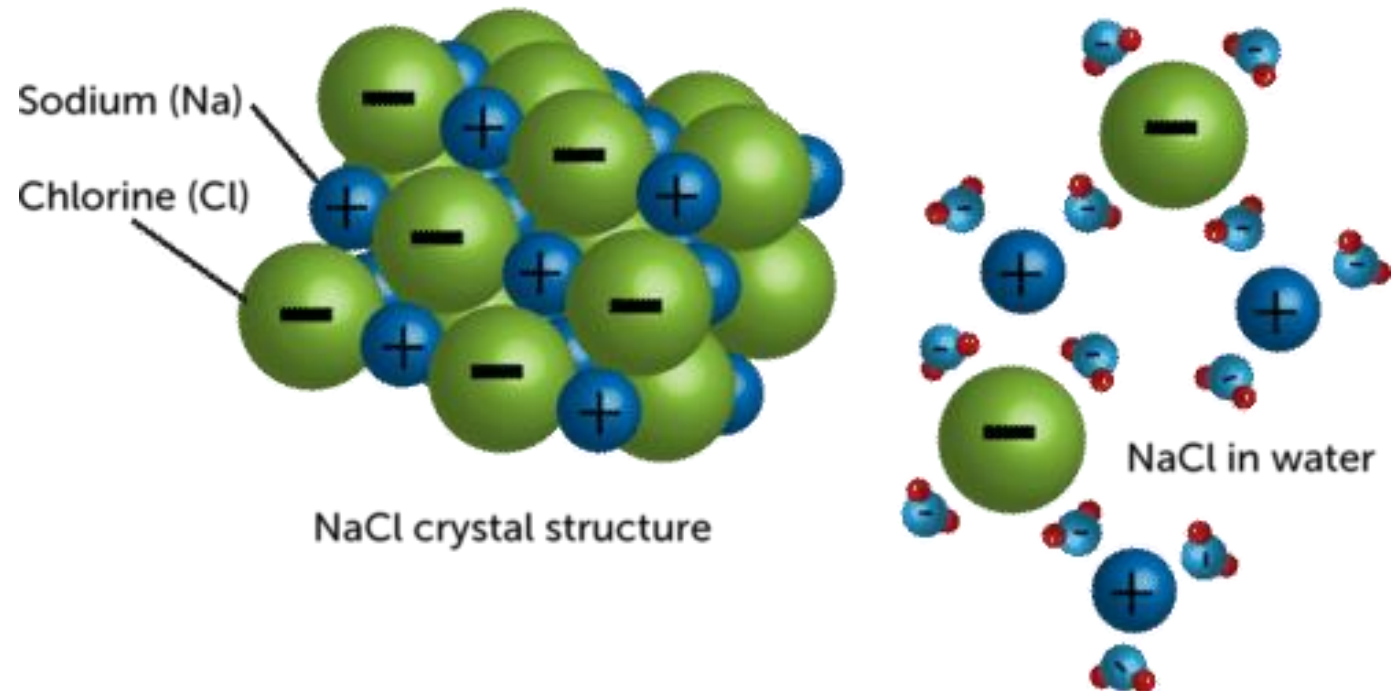
(a)

Field Museum Library/Getty Images.

# NaCl in water (remember electrolytes)

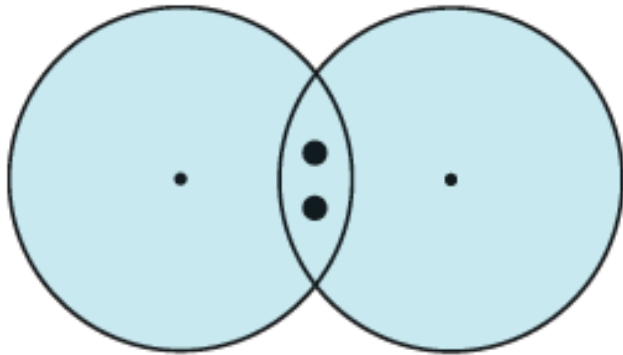
- Solid NaCl does not conduct electricity as charges are not motile
- In water,  $\text{Cl}^-$  and  $\text{Na}^+$  become motile and conduct electricity

## How Salt Dissolves in Water

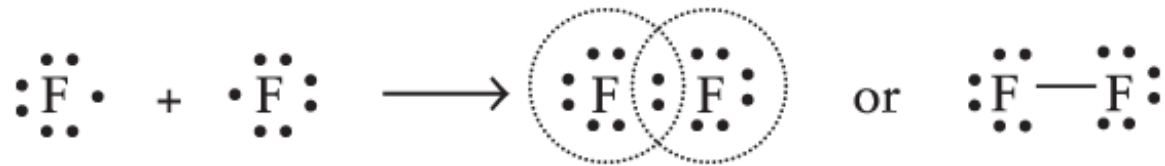


# Covalent bonding

- Bonds between nonmetals
- **Covalent bonds** form by atoms sharing electrons until they reach a *noble-gas configuration*.
- Lewis called this principle the **octet rule**.



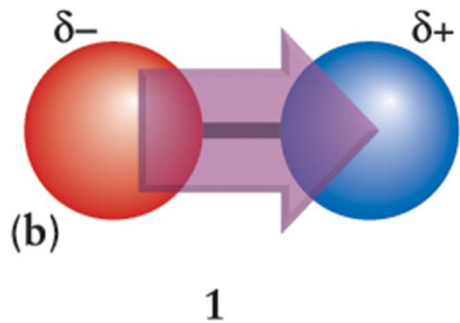
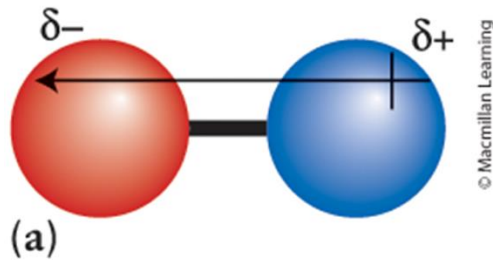
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1 Shared electron pair

# Are the electrons shared equally? Electronegativity

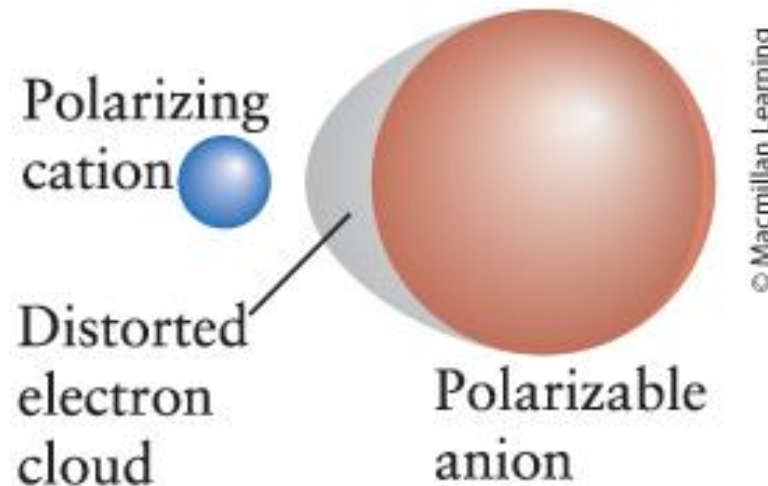
**Electronegativity** = electron-pulling ability of an atom in a molecule



- The **partial charges** ( $+\delta$ ,  $-\delta$ )—not true charges.
- (a) is an older convention whereas (b) is the newer convention. Style (b) is the currently adopted method.

# EPFL Differences in electronegativity create polarity

- The atom with the **highest electronegativity** has the tendency to drag electrons towards itself.
- The electron density is then not in the middle but closer to the most electronegative atom.



# Electronegativity difference



- There is no specific dividing line between ionic and covalent bonding.
- Electronegativity difference  $> 1.7$  means likely ionic
- Electronegativity difference  $< 1.7$  means likely covalent

Ionic and covalent bonding are two extreme bonding models. Most bonds lie somewhere between purely ionic and purely covalent.

