

Voda, samá voda



Pavel Jungwirth
UOCHB AV ČR



20. 1. 2009

Slepá bába a Aristotelovské prvky

Samá voda...



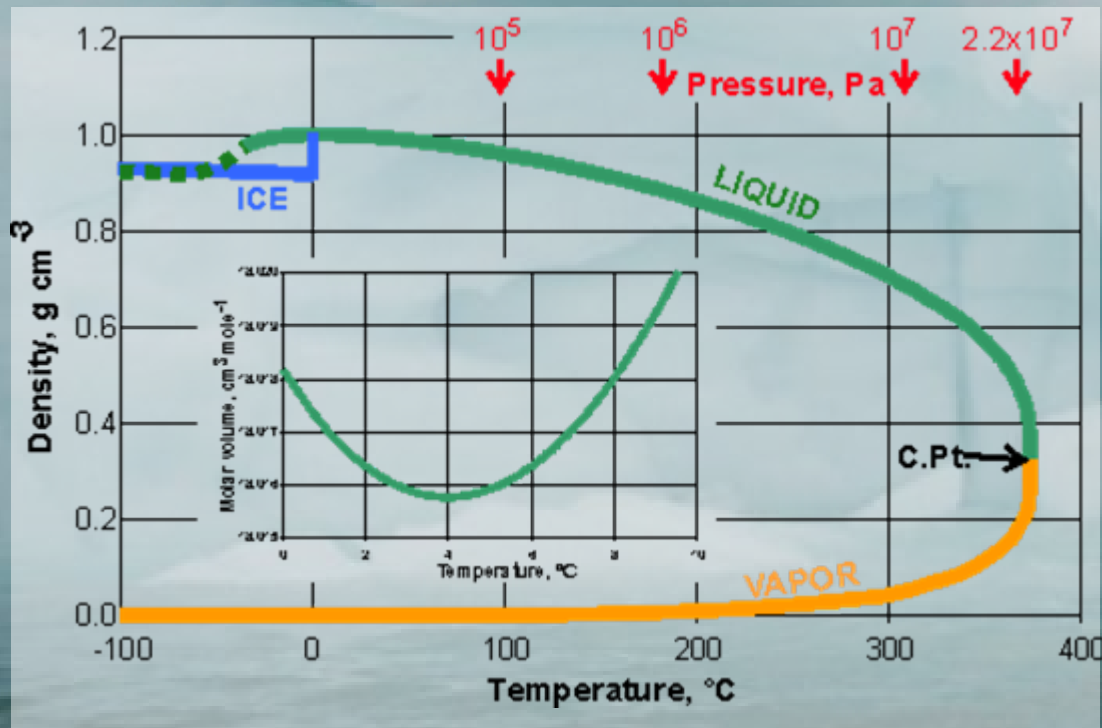
Přihorlivá...



