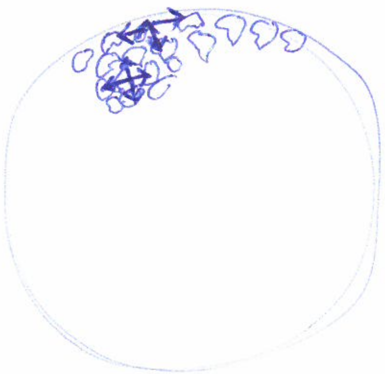
Structural elements of living matter

- living matter : a special organization of matter that is able to - metabolize
  - reproduce itself

- structure : - how components of a system are organized
  - it implies a certain pattern or <u>periodicity</u>

crystals ⟺	liquids
- more organized	- less organized
- periodicity = lattice constant	- only local order
- elementary cell	- no elementary cell only local short-lived structures

(1) water : - medium of life, all biochemical reactions
- <u>anomalous</u> material = it's unusual though it is abundant
  - high boiling (point) temperature
  - high freezing temperature
  - high surface tension
    - liquids tend to minimize their surface due to:
      - cohesive forces: - cancel out each other in bulk ~~water~~ liquid
        - but "attract" the molecules toward the bulk on the surface



- surface tension is the work required to increase the surface area of liquid by one square meter

$$\gamma = \frac{\Delta E}{\Delta A}$$

ΔE ← work = energy change [J]

ΔA ← area [m^2]

γ ← surface tension [$\frac{J}{m^2}$]

- high specific heat capacity: the heat required to increase the temperature of 1 kg liquid by 1°C ≙ 1 K

$$c = \frac{Q}{m \cdot \Delta T}$$

- Q ← heat (energy change) [J]
- c ← specific heat capacity $\left[\frac{J}{kg \cdot K}\right]$
- m ← mass [kg]
- ΔT ← temperature change [K]

- highest density at ≈ 4 °C

Explanation: bonding system

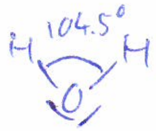
$r(H) = 120\ pm$ radius of H atom

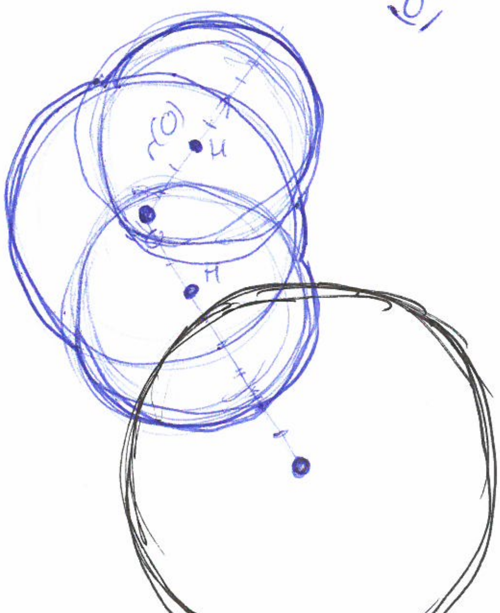
$r(O) = 152\ pm$ radius of O atom

$d(O-H) = 96\ pm$ distance between H and O nuclei in OH bond

⇓

shorter than $r(O)$ and even than $r(H)$





- the H nucleus is "inside" the O electron shell
- the O nucleus is also "inside" the H electron shell

BUT: water forms H-bonds

- X–H ···|X'   X, X': F, N, or O
- strongest secondary interaction
- weakest primary?
  - weak dative polar covalent bond
    - dative ↓ electron pair is provided by one atom
    - polar ↓ $EN(X') > EN(H)$
    - covalent ↓ e^- pair is shared

$d(O| \cdots H) = 177\ pm$

- these distances actually describe a very compacted system

ice crystal	liquid water at 4°C
- tetrahedral structure	- no long range structure
- more organized	- less organized
- less compact	- more compact
- lower density	- density is higher

ice → water 4°C: structure collapses gradually, increasing density

water 4°C → water 100°C: molecular motions increase, average distance between molecules increase, density decreases

- water is not the only molecule having hydrogenes...
- compare other non-metal hydrides: - all the other hydrides are gases at STP
  - the reason: water has the strongest average attractive force between molecules

