Fyzika biopolymerů

Voda

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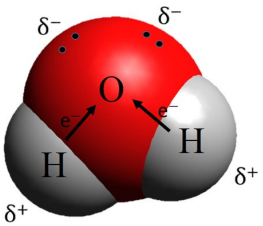
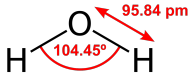
Voda

je nezbytná pro existenci života jak jej známe





Vlastnosti vody

TABLE 4.1 Common Properties of Water

Molecular Formula	**H_2O**
Mass	18.0153 amu (or g/mol) 2.99072×10^{-26} kg/molecule
Molecular volume (liquid)	14.6 Å^3/molecule (van der Waals)
Concentration	55.345 M (mol/L)
Number density	3.34×10^{28} m^{-3}
Density	997.05 kg/m^3 (liquid, 25°C, 1 atm) 999.97 kg/m^3 (liquid, 3.984°C, 1 atm) 916.72 kg/m^3 (solid, 0°C, 1 atm)
Melting point	0°C (273.15 K)
Boiling point	100.0°C
Specific heat (constant pressure)	4182 J/(kg·K)
Dielectric constant	$78.5\varepsilon_0$
Viscosity (dynamic)	0.8909×10^{-3} Pa s (25°C) 1.0016×10^{-3} Pa s (20°C)
Surface tension	0.07198 J/m^2

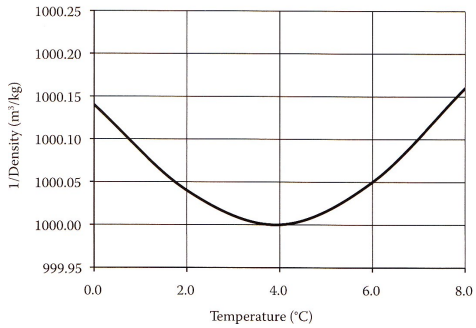
74 anomalií vody

http://www1.lsbu.ac.uk/water/water_anomalies.html

- Phase anomalies P1-P13
- Density anomalies D1-D22
- Material anomalies M1-M18
- Thermodynamic anomalies T1-T11
- Physical anomalies F1-F10

Hustota vody

- charakteristická vlastnost vody
- významná pro existenci života na Zemi
- hustotní maximum při 4 °C → led má menší hustotu než kapalná voda, a proto plave na hladině



Zvláštnosti vody

měrná tepelná kapacita

- voda má silnou schopnost absorbovat teplo (teplota takového systému roste jen zvolna)

TABLE 4.3 Heat Storage:[a] $Q = mc_p\Delta T$

Substance	c_p (kcal/kg·K)
Lead	0.031
Mercury	0.033
Copper	0.092
Glass	0.20
Marble	0.21
Aluminum	0.214
Ice (−10°C)	0.53
Ethanol	0.581
Sea water	0.93
Water	**1.00**

[a] Specific heats of substances at constant pressure.

Zvláštnosti vody

tepelná vodivost

- voda má velkou tepelnou vodivost, asi 4x větší než jiné kapaliny

TABLE 4.4 Heat Transport: Thermal Conductivities of Selected Substances

Substance	Thermal Conductivity ($W\ m^{-1}\ K^{-1}$)
Air	0.0256
Nitrogen (300 K/80 K)	0.026/0.13
Carbon tetrachloride	0.10
Diphenyl	0.14
Toluene	0.13
Water	**0.60**
Styrofoam	0.010
Ice (0°C)	2.2
Copper	390
Diamond	2450

Zvláštnosti vody

skupenské teplo

- skupenské teplo fázových přechodů je asi 3x větší než u jiných kapalin

Table 4.5 Latent Heats of Fusion, Vaporization, and Corresponding Temperatures for Water and Several Other Substances

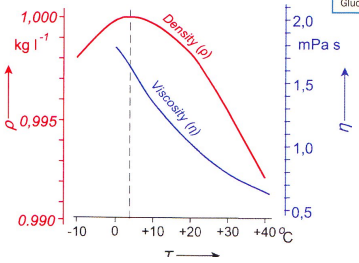
	Melting Point (°C)	Latent Heat of Fusion, L_f (J/kg)	Boiling Point (°C)	Latent Heat of Vaporization, L_v (J/kg)
Ethanol	−114.4	10.8×10^4	78.3	8.55×10^5
Methanol	−96	9.92×10^4	64.7	10.7×10^5
Acetone	−94.7	9.80×10^4	56.5	5.51×10^5
Mercury	−38.9	1.14×10^4	356.6	2.96×10^5
Water	**0.0**	$\mathbf{33.5 \times 10^4}$	**100.0**	$\mathbf{22.6 \times 10^5}$
Benzene	5.5	12.6×10^4	80.1	13.7×10^5
Glycerol	17	20.6×10^4	290	9.57×10^5