# Periodic Table of the Elements



|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| GROUP 1<br>IA  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 2<br>IIA  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 13<br>IIIA  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 14<br>IVA   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 15<br>VA   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 16<br>VIA   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 17<br>VIIA  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 18<br>VIIIA  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 1<br>H<br>Hydrogen<br>1.00794<br>9.0010 13.5964<br>258.14 -252.87<br>(1) 1<br>[1s] <sup>1</sup><br>+1    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 2<br>He<br>Helium<br>4.002602<br>6.1719 26.5814<br>(1) 2<br>[1s] <sup>2</sup><br>0                      |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 3<br>B<br>Boron<br>10.811<br>2.46 8.2500<br>2075 4000<br>(2) 40<br>[He] 2s <sup>2</sup> 2p <sup>1</sup><br>+3                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 4<br>C<br>Carbon<br>12.0107<br>2.26 2.50<br>3015 4000<br>(4) 42<br>[He] 2s <sup>2</sup> 2p <sup>2</sup><br>+2, 4                        |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 5<br>N<br>Nitrogen<br>14.0064<br>2.86 2.86<br>-210.1 -195.79<br>(5) 75<br>[He] 2s <sup>2</sup> 2p <sup>3</sup><br>+3, 5, 3, 1, 2, 3                  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 6<br>O<br>Oxygen<br>15.9994<br>3.46 3.46<br>-218.3 -182.9<br>(6) 75<br>[He] 2s <sup>2</sup> 2p <sup>4</sup><br>-2                                     |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 7<br>F<br>Fluorine<br>18.9984<br>3.94 3.94<br>-253.15 -188.12<br>(7) 75<br>[He] 2s <sup>2</sup> 2p <sup>5</sup><br>-1                             |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 8<br>Ne<br>Neon<br>20.1797<br>3.8 3.8<br>-248.58 -182.46<br>(8) 75<br>[He] 2s <sup>2</sup> 2p <sup>6</sup><br>0                                    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 9<br>Li<br>Lithium<br>6.941<br>0.46 1.57<br>635 538.17<br>180.56 1042<br>(3) 130<br>[He] 2s <sup>1</sup><br>+1                                      |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 10<br>Be<br>Beryllium<br>9.012182<br>1.848 9.3227<br>185.56 1242<br>(4) 112<br>HCP<br>[He] 2s <sup>2</sup><br>0                                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 11<br>Na<br>Sodium<br>22.989769<br>0.95 0.50<br>97.72 103<br>(11) 138<br>BCC<br>[Ne] 3s <sup>1</sup><br>+1                                     |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 12<br>Mg<br>Magnesium<br>24.304<br>1.21 1.31<br>97.32 103<br>(12) 138<br>HCP<br>[Ne] 3s <sup>2</sup><br>0                            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 13<br>Al<br>Aluminum<br>26.981538<br>1.81 1.81<br>90.12 103<br>(13) 142<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>1</sup><br>+3                              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 14<br>Si<br>Silicon<br>28.0855<br>1.56 1.56<br>168.32 2519<br>(14) 142<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>2</sup><br>+2, 4                            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 15<br>P<br>Phosphorus<br>30.973761<br>2.19 2.19<br>100.12 2519<br>(15) 142<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>3</sup><br>+3, 5                              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 16<br>S<br>Sulfur<br>32.06<br>2.50 2.50<br>100.12 2519<br>(16) 142<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>4</sup><br>-2, 4, 6                                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 17<br>Cl<br>Chlorine<br>35.453<br>3.16 3.16<br>-101.5 238.5<br>(17) 98<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>5</sup><br>-1, 3, 5, 7                             |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 18<br>Ar<br>Argon<br>39.948<br>1.78 1.78<br>-185.7 255.3<br>(18) 97<br>FCC<br>[Ne] 3s <sup>2</sup> 3p <sup>6</sup><br>0                            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 4<br>K<br>Potassium<br>39.0983<br>0.82 1.38<br>63.5 103<br>(19) 227<br>BCC<br>[Ar] 4s <sup>1</sup><br>+1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 20<br>Ca<br>Calcium<br>40.078<br>1.88 1.88<br>84.28 103<br>(20) 182<br>FCC<br>[Ar] 4s <sup>2</sup><br>0 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 21<br>Sc<br>Scandium<br>44.955910<br>1.35 1.35<br>2486 55119<br>[Ar] 182<br>HCP<br>[Ar] 3d <sup>1</sup> 4s <sup>2</sup><br>+3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 22<br>Ti<br>Titanium<br>47.88<br>1.54 1.63<br>1462 5381<br>[Ar] 142<br>HCP<br>[Ar] 3d <sup>2</sup> 4s <sup>2</sup><br>+2, 3, 4          |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 23<br>V<br>Vanadium<br>50.9415<br>1.63 1.63<br>1910 5381<br>[Ar] 134<br>BCC<br>[Ar] 3d <sup>3</sup> 4s <sup>2</sup><br>+2, 3, 4, 5                   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 24<br>Cr<br>Chromium<br>51.9961<br>1.65 1.65<br>1907 5381<br>[Ar] 138<br>BCC<br>[Ar] 3d <sup>5</sup> 4s <sup>1</sup><br>+2, 3, 4, 6                   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 25<br>Mn<br>Manganese<br>54.938044<br>1.55 1.55<br>1912 5381<br>[Ar] 137<br>FCC<br>[Ar] 3d <sup>5</sup> 4s <sup>2</sup><br>+2, 3, 4, 6, 7         |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 26<br>Fe<br>Iron<br>55.845<br>1.83 1.83<br>1538 5381<br>[Ar] 136<br>BCC<br>[Ar] 3d <sup>6</sup> 4s <sup>2</sup><br>+2                              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 27<br>Co<br>Cobalt<br>58.933194<br>1.85 1.85<br>1495 5381<br>[Ar] 136<br>HCP<br>[Ar] 3d <sup>7</sup> 4s <sup>2</sup><br>+2, 3                       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 28<br>Ni<br>Nickel<br>58.6934<br>1.91 1.91<br>1455 5381<br>[Ar] 136<br>FCC<br>[Ar] 3d <sup>8</sup> 4s <sup>2</sup><br>+2                       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 29<br>Cu<br>Copper<br>63.546<br>1.98 1.98<br>1083.2 2387<br>[Ar] 128<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>1</sup><br>+1, 2                  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 30<br>Zn<br>Zinc<br>65.38<br>1.85 1.85<br>419.53 507<br>[Ar] 134<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup><br>+2               |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 31<br>Ga<br>Gallium<br>69.723<br>1.81 1.81<br>302.9 2387<br>[Ar] 135<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>1</sup><br>+3                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 32<br>Ge<br>Germanium<br>72.64<br>2.01 2.01<br>375.2 2387<br>[Ar] 132<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup><br>+2, 4            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 33<br>As<br>Arsenic<br>74.921594<br>2.15 2.15<br>375.2 2387<br>[Ar] 119<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup><br>+3, 5                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 34<br>Se<br>Selenium<br>78.96<br>2.55 2.55<br>375.2 2387<br>[Ar] 116<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup><br>+2, 4, 6              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 35<br>Br<br>Bromine<br>79.904<br>2.96 2.96<br>-73.3 2387<br>[Ar] 114<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup><br>+1, 5                    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 36<br>Kr<br>Krypton<br>83.798<br>3 3<br>-153.2 2387<br>[Ar] 118<br>FCC<br>[Ar] 3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup><br>0               |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 5<br>Rb<br>Rubidium<br>85.4678<br>0.82 0.95<br>38.2 103<br>(21) 248<br>BCC<br>[Kr] 5s <sup>1</sup><br>+1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 38<br>Sr<br>Strontium<br>87.62<br>0.95 0.95<br>38.2 103<br>(22) 248<br>FCC<br>[Kr] 5s <sup>2</sup><br>0 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 39<br>Y<br>Yttrium<br>88.905848<br>1.22 1.22<br>1525 3345<br>[Kr] 182<br>HCP<br>[Kr] 4d <sup>1</sup> 5s <sup>2</sup><br>+3    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 40<br>Zr<br>Zirconium<br>91.224<br>1.35 1.35<br>1525 3345<br>[Kr] 182<br>HCP<br>[Kr] 4d <sup>2</sup> 5s <sup>2</sup><br>+4              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 41<br>Nb<br>Niobium<br>92.90638<br>1.43 1.43<br>2477 4744<br>[Kr] 146<br>BCC<br>[Kr] 4d <sup>4</sup> 5s <sup>1</sup><br>+3, 5                        |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 42<br>Mo<br>Molybdenum<br>95.94<br>2.15 2.15<br>3025 4744<br>[Kr] 138<br>BCC<br>[Kr] 4d <sup>5</sup> 5s <sup>1</sup><br>+2, 3, 4, 5, 6                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 43<br>Tc<br>Technetium<br>98.9062<br>1.9 1.9<br>2527 4744<br>[Kr] 136<br>HCP<br>[Kr] 4d <sup>5</sup> 5s <sup>2</sup><br>+4, 7                     |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 44<br>Ru<br>Ruthenium<br>101.07<br>2.26 2.26<br>2334 4744<br>[Kr] 134<br>FCC<br>[Kr] 4d <sup>7</sup> 5s <sup>1</sup><br>+2, 3, 4, 5, 6             |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 45<br>Rh<br>Rhodium<br>102.9055<br>2.26 2.26<br>1962 5381<br>[Kr] 134<br>FCC<br>[Kr] 4d <sup>8</sup> 5s <sup>1</sup><br>+3, 4                       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 46<br>Pd<br>Palladium<br>106.3676<br>2.29 2.29<br>1962 5381<br>[Kr] 137<br>FCC<br>[Kr] 4d <sup>10</sup><br>+4                                  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 47<br>Ag<br>Silver<br>107.8682<br>1.93 1.93<br>961.78 2387<br>[Kr] 146<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>1</sup><br>+1                   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 48<br>Cd<br>Cadmium<br>112.411<br>1.69 1.69<br>321.87 107<br>[Kr] 151<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup><br>+2          |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 49<br>In<br>Indium<br>114.818<br>1.78 1.78<br>327.4 107<br>[Kr] 97<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>1</sup><br>+3                  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 50<br>Sn<br>Tin<br>118.710<br>1.86 1.86<br>327.4 107<br>[Kr] 141<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup><br>+2, 4                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 51<br>Sb<br>Antimony<br>121.757<br>2.85 2.85<br>630.83 1587<br>[Kr] 138<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup><br>+3, 5                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 52<br>Te<br>Tellurium<br>127.60<br>2.55 2.55<br>443.51 107<br>[Kr] 135<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup><br>+2, 4, 6            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 53<br>I<br>Iodine<br>126.90544<br>2.66 2.66<br>113.7 107<br>[Kr] 133<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup><br>+1, 5, 7                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 54<br>Xe<br>Xenon<br>131.29<br>2.66 2.66<br>-116.3 -91<br>[Kr] 136<br>FCC<br>[Kr] 4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup><br>0            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 6<br>Cs<br>Cesium<br>132.90545<br>0.79 0.89<br>28.4 103<br>(23) 248<br>BCC<br>[Xe] 6s <sup>1</sup><br>+1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 56<br>Ba<br>Barium<br>137.327<br>0.89 0.89<br>28.4 103<br>(24) 222<br>BCC<br>[Xe] 6s <sup>2</sup><br>0  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 57-71<br>Lanthanide Series  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 72<br>Hf<br>Hafnium<br>178.49<br>1.3 1.3<br>1525 3345<br>[Kr] 138<br>BCC<br>[Xe] 4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup><br>+4 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 73<br>Ta<br>Tantalum<br>180.94788<br>1.5 1.5<br>1669 3345<br>[Kr] 146<br>BCC<br>[Xe] 4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup><br>+3, 4, 5, 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 74<br>W<br>Tungsten<br>183.84<br>2.26 2.26<br>3422 5381<br>[Kr] 137<br>HCP<br>[Xe] 4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup><br>+2, 3, 4, 5, 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 75<br>Re<br>Rhenium<br>186.207<br>1.9 1.9<br>3186 5381<br>[Kr] 137<br>HCP<br>[Xe] 4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup><br>+4, 6, 7, 1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 76<br>Os<br>Osmium<br>190.23<br>2.2 2.2<br>2415 4744<br>[Kr] 136<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup><br>+2, 3, 4, 5, 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 77<br>Ir<br>Iridium<br>192.222<br>2.26 2.26<br>2415 4744<br>[Kr] 138<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup><br>+3, 4, 5, 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 78<br>Pt<br>Platinum<br>195.084<br>2.26 2.26<br>1962 5381<br>[Kr] 139<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>9</sup> 6s <sup>1</sup><br>+2, 4 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 79<br>Au<br>Gold<br>196.966569<br>2.54 2.54<br>1063 2387<br>[Kr] 144<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>1</sup><br>+1, 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 80<br>Hg<br>Mercury<br>200.59<br>2 2<br>234.3 107<br>[Kr] 181<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup><br>+2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 81<br>Tl<br>Thallium<br>204.38<br>1.62 1.62<br>304 107<br>[Kr] 179<br>HCP<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>1</sup><br>+3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 82<br>Pb<br>Lead<br>207.2<br>2.33 2.33<br>327.4 107<br>[Kr] 178<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>2</sup><br>+2, 4 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 83<br>Bi<br>Bismuth<br>208.9804<br>2.62 2.62<br>271.3 107<br>[Kr] 145<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>3</sup><br>+3, 5 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 84<br>Po<br>Polonium<br>209<br>2.0 2.0<br>-210.1 -182.9<br>[Kr] 142<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>4</sup><br>-2, 4 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 85<br>At<br>Astatine<br>210<br>2.2 2.2<br>-210.1 -182.9<br>[Kr] 145<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>5</sup><br>+3, 5, 7 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 86<br>Rn<br>Radon<br>222<br>3 3<br>-210.1 -182.9<br>[Kr] 146<br>FCC<br>[Xe] 4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 6p <sup>6</sup><br>0 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 7<br>Fr<br>Francium<br>223<br>0.7 0.9<br>-253.15 -188.12<br>[Rn] 7s <sup>1</sup><br>+1                   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 88<br>Ra<br>Radium<br>226<br>0.9 0.9<br>-253.15 -188.12<br>[Rn] 7s <sup>2</sup><br>0                    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 89-103<br>Actinide Series   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 104<br>Rf<br>Rutherfordium<br>261<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>2</sup> 7s <sup>2</sup><br>+4                             |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 105<br>Db<br>Dubnium<br>262<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup><br>+5  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 106<br>Sg<br>Seaborgium<br>263<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup><br>+6  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 107<br>Bh<br>Bohrium<br>264<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup><br>+7   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 108<br>Hs<br>Hassium<br>265<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup><br>+8  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 109<br>Mt<br>Meitnerium<br>266<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup><br>+9  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 110<br>Ds<br>Darmstadtium<br>267<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>8</sup> 7s <sup>2</sup><br>+10                                    |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 111<br>Rg<br>Roentgenium<br>268<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>9</sup> 7s <sup>2</sup><br>+11                                     |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 112<br>Cn<br>Copernicium<br>269<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup><br>+12                          |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 113<br>Uut<br>Ununtrium<br>271<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>1</sup><br>+3                                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 114<br>Uuq<br>Ununquadium<br>272<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>2</sup><br>+2, 4                            |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 115<br>Uup<br>Ununpentium<br>273<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>3</sup><br>+3, 5                                  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 116<br>Uuh<br>Ununhexium<br>274<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>4</sup><br>+2, 4                                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 117<br>Uus<br>Ununseptium<br>275<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>5</sup><br>+3, 5, 7                                |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 118<br>Uuo<br>Ununoctium<br>276<br>6.9 6.9<br>[Rn] 5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>6</sup><br>0                          |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 8<br>La<br>Lanthanum<br>138.90547<br>1.39 1.39<br>[Xe] 5d <sup>1</sup> 6s <sup>2</sup><br>+3             |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 58<br>Ce<br>Cerium<br>140.12<br>1.32 1.32<br>[Xe] 4f <sup>1</sup> 6s <sup>2</sup><br>+3                 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 59<br>Pr<br>Praseodymium<br>140.90765<br>1.15 1.15<br>[Xe] 4f <sup>2</sup> 6s <sup>2</sup><br>+3                              |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 60<br>Nd<br>Neodymium<br>144.24<br>1.34 1.34<br>[Xe] 4f <sup>4</sup> 6s <sup>2</sup><br>+3  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 61-71<br>Pm<br>Promethium Series   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 62<br>Sm<br>Samarium<br>150.36<br>1.17 1.17<br>[Xe] 4f <sup>6</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 63<br>Eu<br>Europium<br>151.964<br>1.28 1.28<br>[Xe] 4f <sup>7</sup> 6s <sup>2</sup><br>+3  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 64<br>Gd<br>Gadolinium<br>157.25<br>1.28 1.28<br>[Xe] 4f <sup>7</sup> 6s <sup>2</sup><br>+3  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 65<br>Tb<br>Terbium<br>158.92534<br>1.2 1.2<br>[Xe] 4f <sup>9</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 66<br>Dy<br>Dysprosium<br>162.50<br>1.22 1.22<br>[Xe] 4f <sup>10</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 67<br>Ho<br>Holmium<br>164.93032<br>1.23 1.23<br>[Xe] 4f <sup>11</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 68<br>Er<br>Erbium<br>167.259<br>1.24 1.24<br>[Xe] 4f <sup>12</sup> 6s <sup>2</sup><br>+3  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 69<br>Tm<br>Thulium<br>168.93421<br>1.25 1.25<br>[Xe] 4f <sup>13</sup> 6s <sup>2</sup><br>+3  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 70<br>Yb<br>Ytterbium<br>173.0547<br>1.25 1.25<br>[Xe] 4f <sup>14</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 71<br>Lu<br>Lutetium<br>174.967<br>1.27 1.27<br>[Xe] 4f <sup>14</sup> 6s <sup>2</sup><br>+3   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |   |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

