

Structural Components

1, Water: $\text{H}-\ddot{\text{O}}-\text{H}$

- size $r(\text{O}) \approx 152 \text{ pm}$ (van der Waals radius)

$r(\text{H}) \approx 120 \text{ pm}$

$d(\text{O}-\text{H}) \approx 90 \text{ pm}$

- within water the H-O distance is less than the r of O : so the nuclei of H's are "immersed" in the electron cloud of oxygen.



- water molecules have H-bonds between them

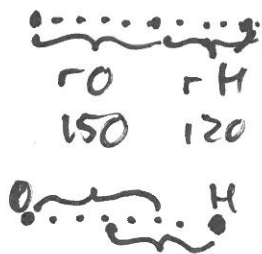
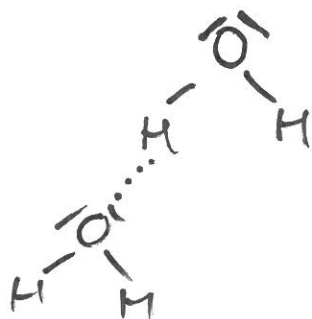
- this is a bond between

- an atom with high electronegativity and free non-bonding electron pair ($\text{H}-\ddot{\text{O}}\cdot$, $\cdot\ddot{\text{N}}\cdot$, $\cdot\ddot{\text{F}}\cdot$)

- a hydrogen atom which is covalently bonded to an atom with high electronegativity ($\text{H}-\ddot{\text{O}}\cdot$, $\text{H}-\ddot{\text{N}}\cdot$, $\text{H}-\ddot{\text{F}}\cdot$)

- H-bond can be considered a weak dative (coordinative) covalent bond

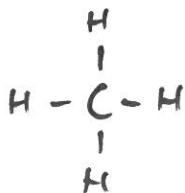
- the H-bond length is about 200 pm



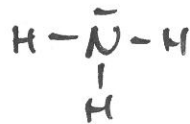
So we can say that water is "densely packed" both in solid (ice) and liquid phase

Anomalous properties of water

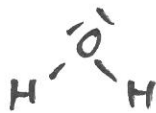
- water is an abundant liquid but its properties are atypical:
 - high boiling point and latent heat of boiling
 - high melting point and latent heat of melting
 - high specific heat capacity
 - high surface tension
 - density variation with temperature
 - ice is slippery
- compared to other nonmetal hydrides, water has very high boiling and melting point \rightarrow the strength of cohesive ~~forces~~ (bonds between water molecules) are responsible



methane



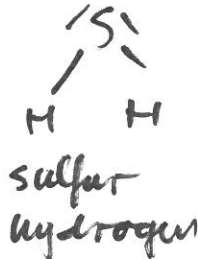
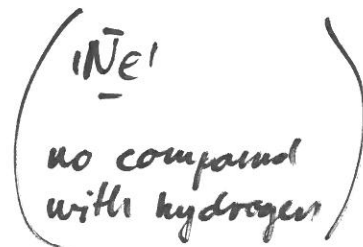
ammonia



water



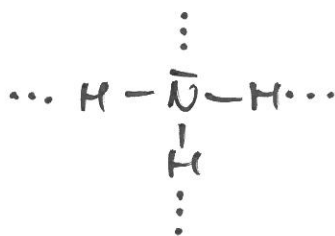
hydrogen fluoride



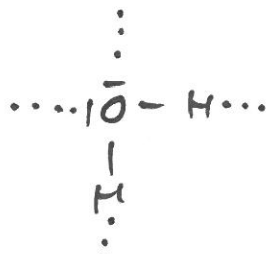
sulfur hydrogen

- does not form H-bonds because
- no nonbonding e^- pair
 - EN of C is low

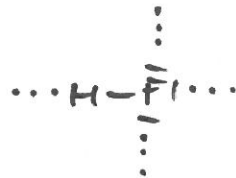
does not form H-bond because EN of S is low



send
accept
average number of bonds 1/molecule



2
2
2/mol
- 2 -



1
3
1/mol

- water wants to minimize its surface
 - water in a space station (where's no gravity) would form spherical drops
 - if the drops are moved close to one another, they would ~~not~~ unite, fuse to form one droplet



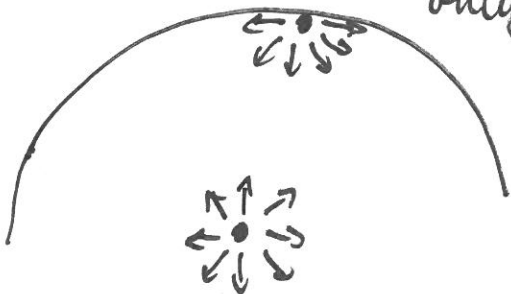
Homework: suppose we have two spherical water droplets with 1g mass each. What is the energy change if they fuse and form one spherical droplet?

$$\gamma_{\text{water}} = 72 \text{ mJ/m}^2$$

- to increase the surface of a liquid we need to invest energy: the energy required to increase the surface by 1 m^2 is called surface energy or surface tension, denoted by γ . Its unit is J/m^2 or N/m . Homework: prove that these units are equal.