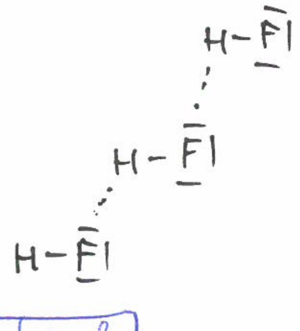
CH_4
- EN of C is too low
- it does not even have a nonbinding e^- - pair

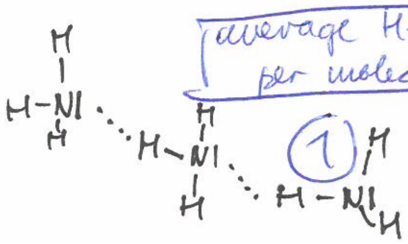
$|NH_3$
can donate 3 H
can receive 1 H → limits number of possible H-bonds
average H-bond per molecule: 1

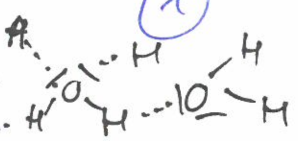
$\langle OH_2$
can donate 2 H
can receive 2 H
average H-bond per molecule: 2

$\langle SH_2$
- EN of S is too low

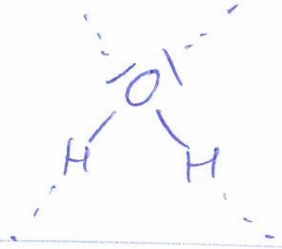
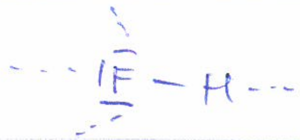
$\overline{|F}H$
can donate 1 H
can receive 3 H → limits number of possible H-bonds
average H bond per molecule: 1







Do not confuse!

	average number of bonds per molecule	number of bonds formed by a single inspected molecule
	$\frac{\text{total number of molecules in system}}{\text{total number of bonds in system}}$	
for $\vert NH_3$	1	 max 4
for OH_2	2	 max 4
for $\overline{\underline{\vert F}}H$	1	 max 4

↑ This matters for bulk properties!

- the strength and number of H-bonds is responsible for ~~...~~ high
  - specific heat
  - boiling / freezing temperatures
  - surface tension and hydrophobic interaction

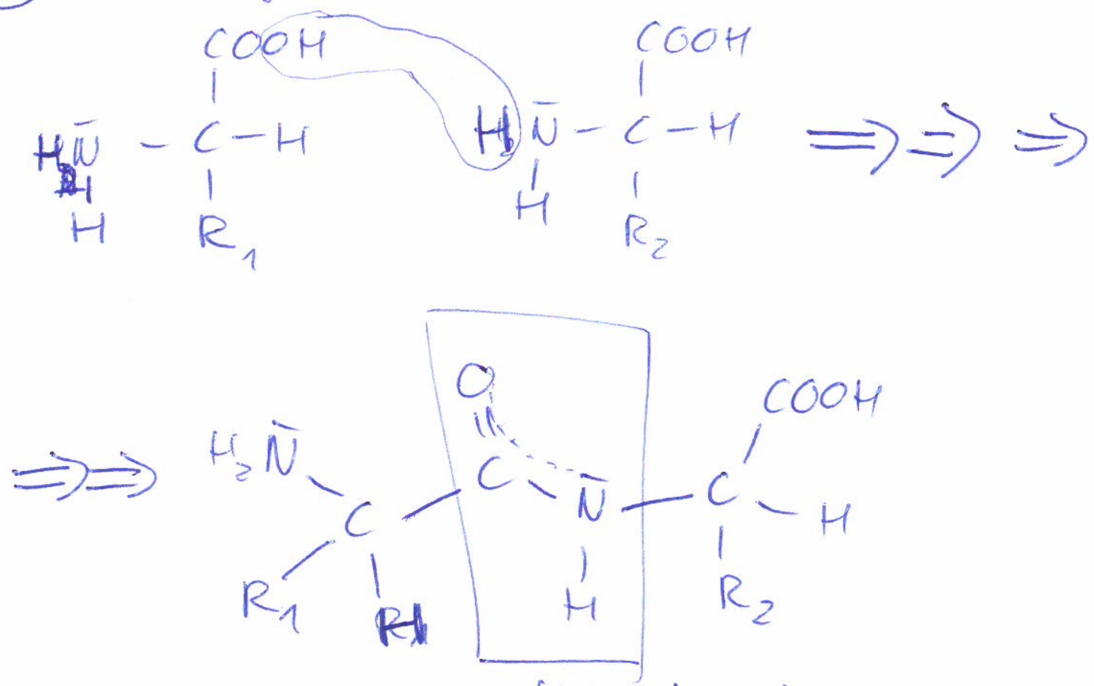
biological "structural elements"

