

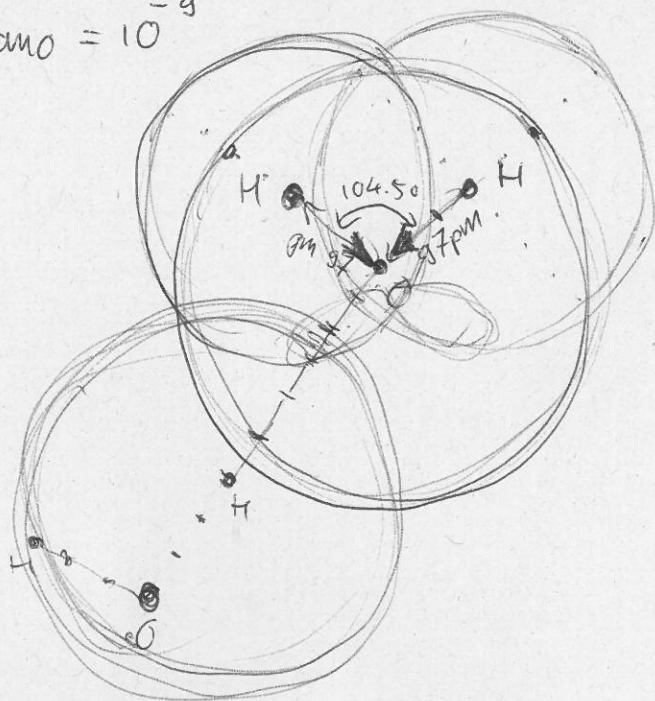
Water

anomalous: - although water is abundant in nature, its properties are rather unique compared to other liquids

properties of a single water molecule

pico = 10^{-12}
nano = 10^{-9}

Ångström = 10^{-10} m



O-H \approx 97 pm
r(O) \approx 150 pm
r(H) \approx 120 pm

O-H \approx 177 pm

- tetrahedral: the non binding e^- pairs take up space as well

- irregular tetrahedron:

the non binding e^- -pairs take up more space than the H-s

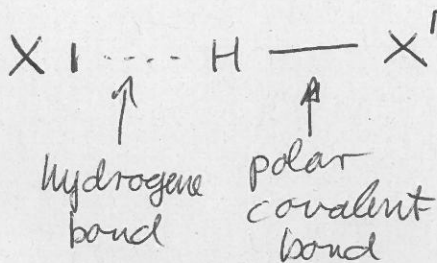
- the H-s electron cloud overlaps to a great extent with that of the O-s.

- because of the 104.5° angle and the EN difference, the water molecule has a permanent dipole moment.

the overlap between the electron clouds of the H and O atoms in a hydrogen bond is also significant

hydrogen bond

X: high EW atom
N, O, F



a hydrogen bond can be considered a weak, polar, dative covalent bond

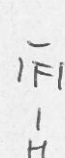
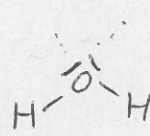
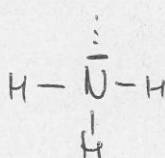
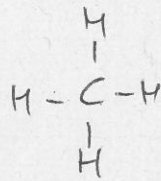
Why does water have extraordinary properties?

1 high boiling and melting point

2 high specific heat capacity (energy required to increase the temperature of 1kg material with 1°C) $C = \frac{\Delta E}{\Delta t \cdot m}$

3 high surface tension (energy required to make an extra 1m² surface) $\gamma = \frac{\Delta E}{\Delta A}$ unit: $\frac{J}{m^2} = \frac{Nm}{m^2} = \frac{N}{m}$

4 density variation with temperature



donated H

(-)

3

2

(1)

accepted H

(+)

(1)

2

3

max no. of H bonds per one mol.