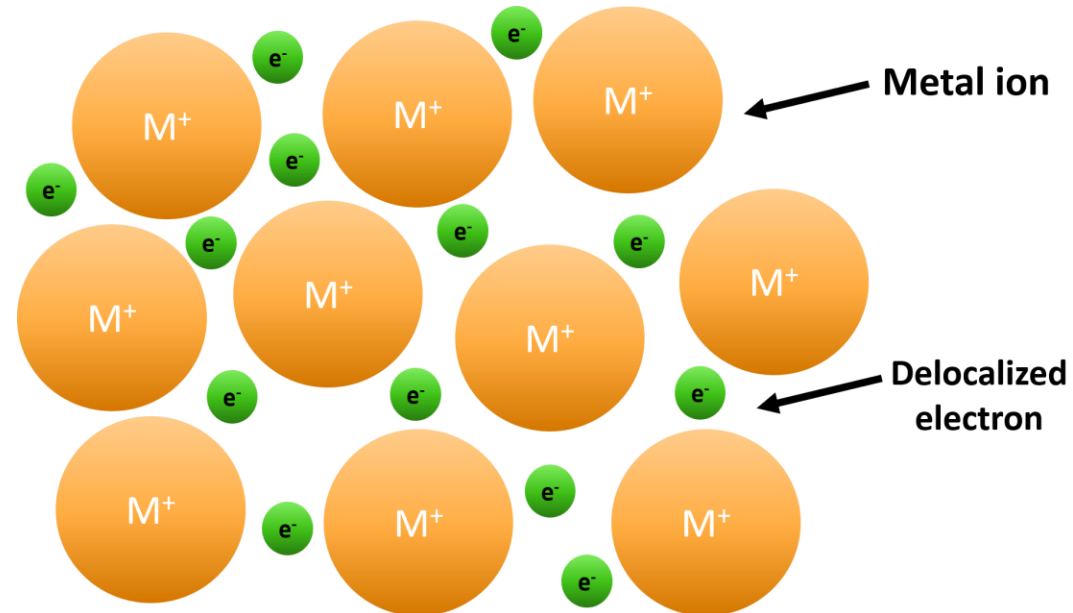
Atomic Number: 1  
Symbol: H  
Name: Hydrogen  
Atomic Weight: 1.00794  
Ground-State Level: 1s  
Electronegativity (Pauling): 2.2  
Ionization Energy (eV): 13.5984  
Boiling Point (°C): -252.87  
Melting Point (°C): -259.14  
Catalytic Activity: 0  
Crystal Structure: FCC  
Electron Configuration: 1s<sup>1</sup>  
Possible Oxidation States: +1, -1

Phase at STP: Gas, Liquid, Solid, Synthetic  
Categories: Alkali Metals, Alkaline Earth Metals, Transition Metals, Rare Earth Metals, Poor Metals, Native Gas, Halogens, Non Metals, Metalloids

Common Constants:  
Absolute Zero: -273.15 °C  
Avogadro's Constant: 6.02214076 × 10<sup>23</sup> mol<sup>-1</sup>  
Boyle's Law Constant: 0.00023662  
Boltzmann constant: 1.3806505 × 10<sup>-23</sup> J/K  
Electron Mass: 9.10938356 × 10<sup>-31</sup> kg  
Electron Radius (Classical): 2.8179403 × 10<sup>-15</sup> m  
Electron Volt: 1.602176634 × 10<sup>-19</sup> J  
Elementary Charge: 1.602176634 × 10<sup>-19</sup> C  
Faraday Constant: 96485.33212 C/mol  
Fine-structure constant: 0.00729735256  
First Radiation Constant: 2.99792458 × 10<sup>8</sup> m/s  
Gravitation Constant: 6.67430 × 10<sup>-11</sup> m<sup>3</sup> kg<sup>-1</sup> s<sup>-2</sup>  
Molar Gas Constant: 8.314472 J mol<sup>-1</sup> K<sup>-1</sup>  
Molar Volume (Ideal Gas): 0.0224141 m<sup>3</sup> mol<sup>-1</sup>  
Planck Constant: 6.62607015 × 10<sup>-34</sup> J s  
Proton-Electron Mass Ratio: 1836.15267343  
Rydberg Constant: 10973731.57 m<sup>-1</sup>  
Second Radiation Constant: 3.76152 × 10<sup>16</sup> m/s  
Speed of Light in a Vacuum: 299 792 458 m/s  
Speed of sound in air at STP: 340.2 m/s  
Standard Pressure: 101 325 Pa

# Metallic binding

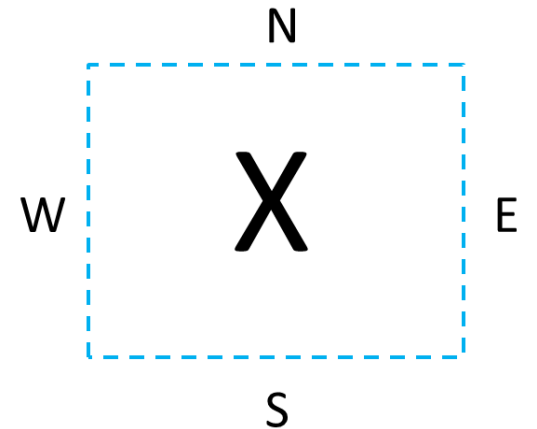
- Valence electrons are shared between all atoms in the metal which ensures the electric conductivity



- Introduction
  - What is a chemical bond
  - What are the different types of bonds
- **Lewis representation**
  - Octet rule
  - Examples
  - Limitations
- Geometric representation (VSEPR)
- Quantum approach

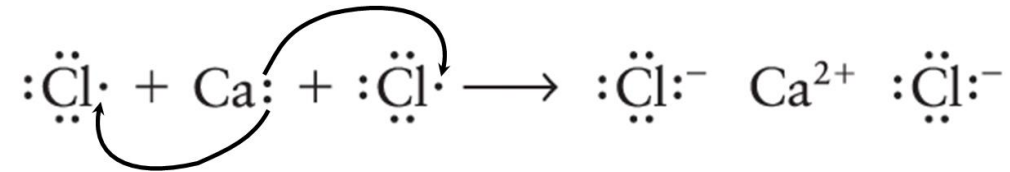
# How can we represent these bonds? Lewis representation

- A single dot represents a valence electron (=electron in the last shell) in the atom
- A pair of dots represents two paired electrons sharing an orbital
- Each symbol is thought of as having four sides, a north, south, east, and west position, where valence electrons are shown as dots



# Lewis structures

For **ionic bonds**, we start by removing valence electrons from the metal and transferring them to the nonmetal atom to complete its valence shell.



- The calcium atom loses its two valence electrons while each chlorine atom has one vacancy electron therefore it forms one bond
- Two chloride ions ( $\text{Cl}^-$ ) *balance the charge* for each calcium ion ( $\text{Ca}^{2+}$ ) resulting in the formula  $\text{CaCl}_2$ ; the overall charge is zero
- There are no  $\text{CaCl}_2$  molecules, only crystals of three-dimensional arrays of  $\text{CaCl}_2$  ions held by the vast array of opposite charges spread throughout the crystal



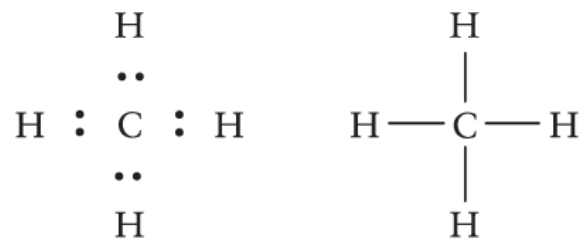
Example: Write the Lewis Structure of  $\text{H}_2\text{O}$ ,  $\text{CO}_2$  and  $\text{N}_2$



# Lewis structures for molecules with covalent bonds



Example: Lewis structure for methane, CH<sub>4</sub>

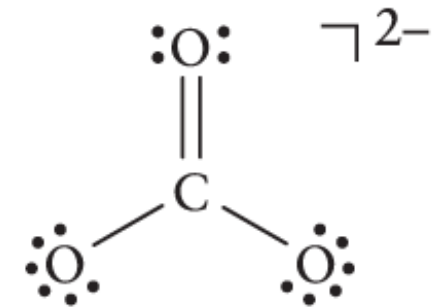
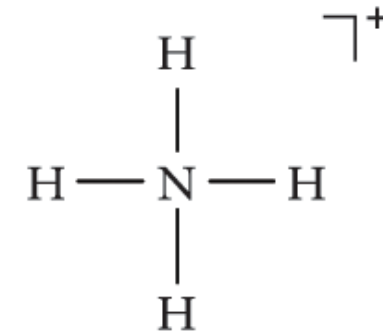


2 Methane, CH<sub>4</sub>

- The first element in the formula is typically the central atom
- Arrange the dots representing electrons so that C has an octet and each H atom has a duplet
- Because the carbon atom is linked by four bonds, the carbon is *tetravalent*: It has a valence of 4.