*Voda ale
není obyčejná;
právě
naopak!*



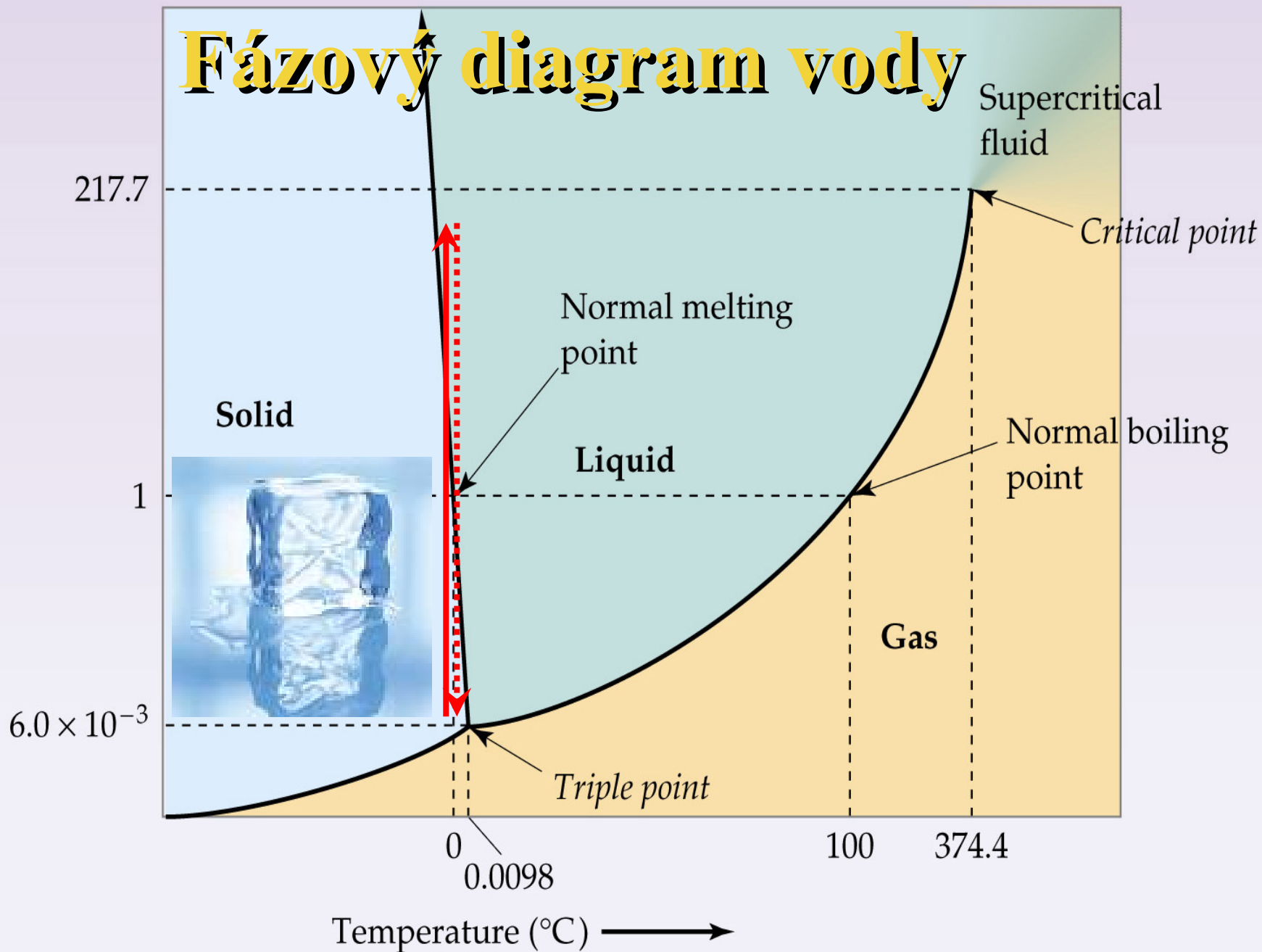
66 anomálií vody



*Nejznámější:
maximum hustoty při
teplotě 4°C*

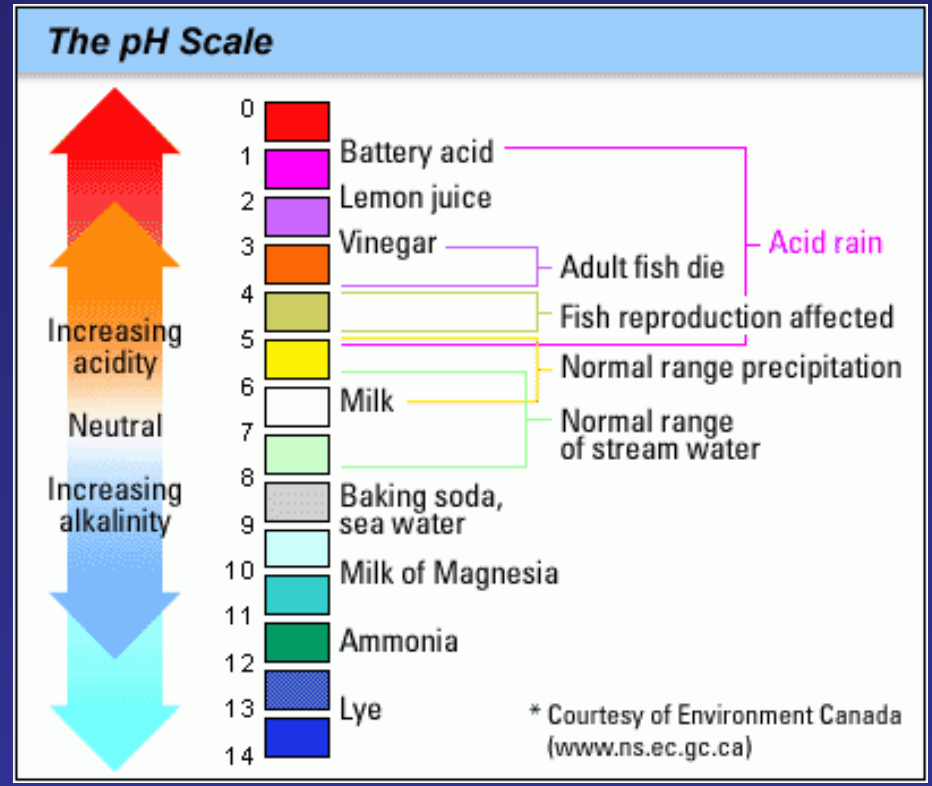
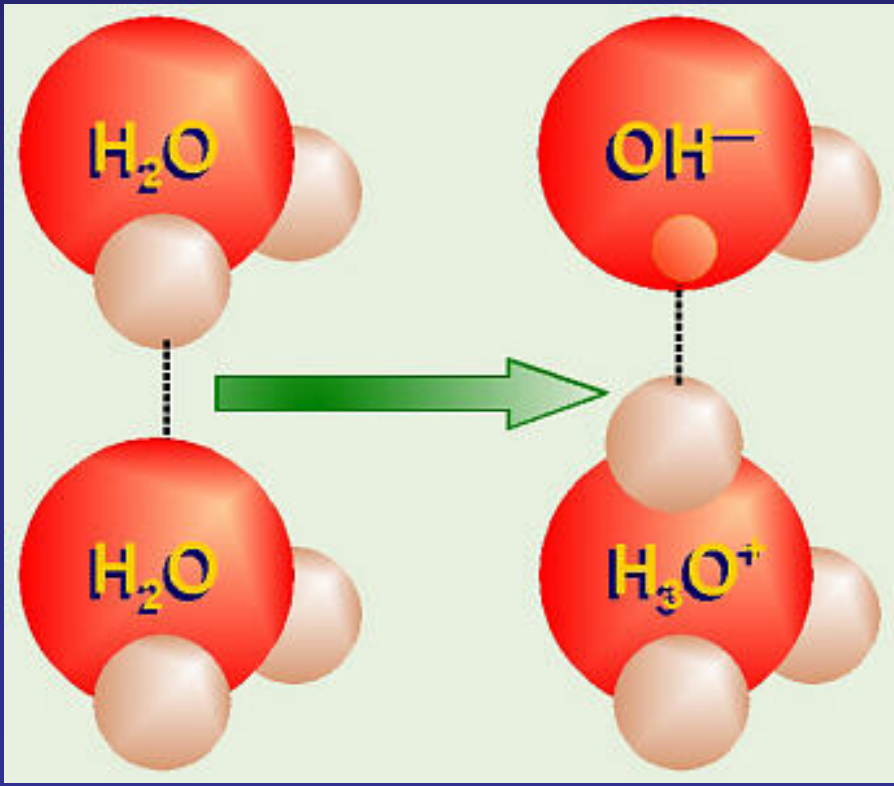
Fázový diagram vody