-

4

4

4

average no. of H-bonds per molecule

1

2

1

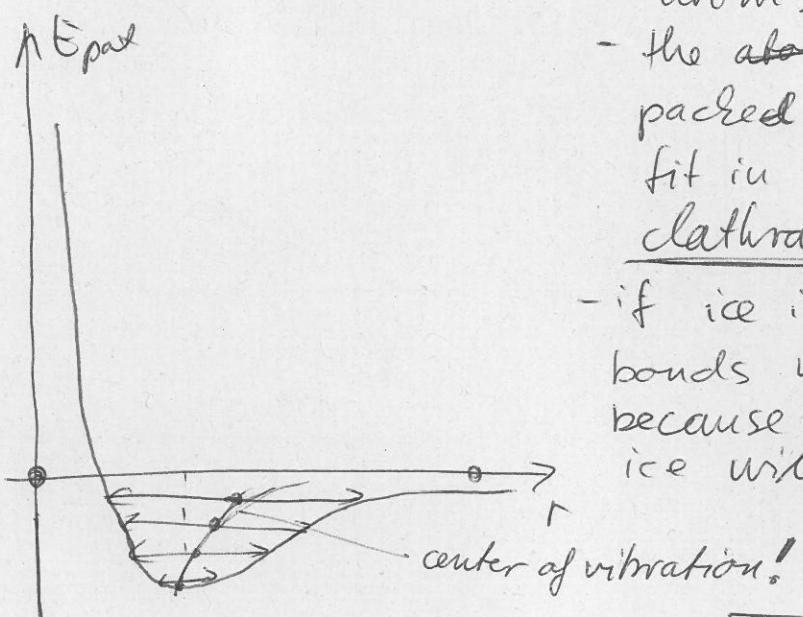
4.) solid water (ice): - tetrahedral structure

- crystal

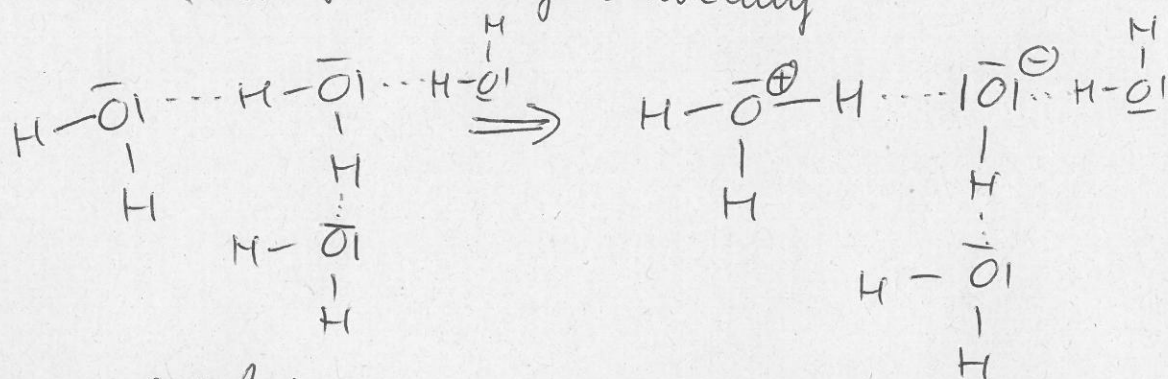
- long term order (where order means periodicity: regular repetition of some property, like position of atoms)

- the ~~atoms~~ molecules in ice are not packed very densely: small atoms fit in between: to form so called clathrates

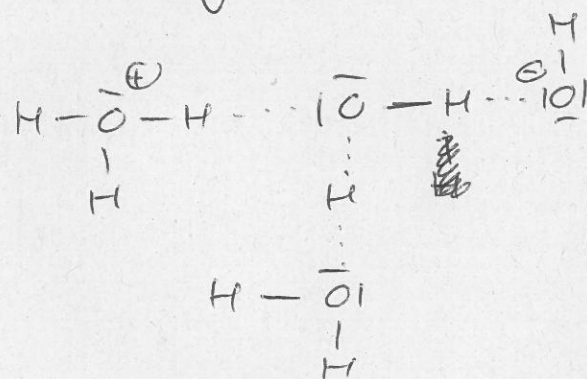
- if ice is heated (e.g. -20°C → -10°C) bonds will vibrate more, and because of asymmetry of vibration, ice will expand



- giving even more heat will melt the ice
- the tetrahedral structure will "collapse"
 - the water will become more "packed"
 - ~~the~~ density increases, maximum is reached at $+4^{\circ}\text{C}$
 - in liquid water there is still some degree of order but it is short range, only a few or few ten ~~atoms~~ or molecules are involved
 - the ordered structures are short-lived, and transform dynamically