# Bonds in Lewis structures

- A **single bond** represents two electrons and is shown with a single line
- A **double bond** represents four electrons and is shown with two lines
- A **triple bond** represents six electrons and is shown with three lines.

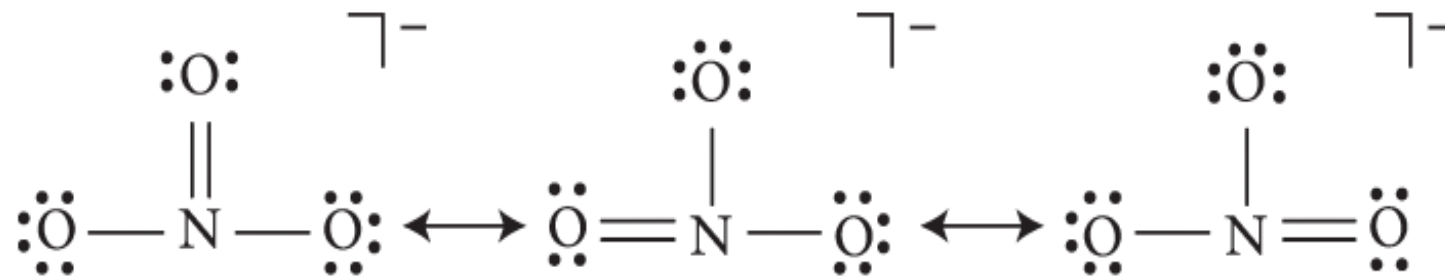


10 Carbonate ion,  $\text{CO}_3^{2-}$

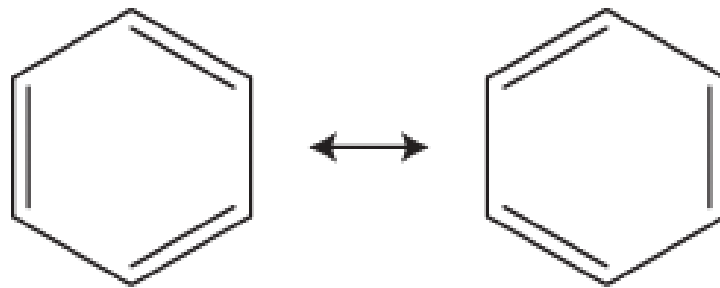


# Resonance structures

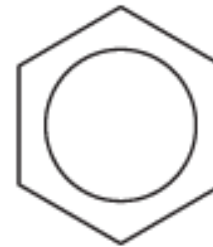
**Delocalized** electrons move from one atom to another



6 Nitrate ion,  $\text{NO}_3^-$



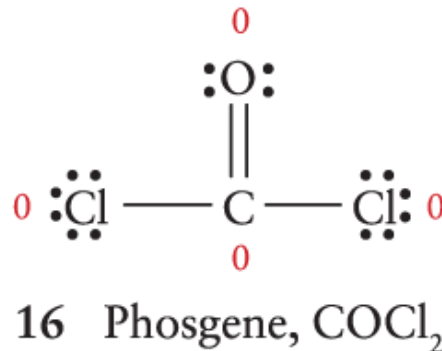
11 Benzene resonance



12 Benzene,  $\text{C}_6\text{H}_6$

# Formal charge (FC)

$$\text{Formal Charge} = V - \left( L + \frac{1}{2}B \right)$$



$$\text{O} \quad 6 - (4 + \frac{1}{2} \times 4) = 0$$

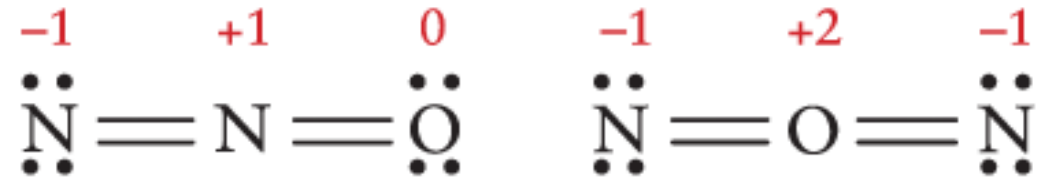
$$\text{Cl} \quad 7 - (6 + \frac{1}{2} \times 2) = 0$$

$$\text{C} \quad 4 - (0 + \frac{1}{2} \times 8) = 0$$

- FC = [number of valence e<sup>-</sup> in the free atom] - [number of electrons in free pairs] - 1/2[number of binding electrons]
- The sum of formal charges is equal to the overall charge of the molecule or ion; electrically neutral molecules have a formal charge of zero.

# Formal charge (FC)

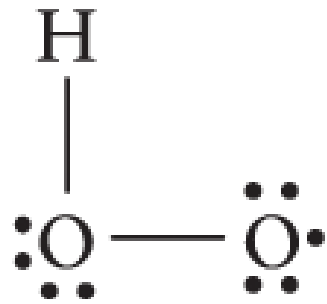
- Formal charges can predict the most *favorable* Lewis structure
- The structure with the lowest formal charges on each atom is the most plausible (lowest energy) structure.



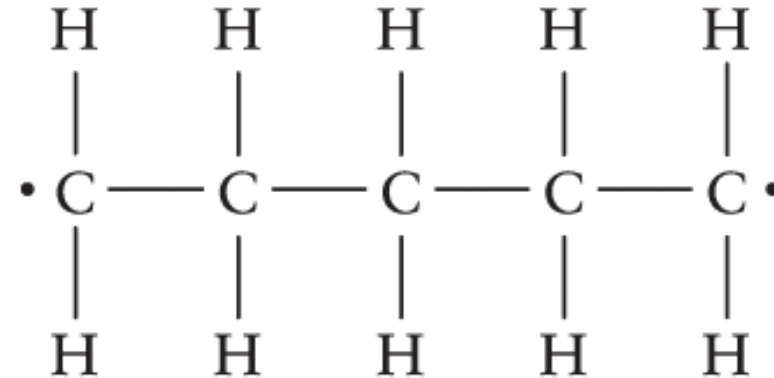
15

# Exceptions to the octet rule

- **Radicals** are something you cannot isolate, are unstable, and are highly reactive. Their formation "violates" the octet rule
- **Antioxidants** (Vitamins A, C, and E) react with radicals before they are able to do damage



4 Hydrogenperoxyl,  $\text{HO}_2\cdot$



3 A biradical

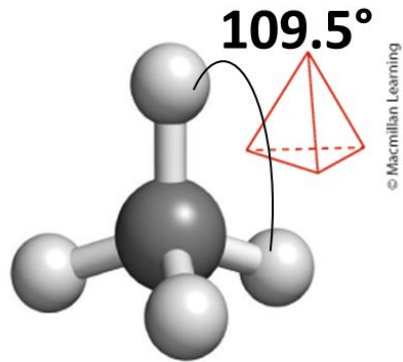
# Exceptions to the octet rule

- Carbon, nitrogen, oxygen, and fluorine obey the octet rule rigorously (only a few atoms but make the majority of molecules on earth).
- Period 3 and subsequent periods can accommodate *more than 8 electrons* in its valence shell, up to 12 electrons.

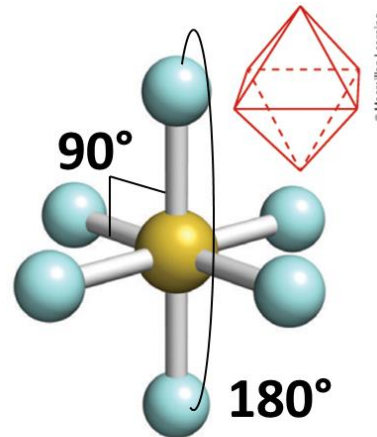
- Introduction
  - What is a chemical bond
  - What are the different types of bonds
- Lewis representation
  - Octet rule
  - Examples
  - Limitations
- **Geometric representation (VSEPR) – applies only to covalent bonds!**
- Quantum approach

# Geometric representation: the basic VSEPR model

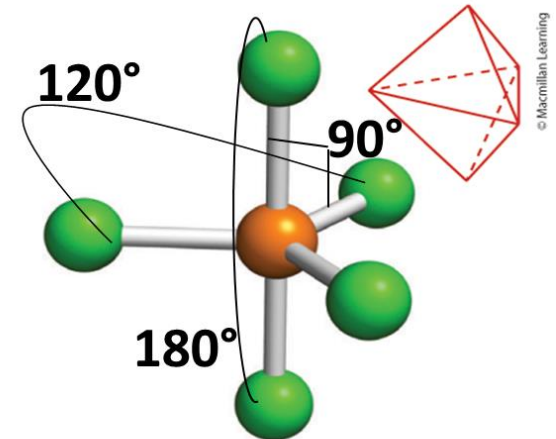
- VSEPR = valence shell electron pair repulsion theory
- Molecules consist of one central atom attached to other atoms, in which electron pairs tend to minimize repulsion energy.
- This creates distinct geometrical shapes, with fixed bond angles.