Pressure (atm) ↑



Temperature (°C) →

Autolýza (autoionizace) vody

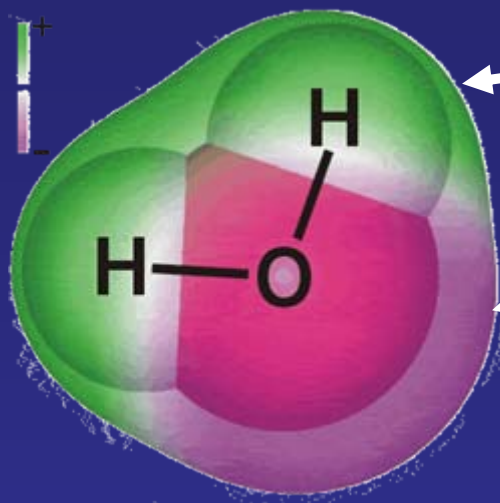


pH-metr

$$pH = -\log_{10} a_{H^+}$$



Molekulová struktura vody

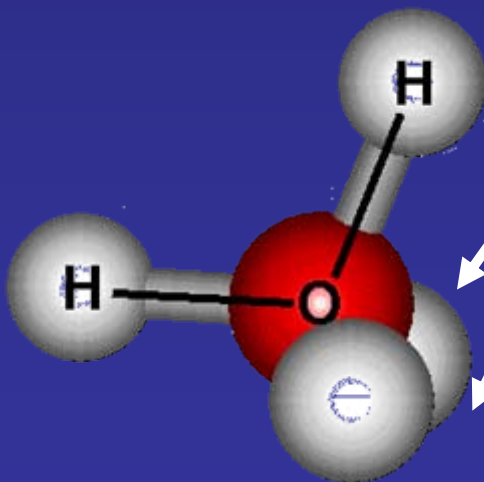


$\sim +0.5 e$

$\sim -1.0 e$

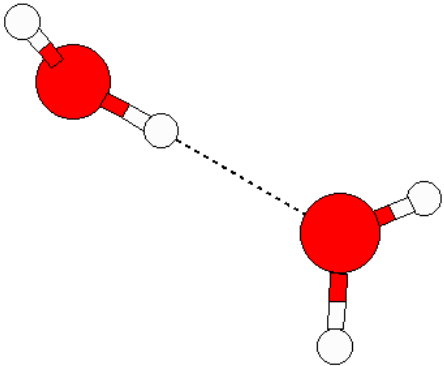
Velký dipólový moment (1.9 Debye)

volné elektronové páry na kyslíku

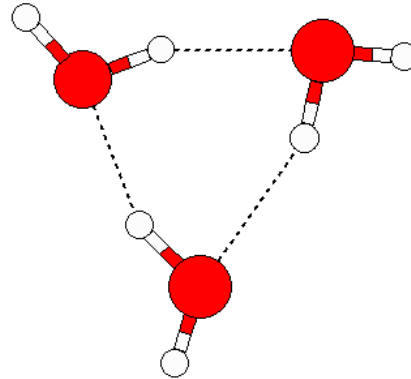


Vodní klastry

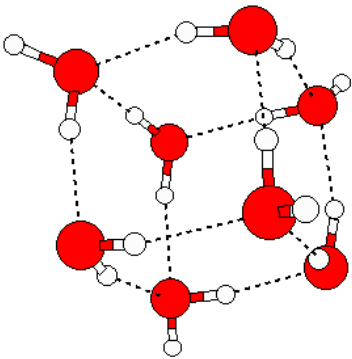
dimer



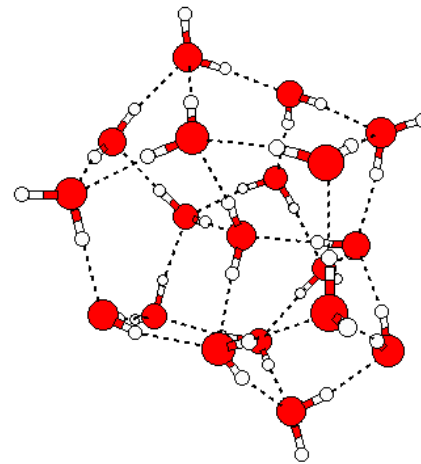
trimer



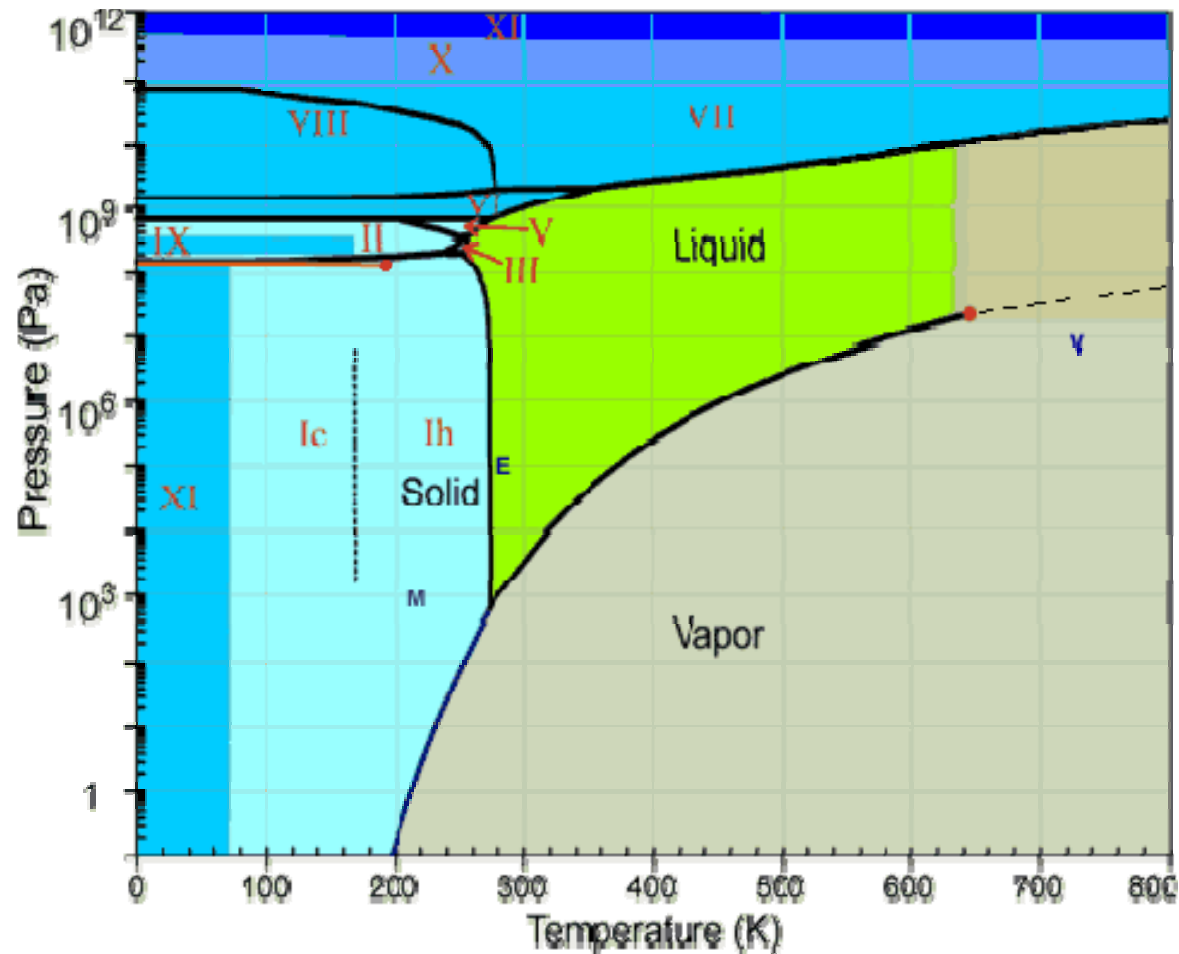
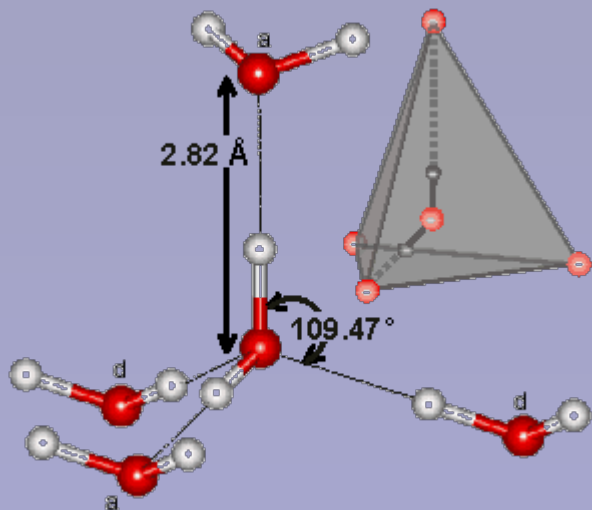
oktamer