Zvláštnosti vody

nízká viskozita

TABLE 4.2 Resistance to Movement: Viscosities of Fluids (25°C)

Fluid	Viscosity (Pa·s)
Air	1.8×10^{-5}
Acetone	3.06×10^{-4}
Methanol	5.44×10^{-4}
Benzene	6.04×10^{-4}
Water	$\mathbf{1.0 \times 10^{-3}}$
Ethanol	1.07×10^{-3}
Methanol	0.544×10^{-3}
Blood	2.3×10^{-3}
Sulfuric acid	2.42×10^{-2}
Motor oil (No. 10)	0.2
Glycerol	1.5
Glucose (solid)	$6.6 \times 10^{+10}$



Zvláštnosti vody

povrchové napětí

- voda má velké povrchové napětí
- znemožňuje vytečení malými otvory

většina kapalin má při nízkém povrchovém napětí i nízkou viskozitu, ale voda má vysoké povrchové napětí a nízkou viskozitu

TABLE 4.6 Surface Tensions and Surface Tension: Viscosity Ratio

Substance	Surface Tensiona (w/air) Σ, (N/m or J/m2)	Σ/η (m/s)
Ethanol	0.0221	20.6
Methanol	0.0227	41.7
Acetone	0.0252	82.4
Benzene	0.0288	47.7
Pyridine	0.0380	—
Sulfuric acid	0.0551	2.28
Glycerol	0.0640	0.0445
Hydrazine	0.0667	—
Water	**0.0728 (25°C)** **0.0588 (100°C)**	**72.8**
Tissue fluids	**0.050**	**—**
Soapy water	**0.037**	**—**
Lung surfactant	**0.001**	**—**
Water (with butanol)	**0.0018**	**—**

[a] Interface with air, except as noted.

Zvláštnosti vody

dielektrická konstanta

- voda má jednu z nejvyšších dielektrických konstant mezi kapalinami

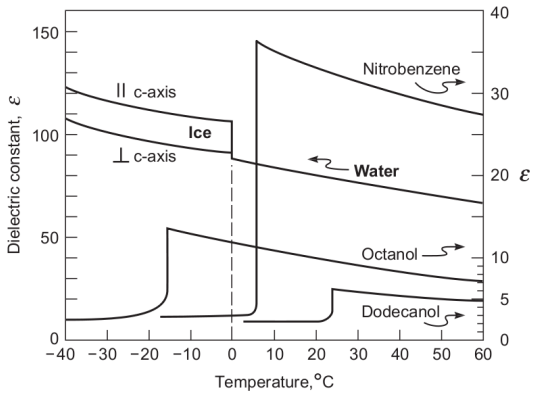
TABLE 4.7 Dielectric Properties of Fluids[a]

Substance	Static Dielectric Constant, ε	Dipole Moment (Debye)
Hexane	1.9	0.00
Benzene	2.3	0.00
Diethyl ether	4.3	1.15
Chloroform	4.8	1.15
Ammonia	16.9	1.47
Acetone	20.7	2.72
Ethanol	24.3	1.68
Methanol	32.6	1.66
Dimethyl sulfoxide	48.9	3.96
Water (298 K)	**78.5**	**1.84 (gas)**
(Liquid, 273 K)	**88**	**2.5–3 (in liquid and solid?)**
(Ice, 273 K)	**91.5**	
Formamide	110.0	3.37

[a] Water has a high dielectric constant and relatively low permanent electric dipole moment.