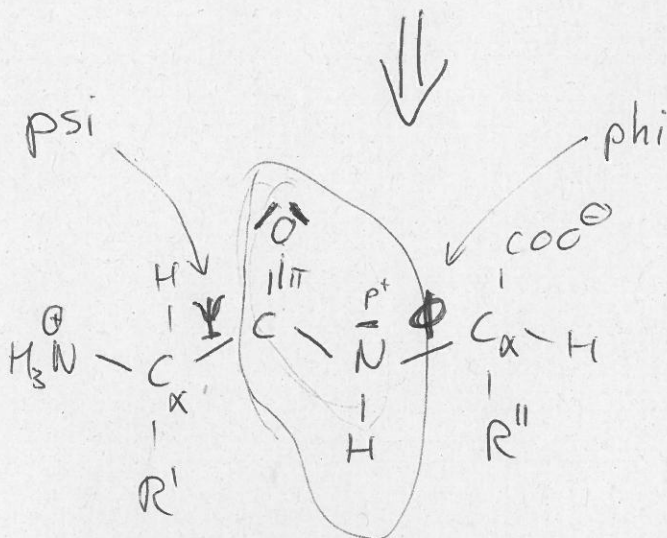
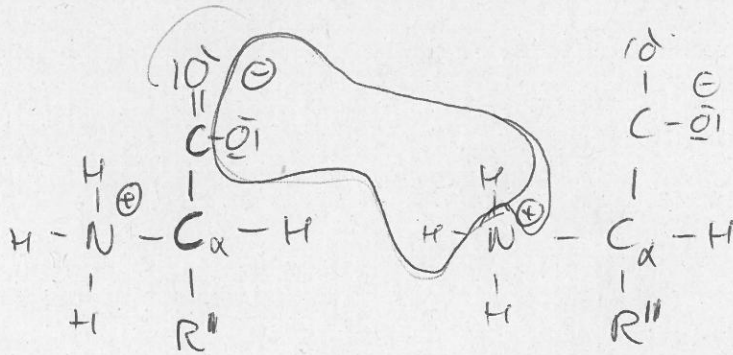
- the $\text{H}-\text{O}$ covalent bonds transform rapidly into $\text{H} \cdots \text{O}$ hydrogen bonds
- hydrogen bonds break up and re-form very quickly (10^{10} times/s)



- the organized structure in liquid water is e.g. the water cluster

Proteins

- directed ~~hetero~~ heteropolymers of the 20 (+2) proteinogenic amino acids



peptide bond
with delocalized
electrons

all atoms involved in the
delocalization will be
in the same plane

COPLANAR

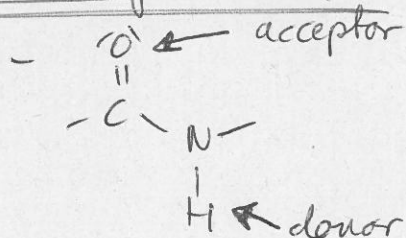
- no free rotation about the $\text{C} = \text{N}$ bond

- only the ψ and ϕ torsional angles allow relatively free rotation. \rightarrow protein structure
- there is a hierarchy in protein structure

primary structure:

- the amino acid sequence = constitution
- stabilized by covalent (peptide) bonds
- chemical methods, sequencing

secondary structure:



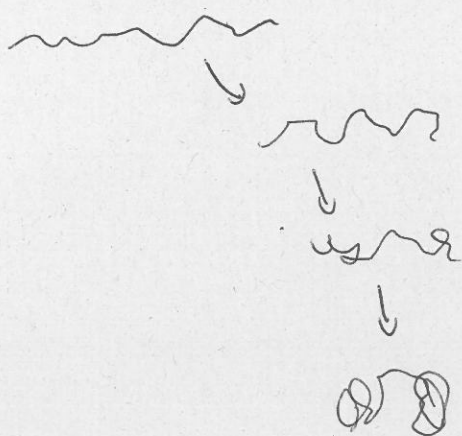
- local order in the size of ψ and ϕ torsional angles involving at least 3 amino-acid residues (units)
- it is stabilized by hydrogen bonds between the polypeptid backbone N and O

- possible angle combinations are shown in the RAMACHANDRAN plot

- typical examples:
 - α helix (right handed)
 - β -sheet (parallel & anti parallel)
 - β -turn

tertiary structure:

- complete protein conformation
- 3D-structure
- stabilized by hydrophobic interactions
- the process of the formation of this structure is called protein folding.



~~tertiary~~

quaternary structure

- proteins consisting of several subunits : polypeptide chains
- hydrophobic interaction

Nucleic acids

primary structure: → nucleotide sequence

secondary structure: → double helix

- A, B, Z

- stabilized by base pairing

tertiary structure: → nucleosome formation
super helix



chromosome