- lipids
- macromolecules → proteins, → nucleic acids

(2) structure of proteins

- directed linear copolymers of 20 amino-acid types (may be modified)

(I) Primary structure: sequence of amino acids



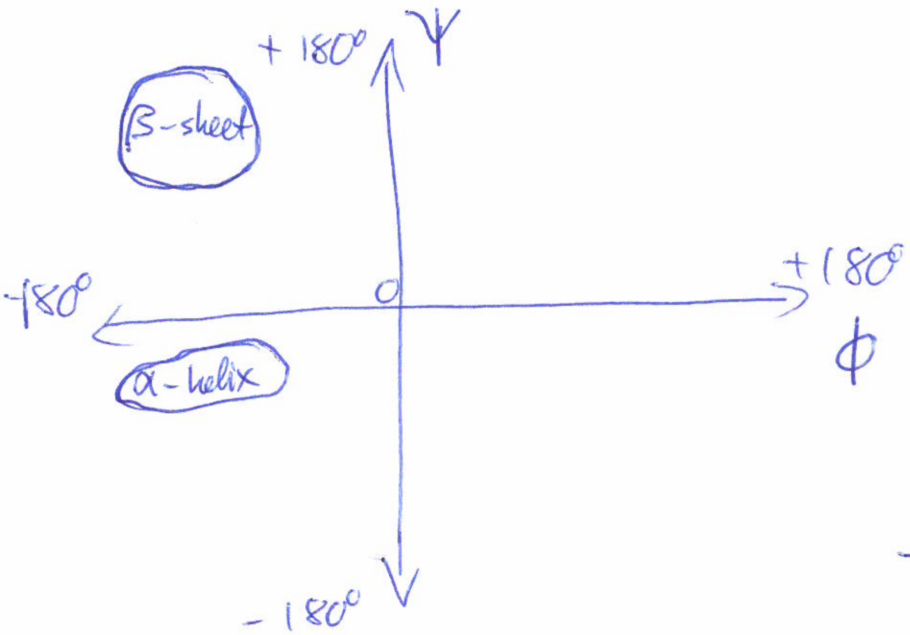
peptide bond

- O, C, N, H are in the same plane due to the delocalized electron system of O=C double bond and N̄ non-binding electron pair
- the structure is stabilized by <u>covalent bond</u>

II Secondary structure: local order in the polypeptide chain

- $\overset{O}{\overset{\|}{C}}-\underset{H}{\underset{|}{\bar{N}}}$ angle is fixed (almost always 180)
- $C_\alpha - \overset{O}{\overset{\|}{C}}$ angle (ψ) and $\underset{H}{\underset{|}{\bar{N}}} - C_\alpha$ angle (ϕ)

may vary, but due to spatial obstructions the rotation about these sigma bonds is limited
- only certain range of angles occure often:
- the plot of ~~pe~~ frequent ψ and ϕ angles is called Ramachandran-plot:



- so the secondary structures are repetitions of characteristic ψ and ϕ angles including at least 3 amino acid ~~residues~~ units
- secondary structures are stabilized by H-bonds formed between atoms of the polypeptide backbone

- not all parts of the polypeptide bond have secondary structure (i.e. repeating ψ and ϕ angle values)

III Tertiary structure: the complete three dimensional structure of a protein molecule

- it is defined by the position of all atoms in the protein
- this "shape" is "encoded" in the molecule
  - hydrophobic side chains are hidden from the aqueous medium
  - hydrophylic is exposed to it
  - the formation is pretty much automatic (does not require help from other cell components in most cases)
- main driving force and stabilizing force: hydrophobic ~~inte~~ interaction ⇒ it is the water that has important role in forming the tertiary structure
- other stabilizing effects:
  - covalent bonds (S-S bridge)
  - salt bridge (acid$^{\oplus}$ .. $^{\ominus}$base)
  - hydrogene bonds

IV Quaternary structure: 3-dimensional shape of protein complexes = more than one polypeptide chain

- forces and formation is similar to III structure