*nona-
dekamer*

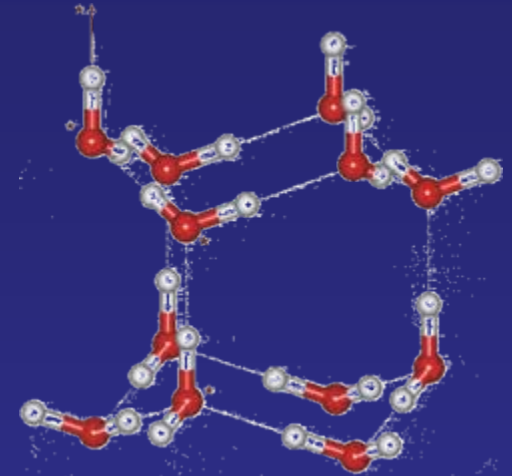
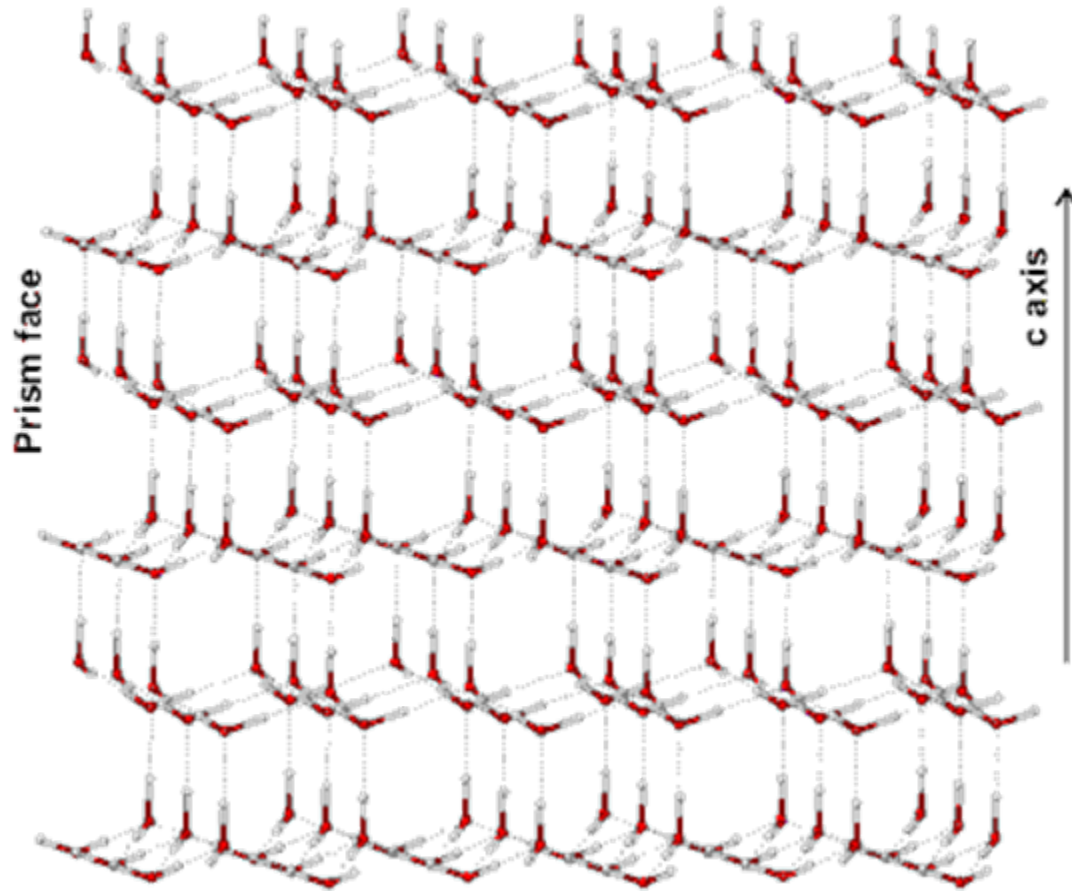


Kondenzované fáze vody: Led(y)