Zvláštnosti vody

dielektrická konstanta



Zvláštnosti vody

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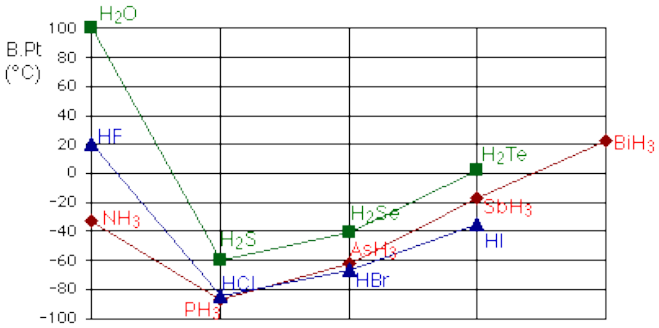
Formamide	110.0	3.37

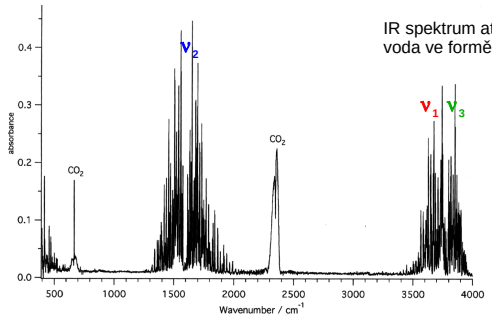
[a] Water has a high dielectric constant and relatively low permanent electric dipole moment.

Zvláštnosti vody

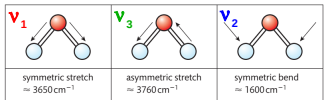
bod varu pro osatní látky s vodíkovými vazbami



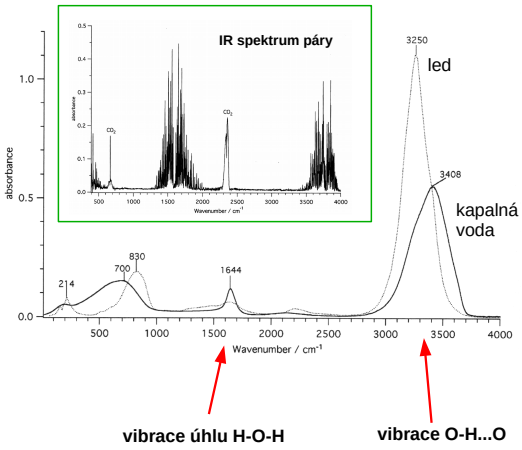
Vibrace molekuly vody



IR spektrum atmosféry
voda ve formě páry



IR

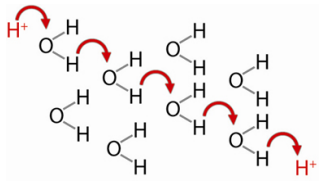


vibrace úhlu H-O-H

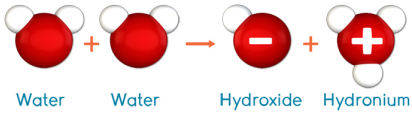
vibrace O-H...O

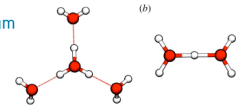
Kapalná voda x led

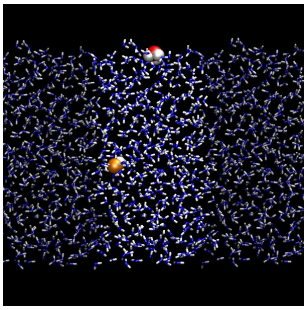
- počet sousedů je v kapalné vodě 5 v ledu 4
- průměrný počet vodíkových vazeb na molekulu je v kapalině ~3.5 v ledu 4
- úhel H-O-H je v kapalině 104.5° = menší než v ledu 109.5°
- molekuly vody mohou vyplňovat mezery přítomné ve struktuře ledu
- v ledu je vyšší protonová vodivost a mobilita (protony přeskakují podél sítě vodíkových vazeb – Grotthussův mechanismus)