4 Methane,  $\text{CH}_4$



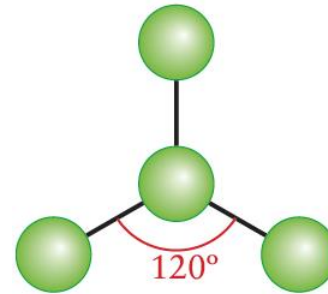
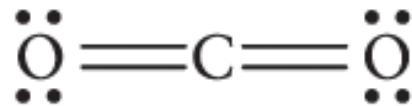
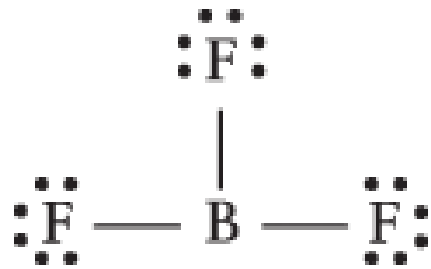
8 Sulfur hexafluoride,  $\text{SF}_6$



6 Phosphorus pentachloride,  $\text{PCl}_5$

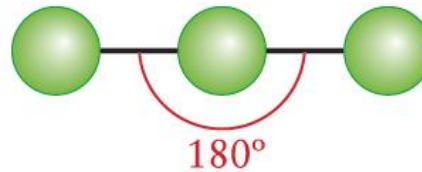
# The basic VSEPR model

- Lewis structures are two-dimensional representations of linked atoms
- The **valence-shell electron pair repulsion model (VSEPR model)** extends Lewis's theory to account for molecular shapes by adding rules for bond angles



(a)

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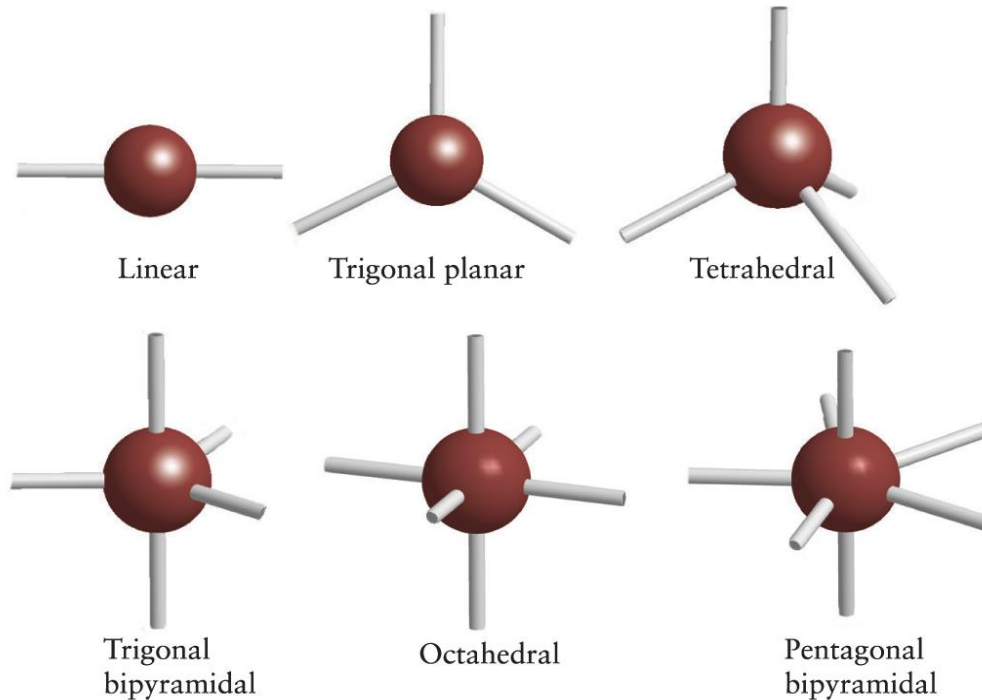
(b)

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# The basic VSEPR model

VSEPR theory states that shapes of molecules correspond to how (1) *electrons pairs* repel one another, and (2) that *electrons pairs* as far apart as possible

**Rule 1.** Regions of high electron density are either **bonding or lone pairs** which repel one another to minimize electron–electron repulsions.

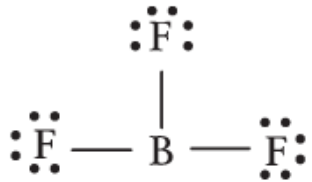


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# Example: arrangement of electron regions of $\text{BF}_3$

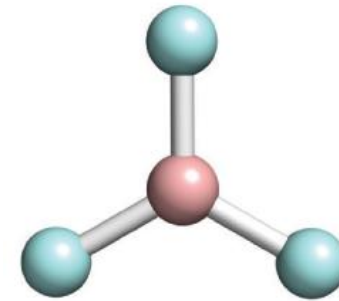


Lewis structure



2 Boron trifluoride,  $\text{BF}_3$

$\text{BF}_3$  has *three electron regions*, therefore it has a trigonal planar shape of electron regions.



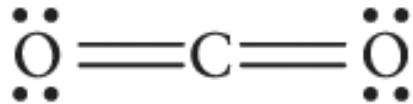
3 Boron trifluoride,  $\text{BF}_3$

VSEPR 3D shape

# VSEPR treats single and multiple bonds the same

**Rule 2.** Electron pairs in multiple bonds are treated the *same* as single bonds.

Lewis Structure



VSEPR 3D shape

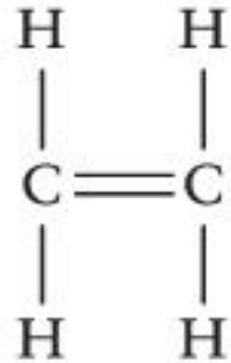


9 Carbon dioxide, CO<sub>2</sub>

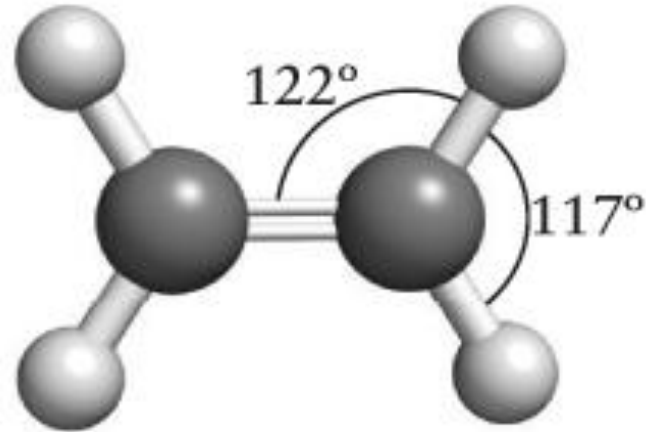
CO<sub>2</sub> has two electron regions, therefore it has a linear shape of electron regions.

# VSEPR for molecules with multiple central atoms

When there is more than one central atom, we consider the bonding about each atom independently.



13 Ethene, C<sub>2</sub>H<sub>4</sub>

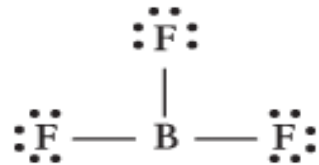


14 Ethene, C<sub>2</sub>H<sub>4</sub>

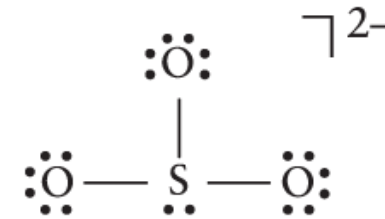
trigonal planar  
around each  
carbon atom

# VSEPR for molecules with central atom lone pairs

- The generic VSEPR formula “ $AX_nE_m$ ” helps identify bonding pair, and lone pairs attachments to the central atom
- “A” represent a central atom, “X” an attached atom, and “E” a lone pair.



$AX_3$



15 Sulfite ion,  $SO_3^{2-}$

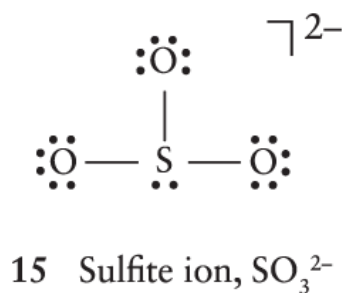
$AX_3E$

**! Lone pairs also count for the geometry of the molecule**

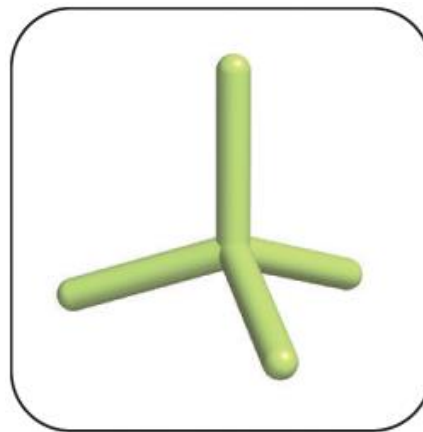
# Electron Arrangement vs. Molecular Shape

If lone pairs are present, the *molecular shape name* differs from the *electron arrangement name*.

**Rule 3.** The **molecular arrangement** only considers positions of **atoms** (not lone pairs) when reporting the *shape of a molecule*.

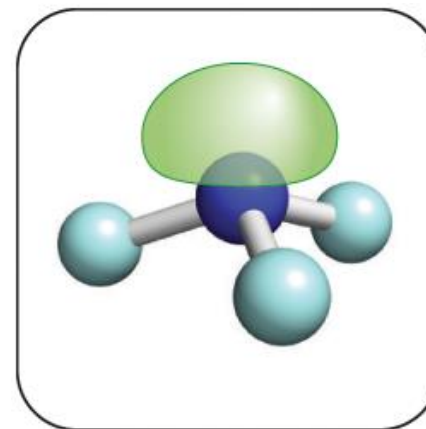


Lewis structure



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Electron group  
Tetrahedral



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Molecular arrangement  
Trigonal pyramidal

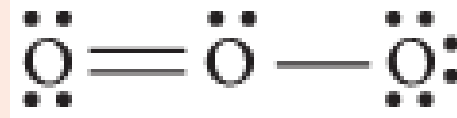
# Lewis structure, VSEPR Electron Arrangement and molecular shape of $O_3$





# Lewis structure, VSEPR Electron Arrangement and molecular shape of O<sub>3</sub>

Draw the Lewis structure.



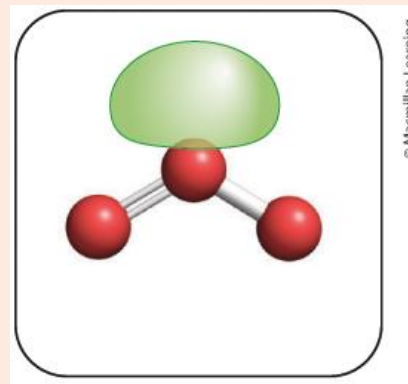
O<sub>3</sub>

Count the bonds and lone pairs on the central atom. Draw the 3D shape. Assign the electron arrangement.



Trigonal  
planar

Identify the shape considering only atoms.



Angular or  
bent

# Some consequences of molecular shapes



Is H<sub>2</sub>O really polar? And CO<sub>2</sub>?

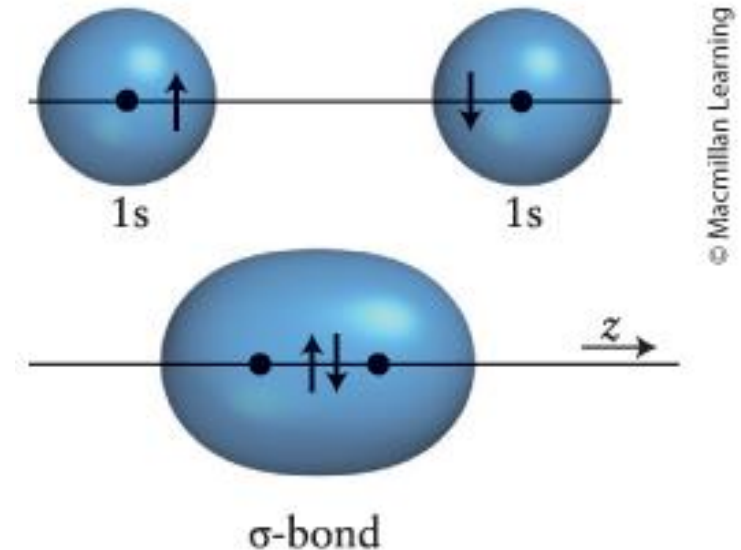
- Introduction
  - What is a chemical bond
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  - Limitations
- Geometric representation (VSEPR)
- **Quantum approach**

# Valence bond theory

- The lewis structures and VSEPR model are very useful qualitative models
- They cannot be used for calculations because they consider electrons as dot-like particles only
- **Valence bond theory** is a description of covalent bonding in terms of atomic orbitals, so taking their wave nature into account
- The idea is that molecular orbitals are hybrids of atomic orbitals
- This theory does not rely on experimental proof, but it explains chemistry well