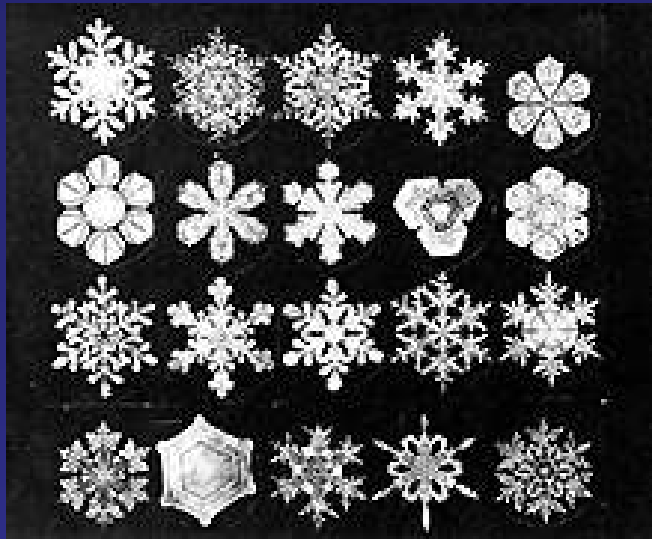


„Normální“ led Ih

Basal plane



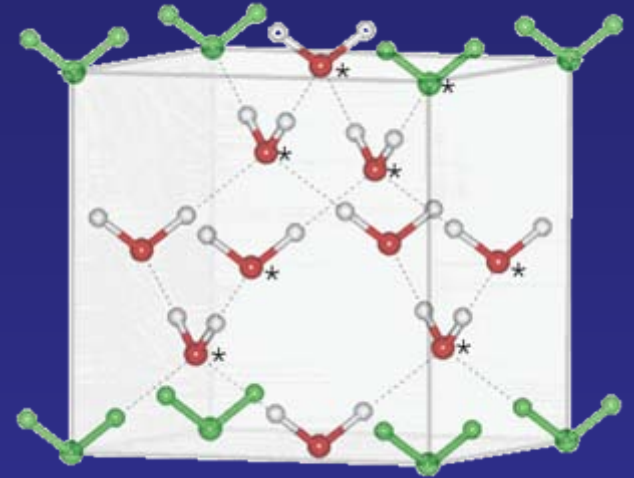
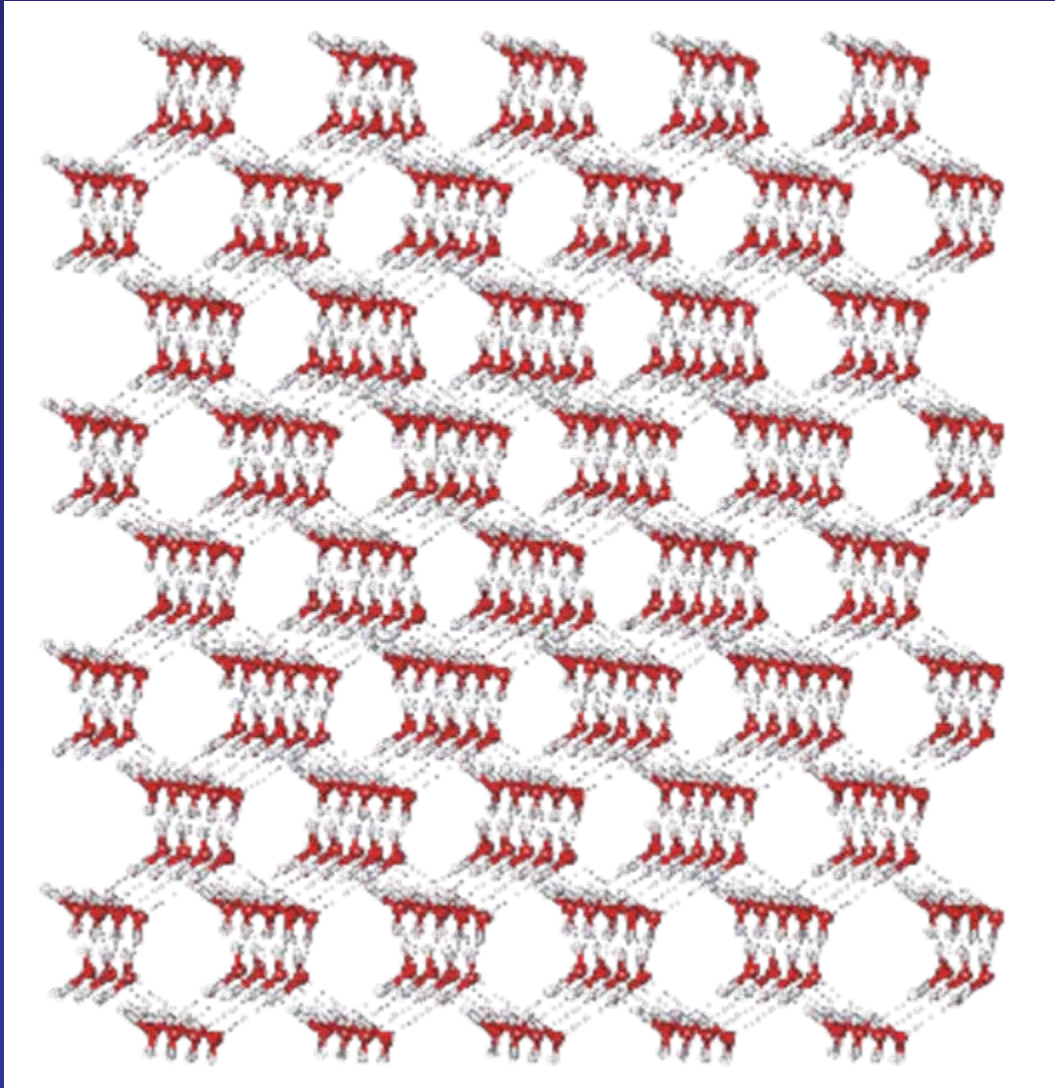
Sněhové vločky