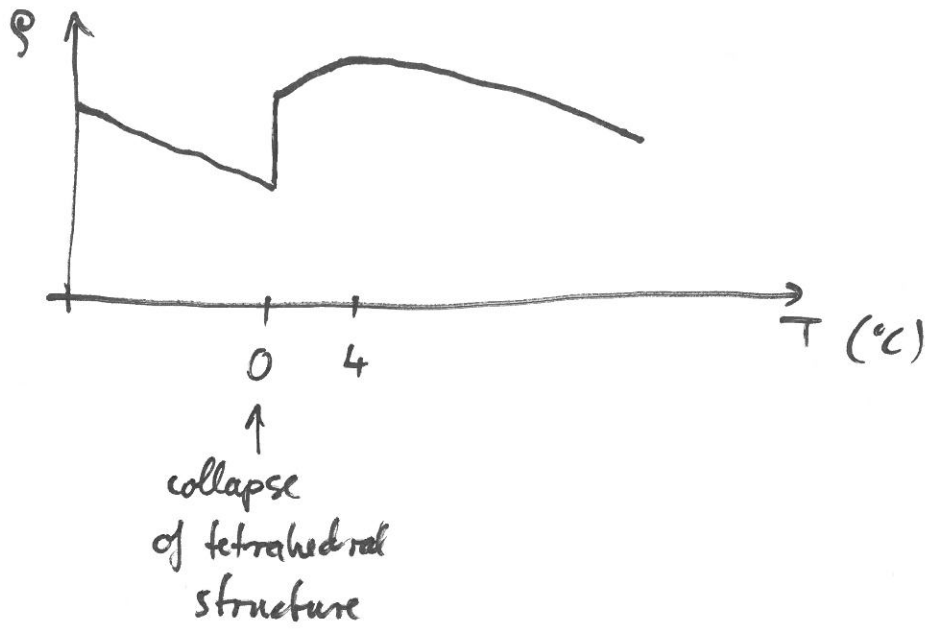
- reason of surface tension:

water molecule on the surface is attracted only on one side \rightarrow net force is inward

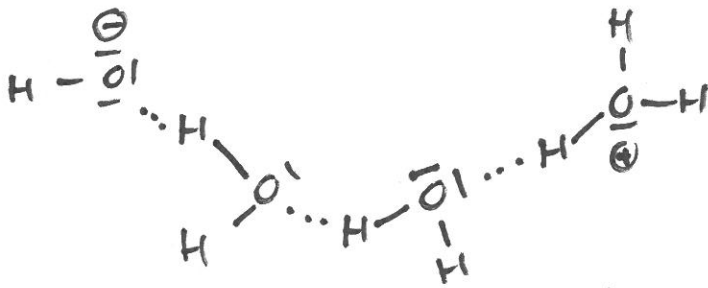
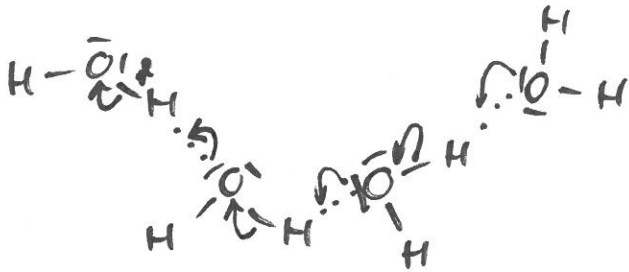


water molecule inside the droplet is attracted due to secondary bonds in directions \rightarrow the net force is zero.