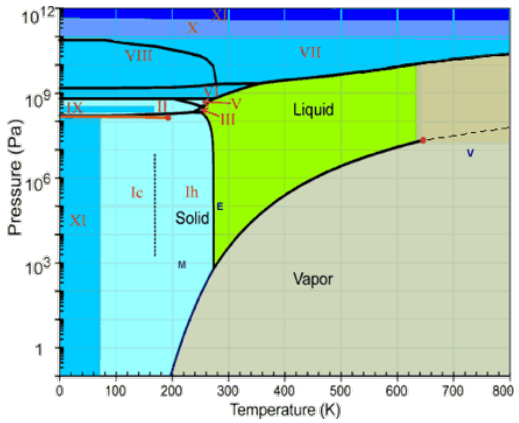
Autoionizační vlastnost vody





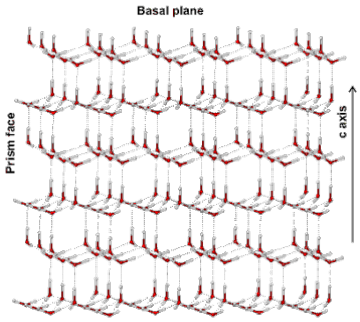


Fázový diagram vody

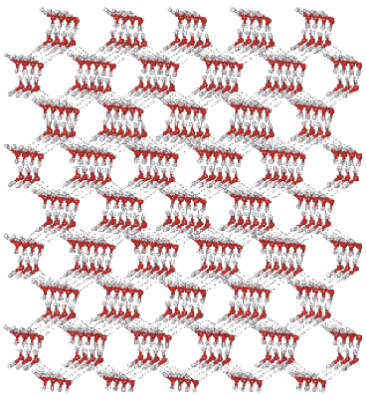


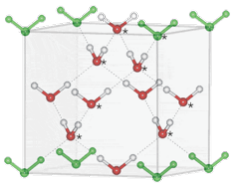
Normální led Ih

hexagonální

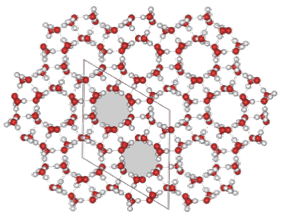
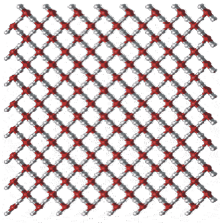
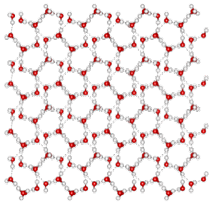
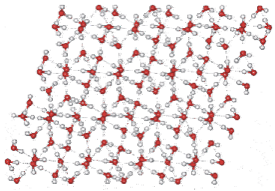


Kubický led Ic





Další ledy

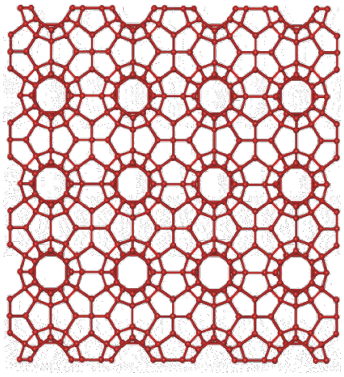
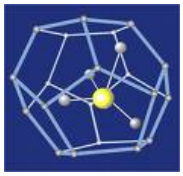





Amorfní voda

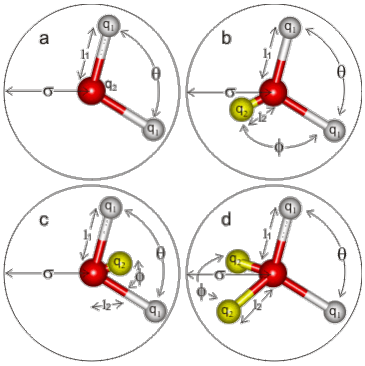
prudce zchlazená voda na cca -150 °C….. sklo


Klatráty

bod varu pro osatní látky s vodíkovými vazbami

Modely vody



SPC, SPC/E, TIP3P, TIP4P, TIP5P…..

http://www1.lsbu.ac.uk/water/water_models.html

Vodní mýty

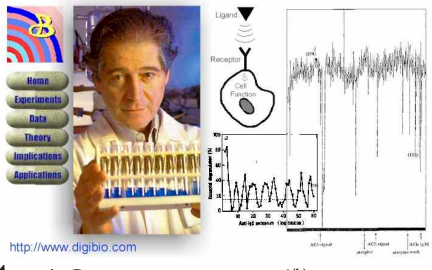
π-voda, neovoda, magnetická voda, polyvoda…

Led č. 9 je stabilní při teplotě výšší než 0 C - Kurt Vonnegut (spisovatel)

Ano, ale jen za enormních tlaků (tisíce atmosfér) - Bernard Vonnegut (vědec)