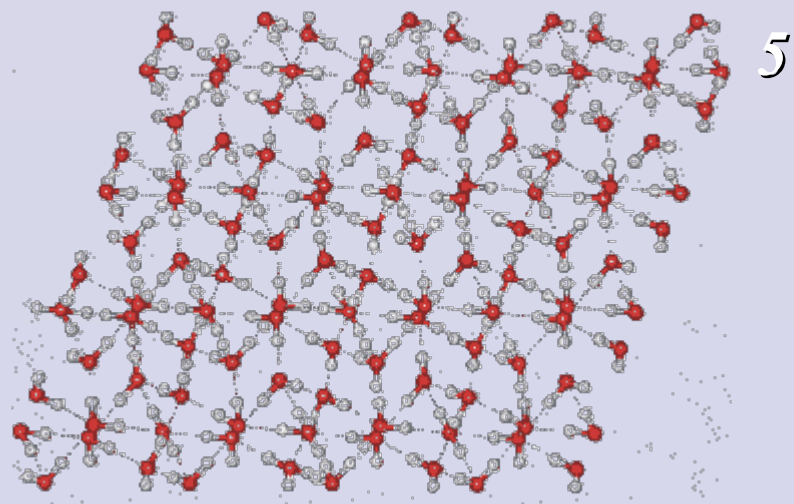
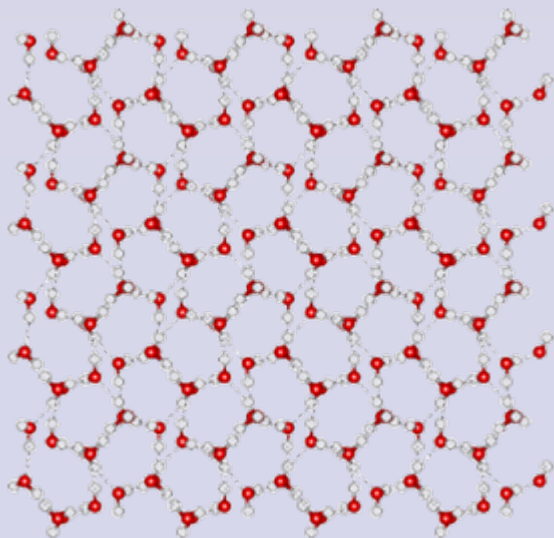
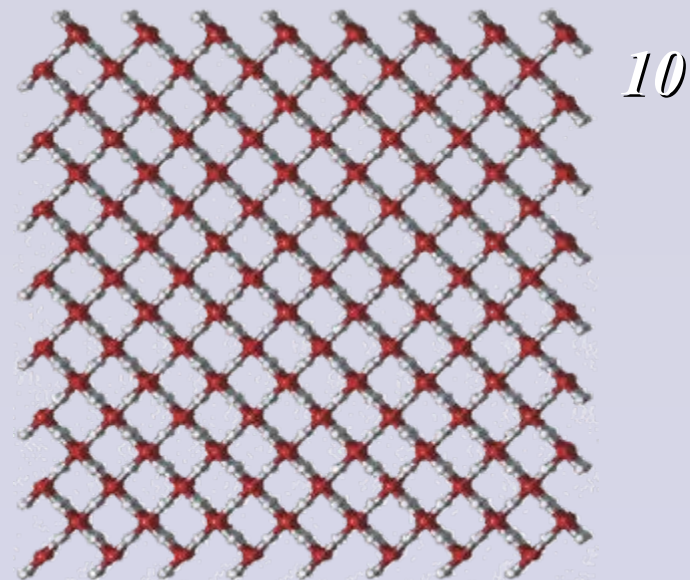
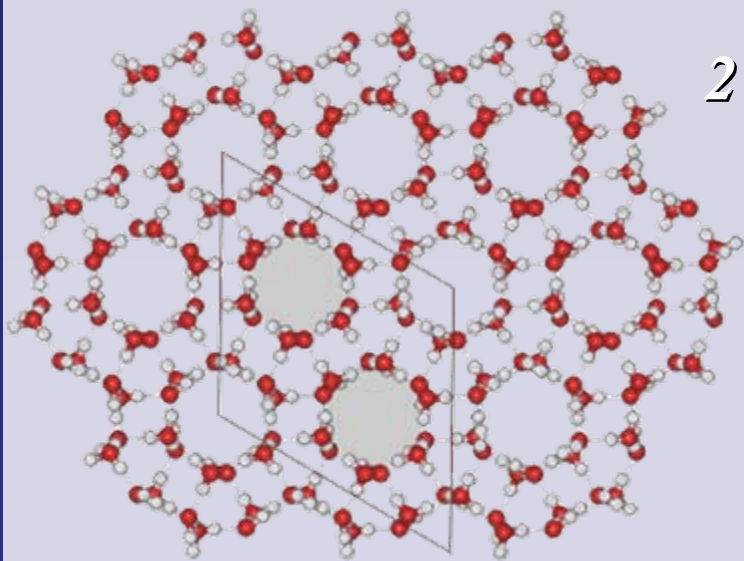
Wilson Bentley
(1865-1931)