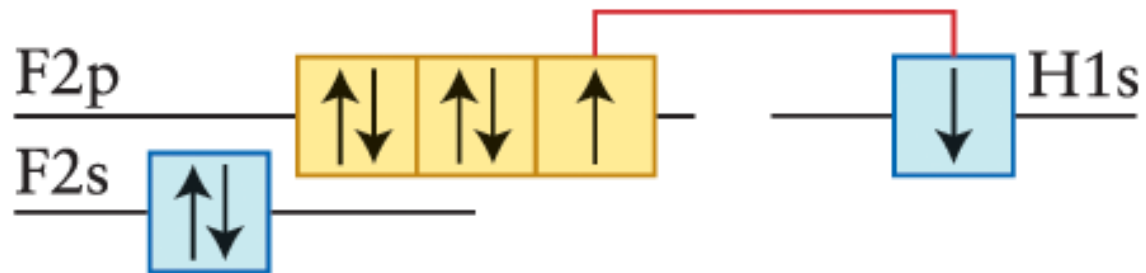
# EPFL Sigma bonds

- The simplest molecule of all is  $H_2$
- A “ground-state” hydrogen atom has one electron in a 1s-orbital
- As two H atoms come together, their 1s-electrons pair (denoted  $\uparrow\downarrow$ ) begin to overlap
- The resulting sausage-shaped distribution of electrons density is between the nuclei and called a  $\sigma$ -bond (a sigma bond).
- a  $\sigma$ -bond is **symmetrical and has no nodal plane**
- = **all single bonds**

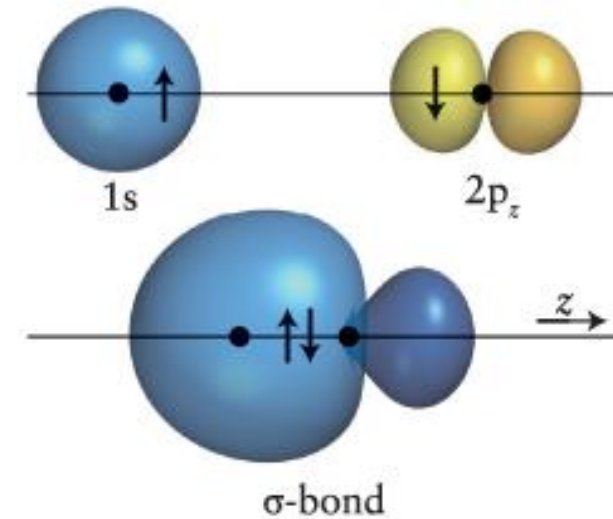


# EPFL Sigma bonds

- F has an unpaired electron atom in the  $2p_z$ -orbital. Hydrogen has an unpaired electron in the  $1s$ -orbital.
- The orbitals **overlap** and merge into a cloud that spreads over both atoms.



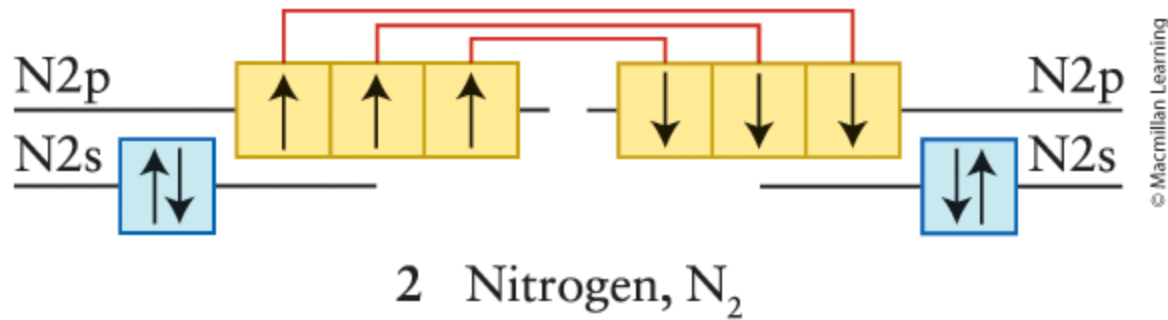
1 Hydrogen fluoride, HF



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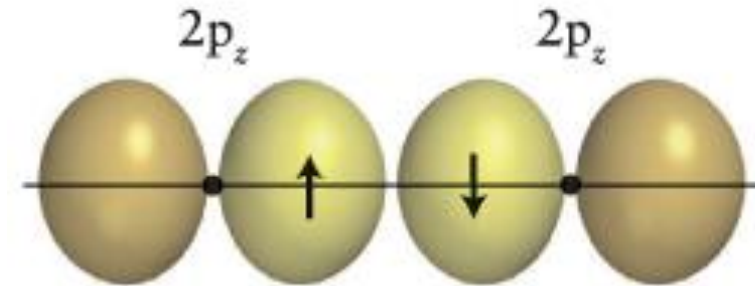
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# Sigma bonds

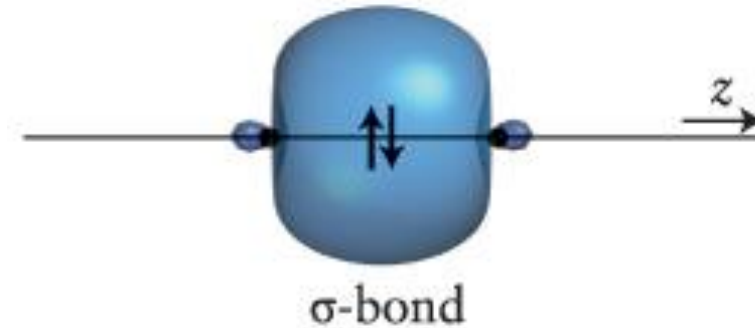


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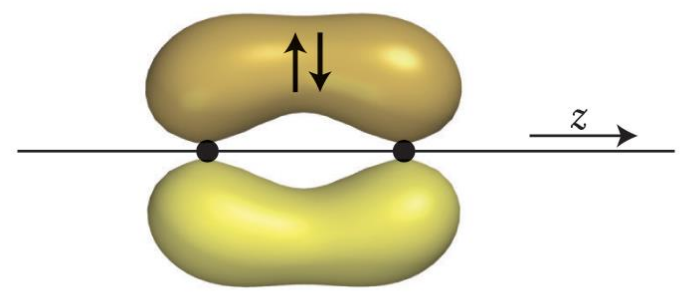
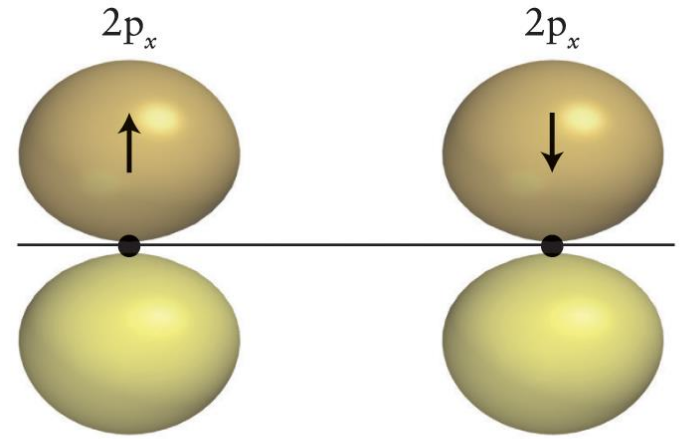
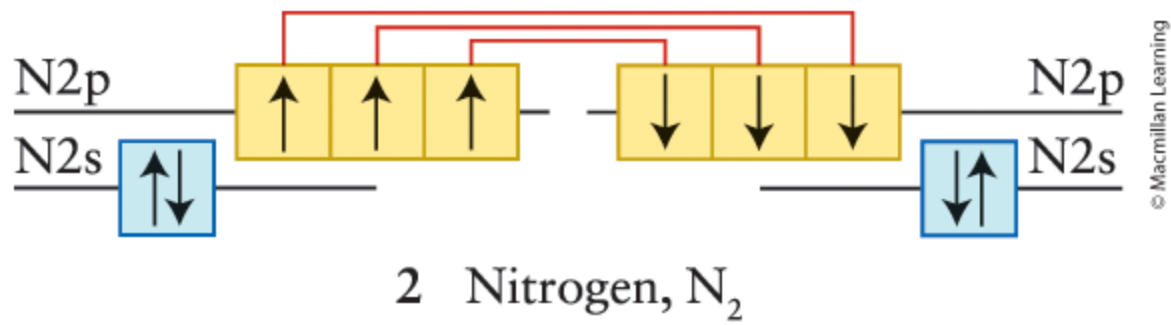
- There is a single electron in each three 2p-orbital
- However, due to bond angles, only one of the three orbitals overlaps end-to-end to form a  $\sigma$ -bond.



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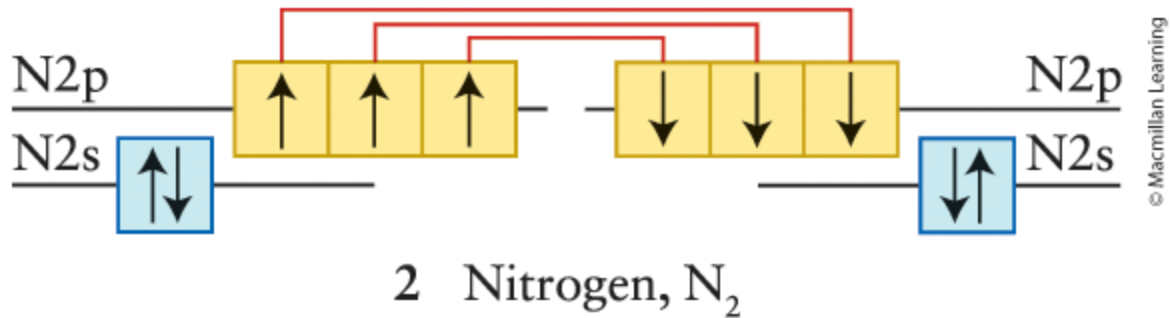