Paměť vody

1987: Jacques Benveniste



http://www.digibio.com

Nature Editor John Maddox

nature

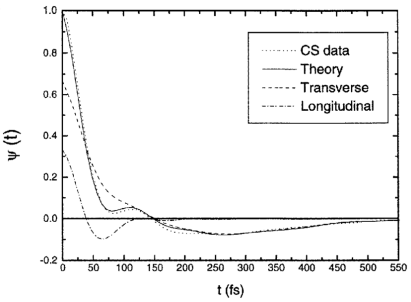
NATURE VOL 338 13 APRIL 1989

It is no disrespect to any of those concerned to compare the dilemma created for *Nature* by these events to that occasioned a year ago by the article in which Professor Jacques Benveniste and colleagues claimed that indefinitely diluted reagents retain their biological effectiveness. The claim flies in the face of orthodox belief, but the data available are insufficient for a careful judgement of its validity. But on this occasion, *Nature* has followed

- Homeopatie - netoxické (ve své době revoluční)
- nejde za efekt placeba

Paměť vody

Autokorelační funkce vody



Homeopatie

+ netoxické (ve své době revoluční)

- nejde za efekt placeba

Polyvoda

1966 – Nikolaj Fedyakin a Boris Deryagin (Technologický Institut Kostroma)

Bod varu: 200 C

Bod tání: -30 C

Specifické infračervené spektrum.

1968: Velká Británie, USA - Desmond Bernal

NATURE VOL. 224 OCTOBER 11 1969

"Anomalous" Water

SIR,—A report on the properties of "anomalous" water appeared recently in *Nature* (**222**, 159; 1969). The probable structure of this phase was reported by Lippincott *et al.*[1] who refer to the phase as polywater, a term descriptive of the structure.

After being convinced of the existence of polywater, I am not easily persuaded that it is not dangerous. The consequences of being wrong about this matter are so serious that only positive evidence that there is no danger would be acceptable. Only the existence of natural (ambient) mechanisms which depolymerize the material would prove its safety. Until such mechanisms are known to exist, I regard the polymer as the most dangerous material on earth.

Every effort must be made to establish the absolute safety of the material before it is commercially produced. Once the polymer nuclei become dispersed in the soil it will be too late to do anything. Even as I write there are undoubtedly scores of groups preparing polywater.

Scientists everywhere must be alerted to the need for extreme caution in the disposal of polywater. Treat it as the most deadly virus until its safety is established.

Yours faithfully,

F. J. DONAHOE

Wilkes College,
Wilkes-Barre,
Pennsylvania 18703, USA.

Zvláštnosti vody

Denis Rousseau, Bell Labs USA

Anomální vlastnosti polyvody díky kontaminaci z kapilár a z potu experimentátorů…

NATURE VOL. 230 MARCH 5 1971

NEWS AND VIEWS

Polywater Drains Away

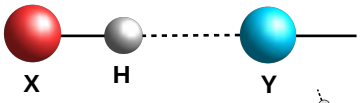
IT now begins to seem as if the concept of polywater is on its last legs. The article by Barnes, Cherry, Finney and Petersen on page 31 of this issue of *Nature* is one of several recent demonstrations that many of the observations put forward in the past few years as evidence of the existence of an anomalous form of water must be accounted for quite differently and much more trivially. On the face of things, at least, polywater seems to be not a distinct, stable (or metastable) form of water, but water contaminated by various substances among which silicates seem to be conspicuous. One of the most striking and direct demonstrations of this was the article by Bascom, Brooks and Worthington last year (*Nature*, **228**, 1290; 1970), which described how electron probe measurements of the residues obtained by condensing polywater had revealed the presence of silicon and sodium atoms. The quantities are indeed sufficiently small to explain why the presence of impurities has been unnoticed for so long. This, however, does not fully account for the way in which experimenters in the late nineteen sixties were apparently happy to record observations of anomalously high viscosity and boiling point without subjecting their samples to the full rigours of modern microanalysis.

Studená fůze

1989: S. Pons & M. Fleischmann

Vodíková vazba

IUPAC: The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation.