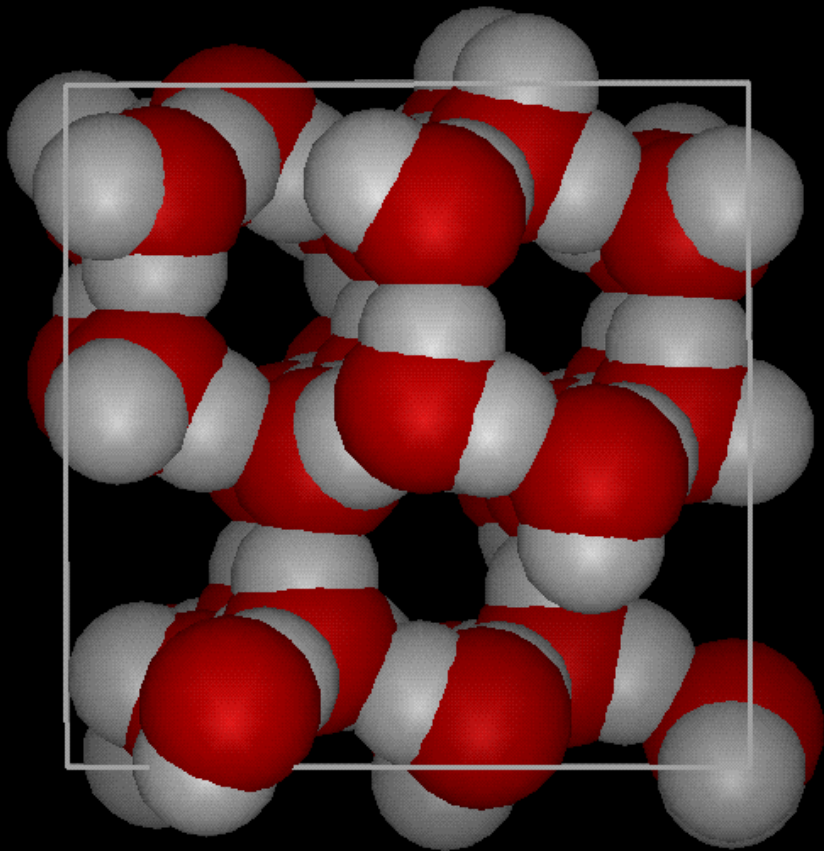
„Kubický led“ Ic



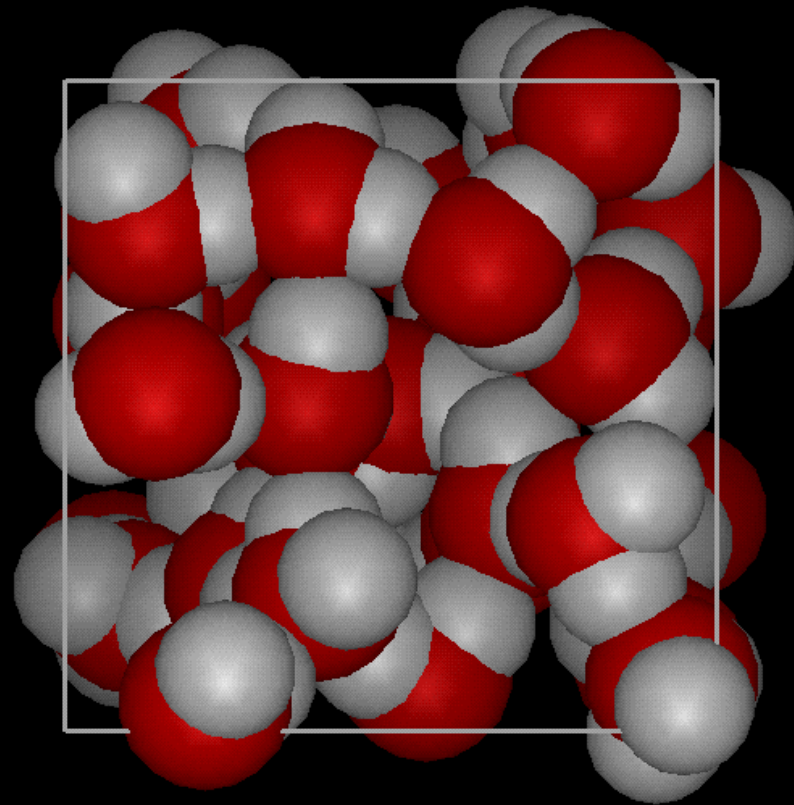
Ledy č. 2-15



Krystalická versus kapalná voda



řidší



hustší

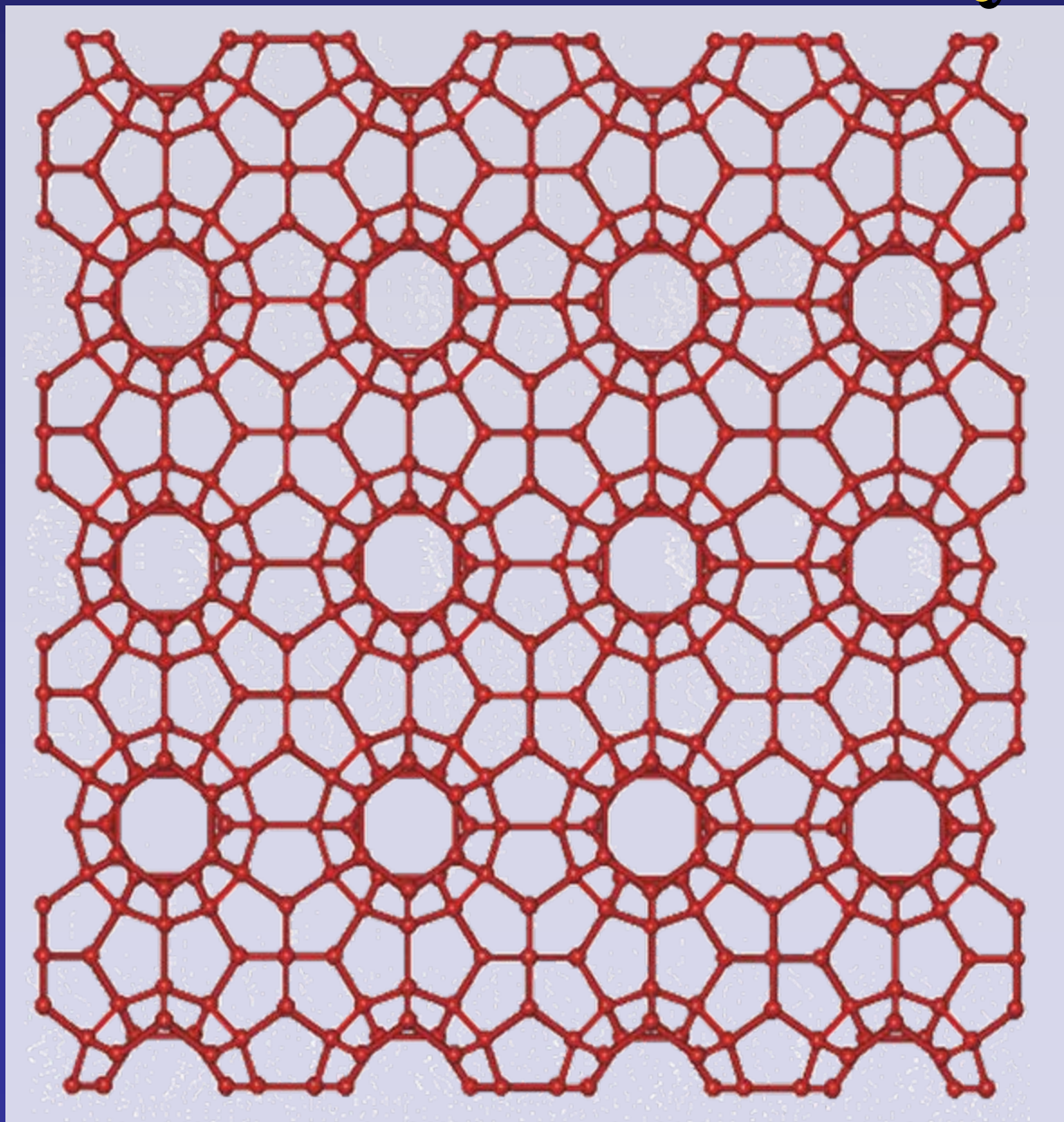


Amorfní tuhá voda („sklo“)



Prudce zchlazená voda na cca -150 °C.

Klatráty



„Hořící“ led

Vodní mýty



Loch Ness

Led č. 9

Led č. 9 je stabilní při teplotě vyšší než 0 °C.