# EPFL Pi bonds

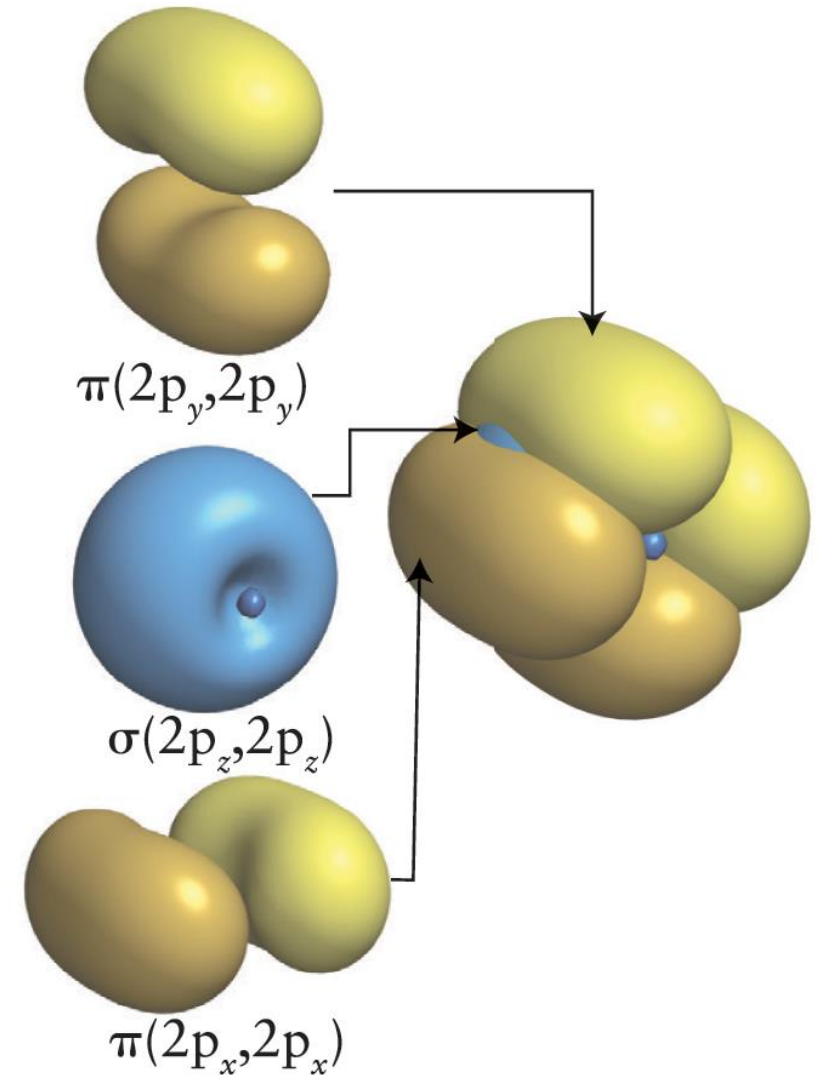


- The other two  $2p$ -orbitals ( $2p_x$  and  $2p_y$ ) are perpendicular to internuclear axis.
- These  $p$ -orbitals can overlap only in a side-by-side arrangement.
- This overlap results in a  $\pi$ -bond.
- A  $\pi$ -bond has a **single nodal plane containing the internuclear axis**

# Pi bonds

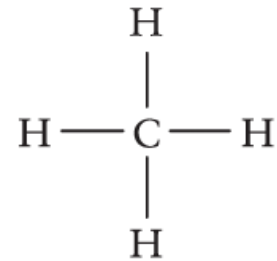
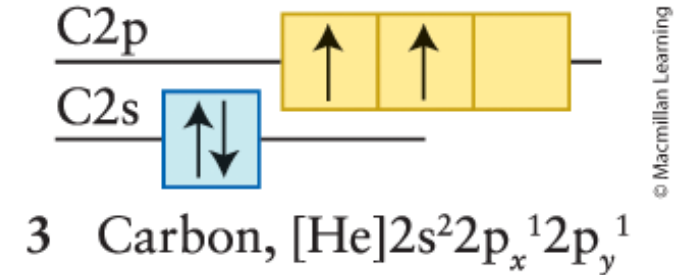


Two  $\pi$ -bonds merge forming a long doughnut-shaped cloud surrounding the  $\sigma$ -bond cloud, resembling a cylindrical hot dog.

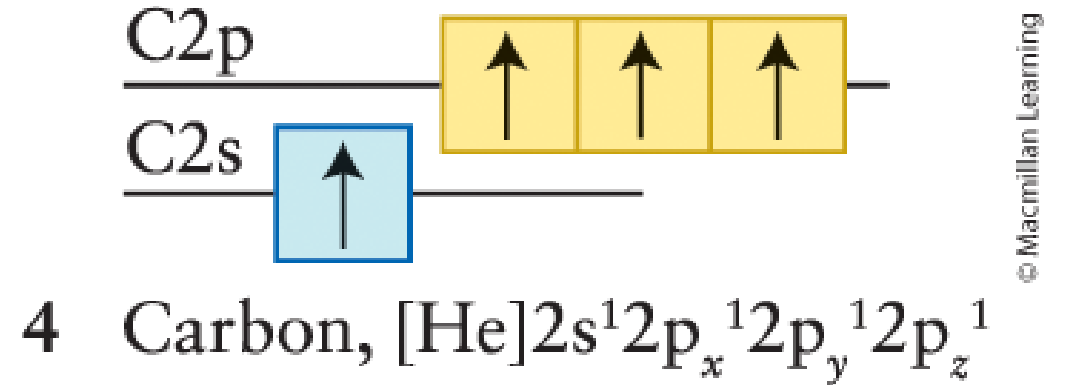
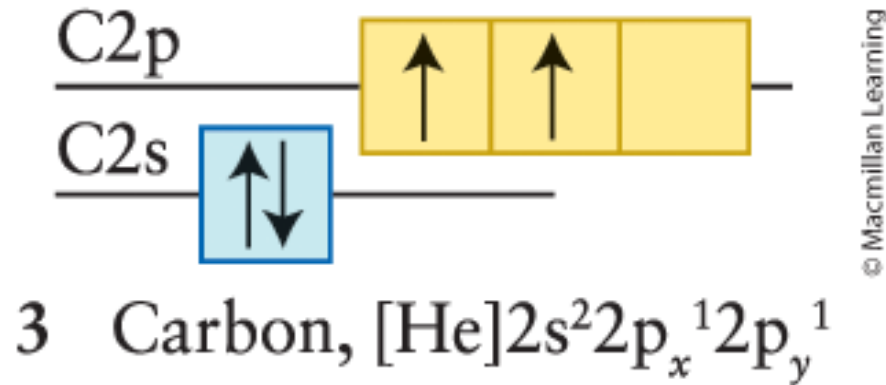


# Exceptions in VB theory – orbitals hybridization (for some atoms, not all of them!)

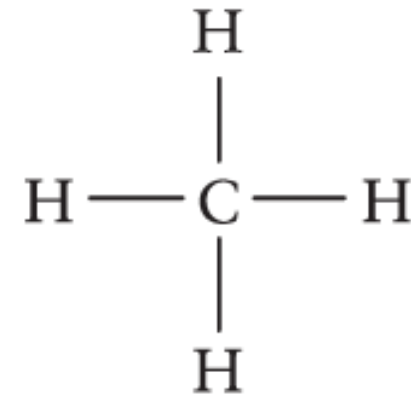
- Orbital hybridization is important for **C, N, O, B, Be, P, S, and transition metals** when they form covalent bonds. It is **not universal** but is most useful for **atoms that need specific molecular geometries**.
- A carbon atom has an electron configuration  $[\text{He}]2s^22p_x^12p_y^1$  with four valence electrons.
- It looks as though a carbon atom should have a valence of 2 and form only two perpendicular bonds.
- However, it always has a valence of 4 (it is commonly "tetravalent").



# Electron promotions

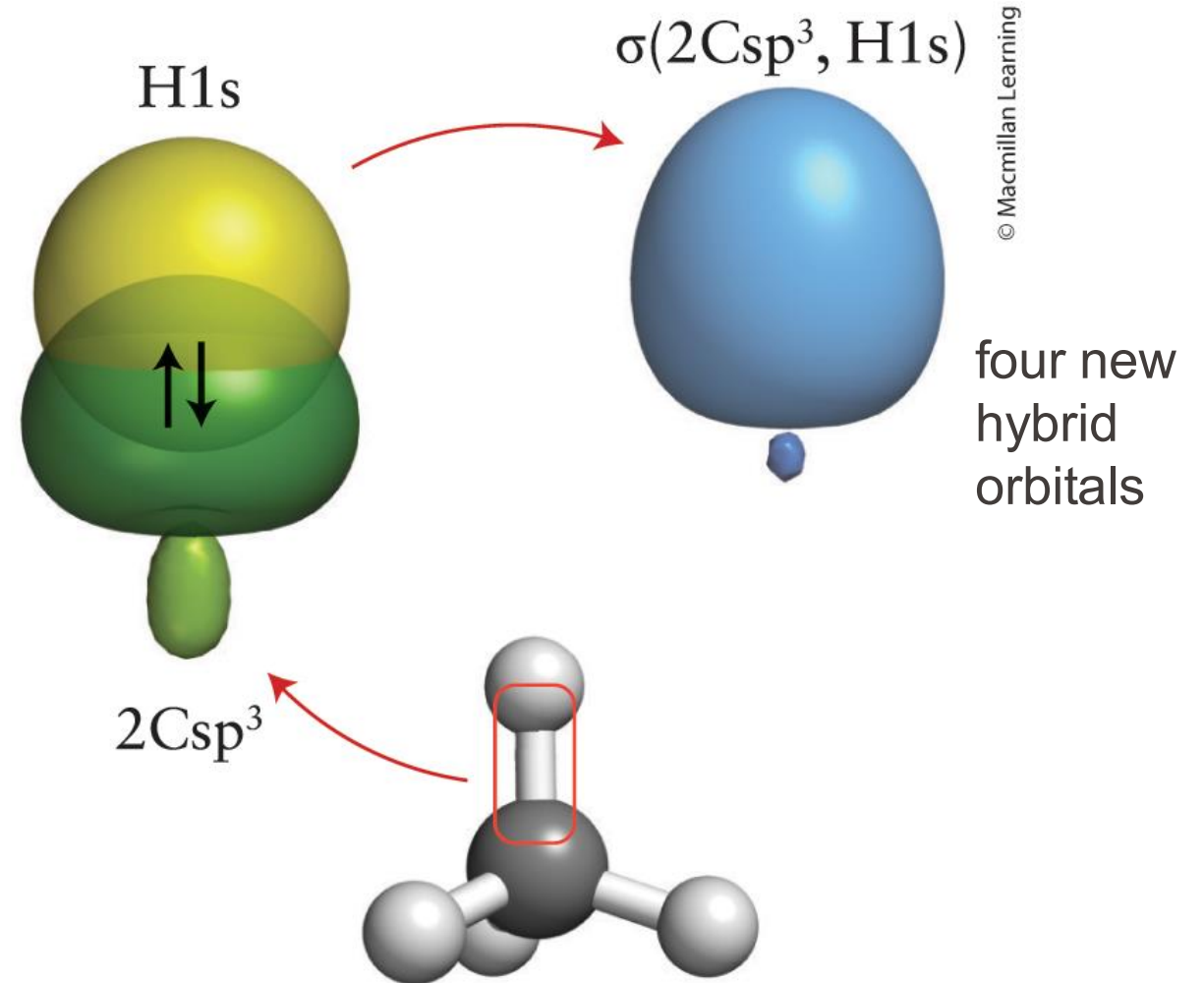


To overcome this, we match theory with our observation that carbon is tetravalent by promoting a 2s-electron into an empty 2p-orbital and we get  $[\text{He}]2s^1 2p_x^1 2p_y^1 2p_z^1$ .