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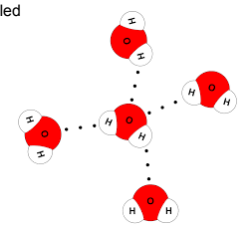
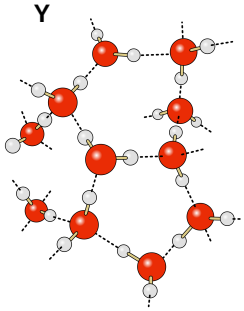


voda

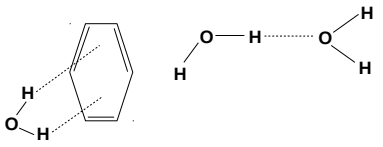


Vodíková vazba

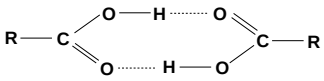
- interakce v důsledku přenosu náboje mezi donorem a akceptorem
- atomy X a H jsou spojeny kovalentní vazbou, která je polarizovaná – s rostoucí elektronegativitou X roste i síla vazby H...Y
- vodíková vazba je obvykle planární – čím více se úhel blíží 180°, tím je vodíková vazba silnější a vzdálenost H...Y menší
- při vzniku vodíkové vazby obvykle dochází k nárůstu délky vazby X-H, což se v IR spektroskopii projeví červeným posunem, ale existují i vodíkové vazby, které způsobují modrý nebo žádný posun vibračních frekvencí v IR
- vodíková vazba vykazuje charakteristické signatury v NMR spektroskopii
- kritérium, že délka vodíkové vazby je menší než součet van der Waalsových poloměrů, neplatí obecně, platí pouze pro silné vodíkové vazby

Příklady vodíkové vazby

slabé

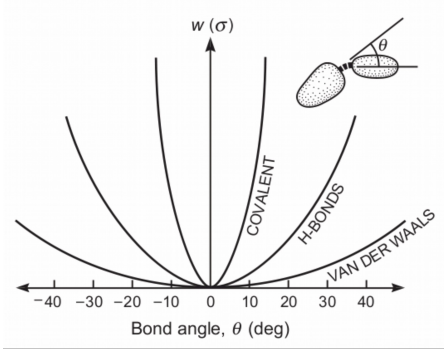


střední

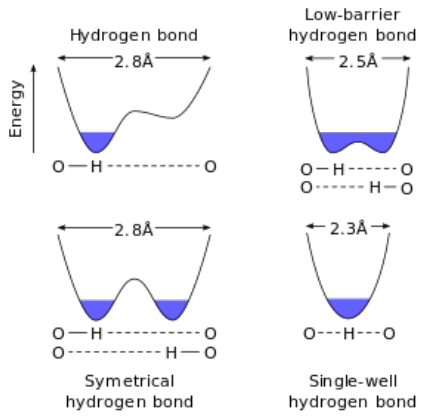


silné

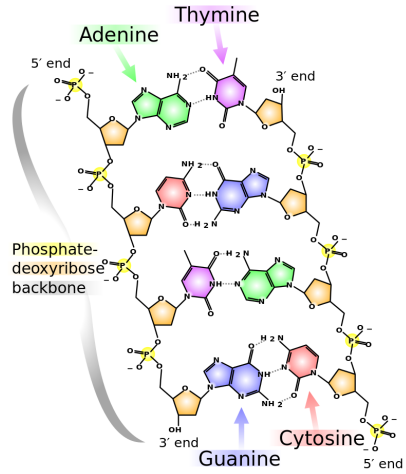
Směrovost vodíkové vazby



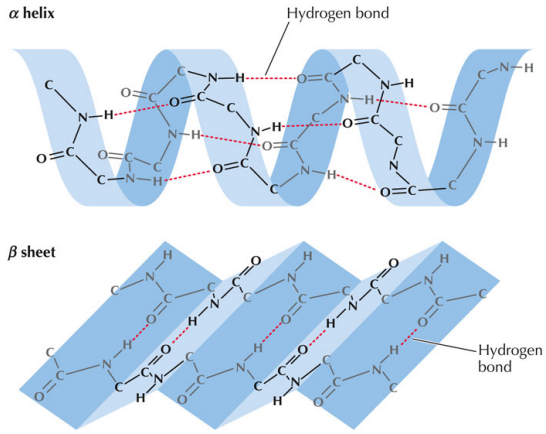
Potenciální energie vodíkové vazby



Vodíkové vazby v biopolymerech - genom



Vodíkové vazby v biopolymerech - proteiny



Vodíkové vazby v biopolymerech - cukry