- density variation of water with temperature



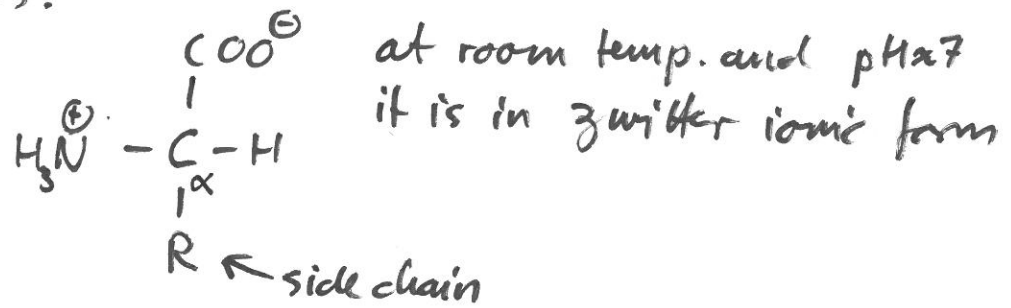
- transportation of H in water



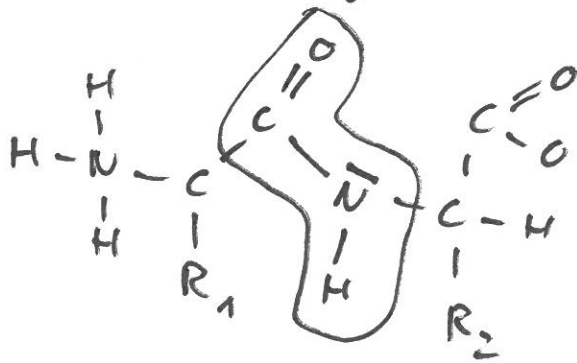
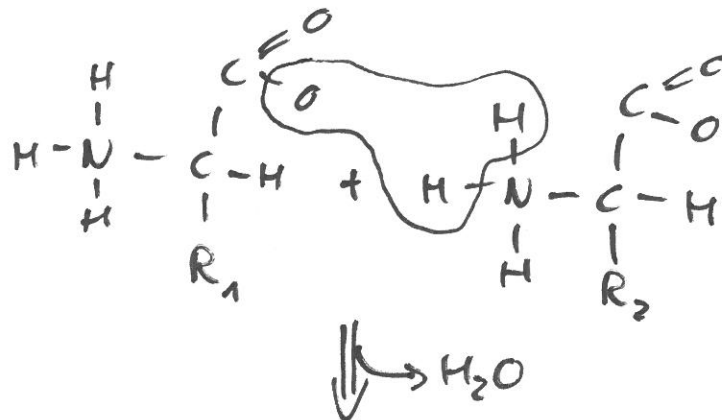
Structure of proteins

proteins are polymers of amino acids

there are 20 different ~~par~~proteinogenic (= forms protein) amino acids:



polymer is formed by condensation of the molecules:



amide (peptide) bond is formed

the π electrons of the $\text{C}=\text{O}$ bond and the p electrons of N are delocalized \rightarrow so the four atoms of the bond are in the same plane.

so the $\text{C} \rightarrow \text{N}$ bond is

not a real sigma bond:

rotation is not allowed.

- we have different levels of protein structure and there is a hierarchy between them.

- PRIMARY structure

- the order of consecutive amino acids within the polypeptide chain

- they are held together by the covalent peptide bonds

Ala - Gly - Val - Leu - Leu - Gly - Asp -

- the structure can be determined by

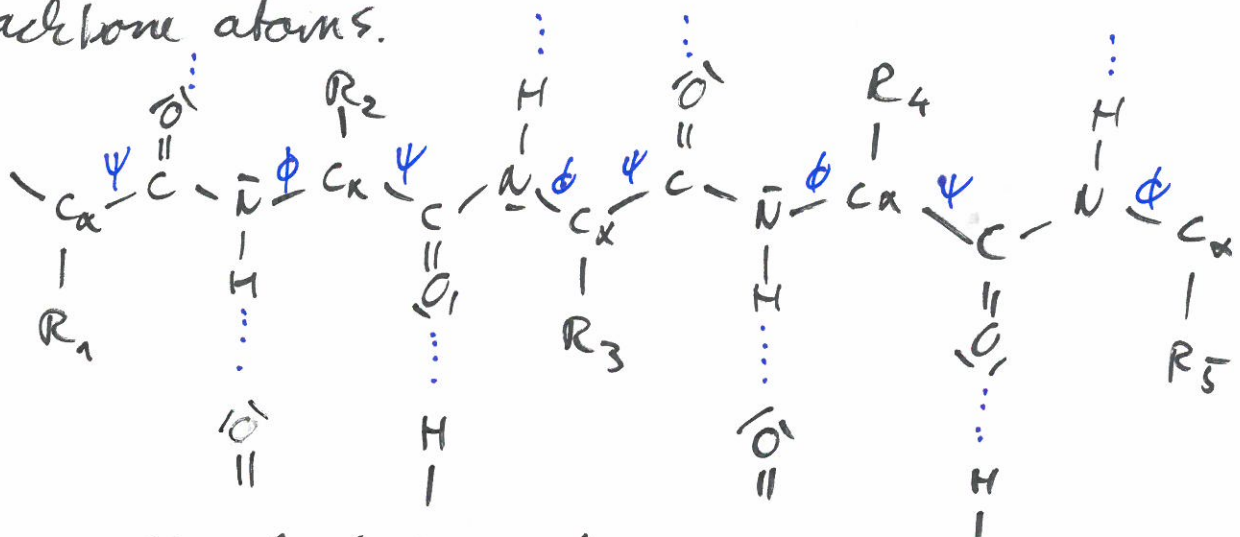
- chemical means (decomposition)

- physical methods (X-ray crystallography, NMR)

- SECONDARY structure

- a local structure characterized by the repetition of the dihedral (torsional) angles (ψ and ϕ) for at least 3 amino acid units

- this structure is stabilized by the H-bonds between backbone atoms.



- types: α -helix (right handed), parallel β -sheet, β -turn, antiparallel β -sheet

- some parts of a protein molecule may have α helix, others β -sheet, again others may be disordered (no 2ndary structure)
- some proteins don't have any secondary structure
- it can be analysed by circular dichroism spectroscopy (see: Polarimetry lab)

- TERTIARY STRUCTURE

- global 3D structure (conformation) of the protein
- it is primarily stabilized by hydrophobic interaction
- it can be determined by X-ray crystallography or NMR or electron microscopy

- QUATERNARY STRUCTURE

- it only applies for proteins with multiple polypeptide chains:
- it is the arrangement of these chains