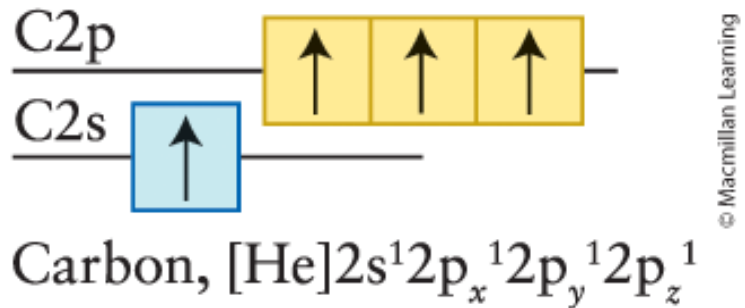
# Hybrid orbitals

- To explain that the structure of methane is tetrahedral, we have to think of orbitals as waves of electron densities that can interfere with each other
- The wavefunctions overlap (with either positive or negative amplitudes) and constructively reinforce each other = **hybridization**

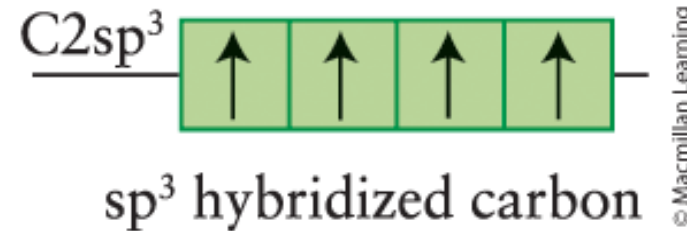


# Hybrid orbitals names

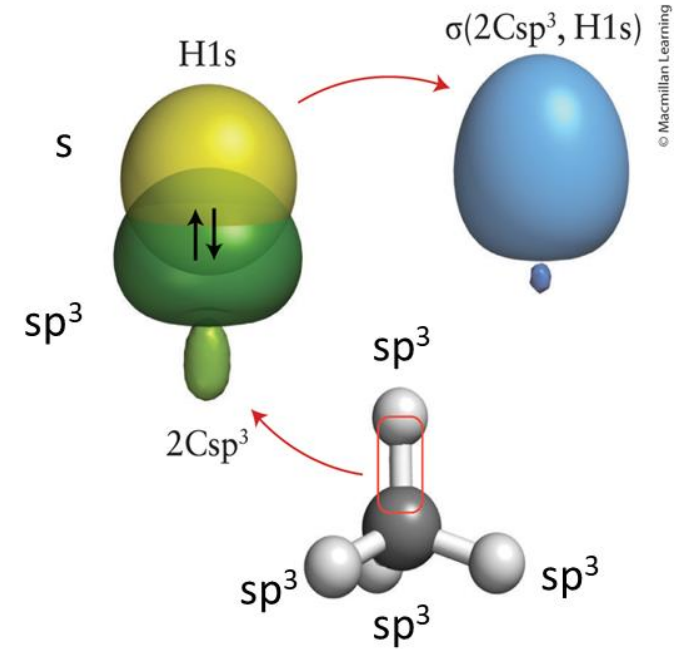
Each of the four **hybrid orbitals** is formed from a **linear combination** of the four original **atomic orbitals**:



Atomic orbitals



Hybrid orbitals



An  **$\text{sp}^3$  hybrid orbital** is a type of **hybrid atomic orbital** formed when **one s orbital** and **three p orbitals** from the same atom mix together to create **four equivalent orbitals**.

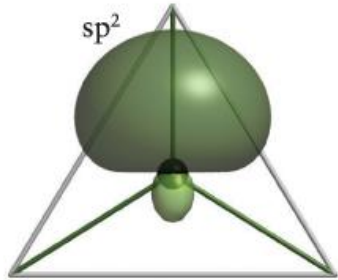
# Linear, Trigonal Planar, and Tetrahedral Hybrid $\sigma$ -Bonds



(a)

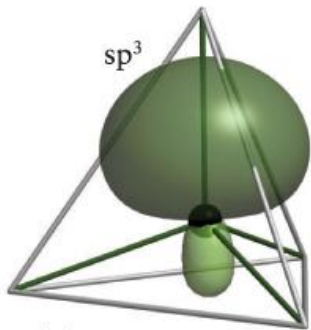
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(a) An s-orbital and p-orbital hybridize into 2  $sp$  hybrid orbitals that point in opposite directions, forming a linear molecular shape.



(b)

(b) An s-orbital and two p-orbitals come together to give 3  $sp^2$  hybrid orbitals.



(c)

(c) An s-orbital and three p-orbitals come together to give 4  $sp^3$  hybrid orbitals.




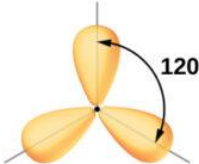
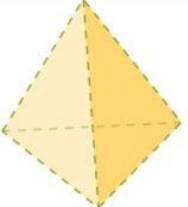
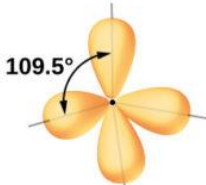

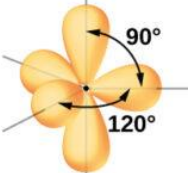
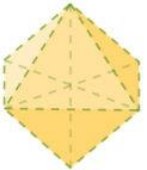
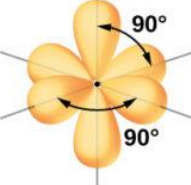
# Link with VSEPR: $AX_nE_m$

If  $n+m=4$  ( $AX_4$ ,  $AX_3E_1$ ,  $AX_2E_2$ ): hybridization  $sp^3$

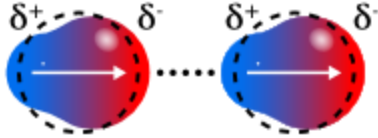
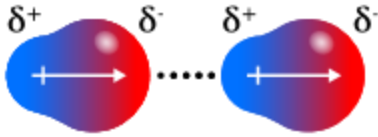
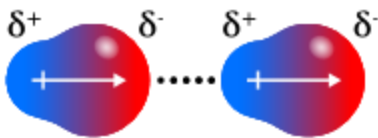
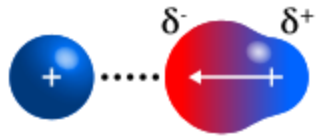
If  $n+m=3$  ( $AX_3$ ,  $AX_2E_1$ ,  $AX_1E_2$ ): hybridization  $sp^2$

# Examples of methane, ethene and ethyne



| Regions of Electron Density | Arrangement  |                      | Hybridization |   |
|-----------------------------|--|----------------------|---------------|---|
|                             |  |                      |               |   |
| 2                           |    | linear               | $sp$          |    |
| 3                           |    | trigonal planar      | $sp^2$        |    |
| 4                           |    | tetrahedral          | $sp^3$        |    |
| 5                           |    | trigonal bipyramidal | $sp^3d$       |    |
| 6                           |  | octahedral           | $sp^3d^2$     |  |

## Recap

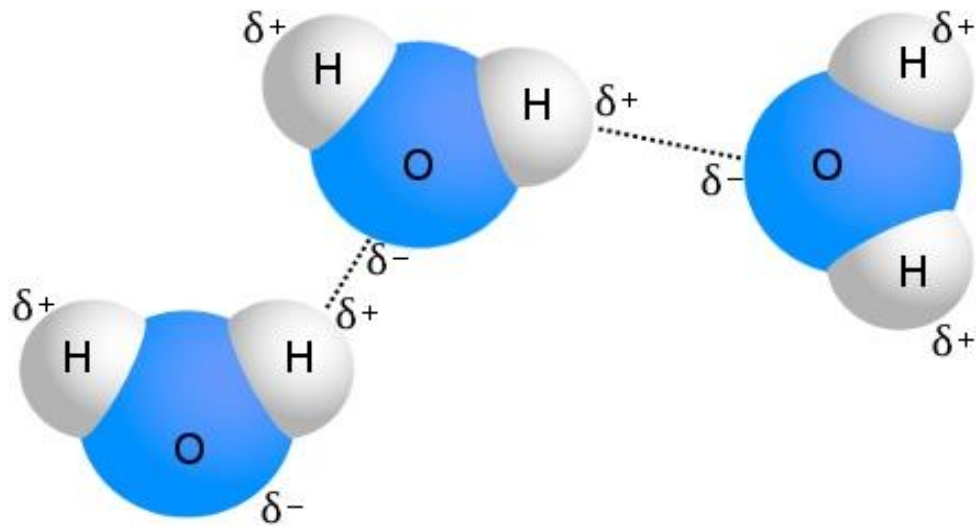
| Types of Intermolecular Forces | Present In                                      | Molecular Perspective  | Strength       |
|--------------------------------|---|--|----------------|
| Dispersion*                    | All molecules and atoms                         |   | 0.05-40 kJ/mol |
| Dipole-Dipole                  | Polar molecules                                 |   | 5-25 kJ/mol    |
| Hydrogen Bonding               | Molecules containing H bonded to F, O, or N     |   | 10-40 kJ/mol   |
| Ion Dipole                     | Mixtures of ionic compounds and polar compounds |  | 40-600 kJ/mol  |

\*Dispersion forces can become very strong (as strong and even stronger than the others) for molecules of high molar mass.

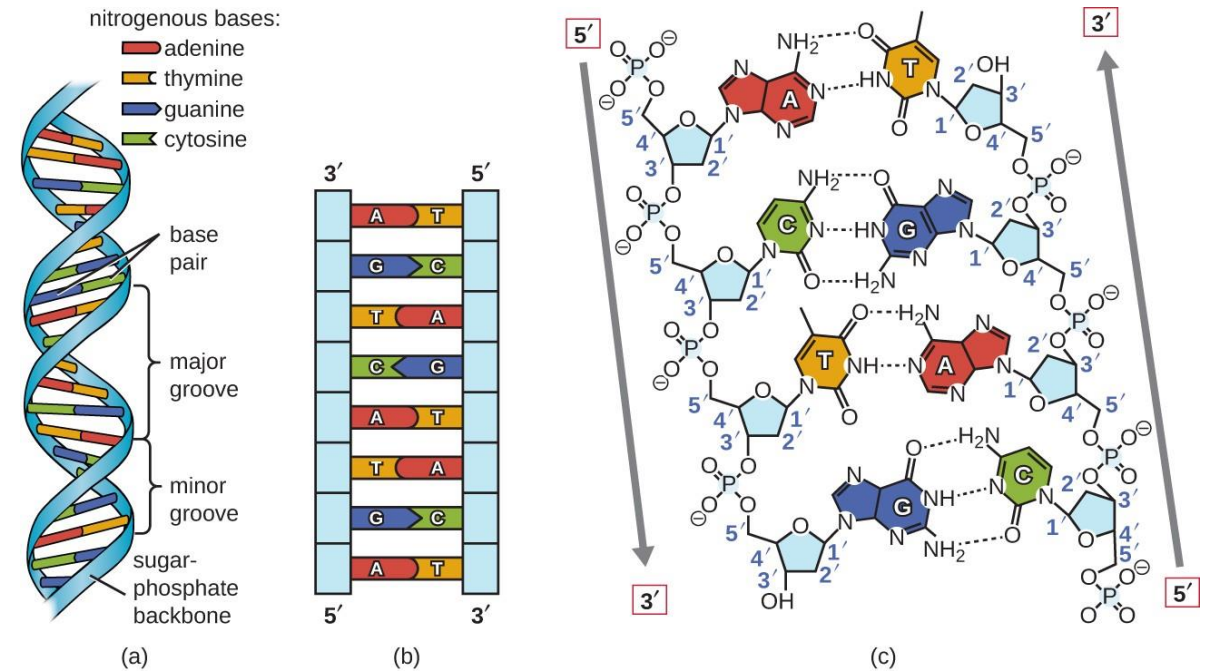
# Hydrogen bonds

- Happens when a hydrogen atom is placed between 2 very electronegative atoms
- Only F, O and N are small and electronegative enough for such bonds

In water



In DNA



Have a beautiful day, see you at the exam 😊  
+ Lecture next Tuesday!