Kurt Vonnegut (spisovatel) – Kolíbka

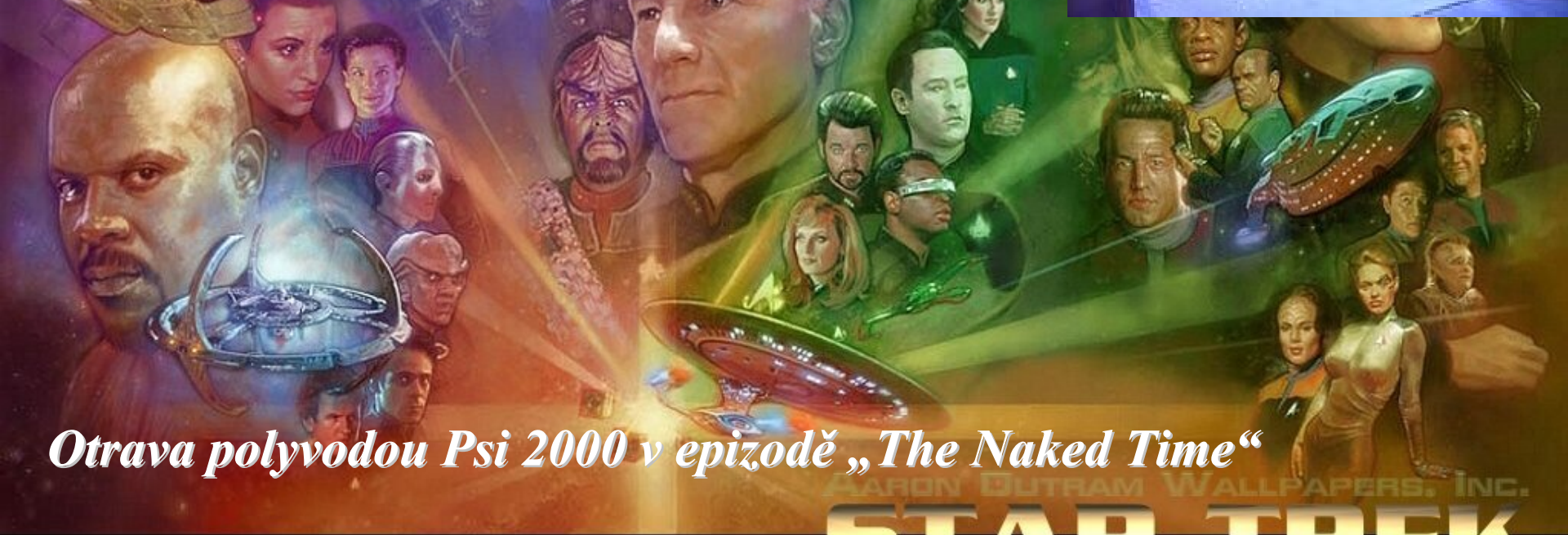


Ano, ale jen za enormních tlaků (tisíce atmosfér).

Bernard Vonnegut (vědec)



Polyvoda



Otrava polyvodou Psi 2000 v epizodě „The Naked Time“

HARRON DUTRAM WALLPAPERS, INC.
STAR TREK
TWENTY-FOURTH CENTURY

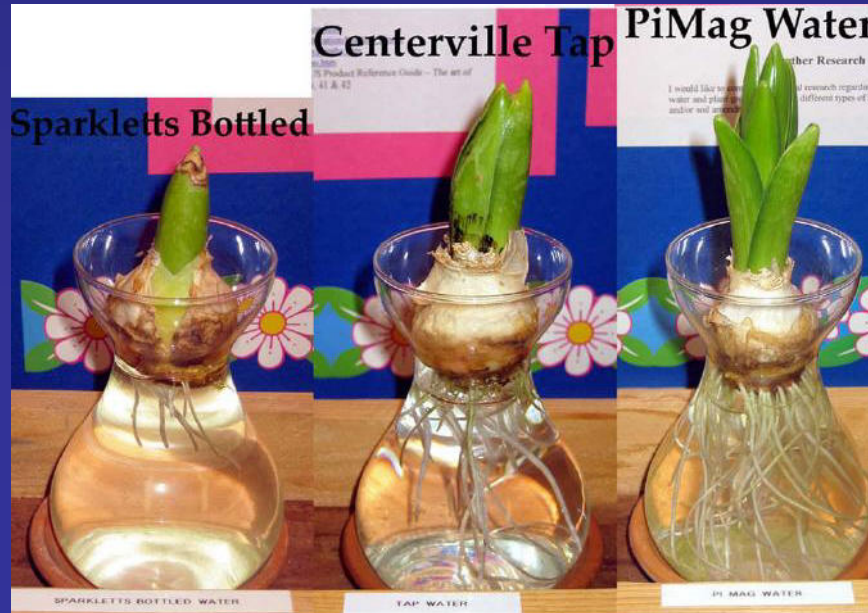


American
Polywater
Corporation

π -voda, neovoda, magnetická voda...



*nejrůznější
komerční
názvy*



Kde se vzala polyvoda?



Technologický
Institut Kostroma



1966 – Nikolaj Fedyakin a Boris Deryagin

Potvrzení polyvody na Západě

Bod varu: 200 °C

Bod tání: -30 °C

Specifické infračervené spektrum.

1968: Velká Británie, USA.



Desmond Bernal

"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.

NATURE VOL. 224 OCTOBER 11 1969

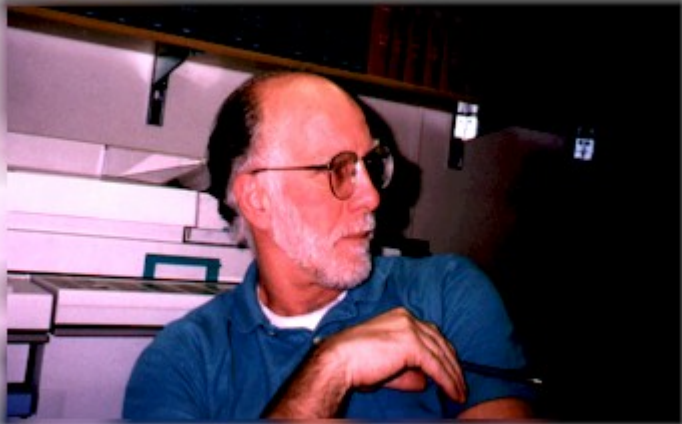
Konec polyvody

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.



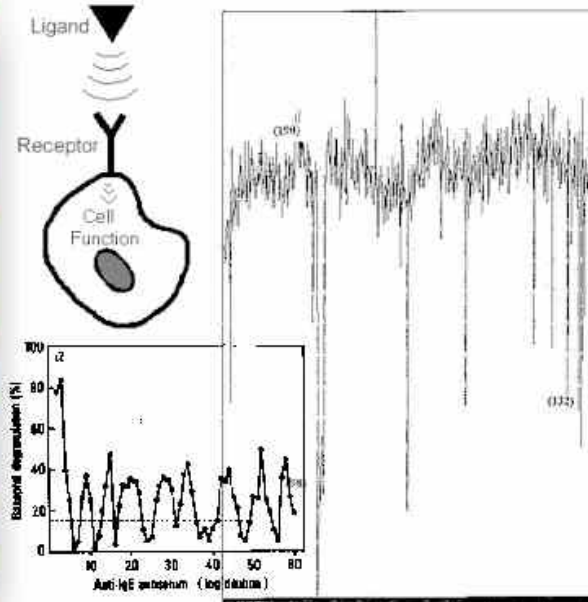
Denis Rousseau, Bell Labs USA

*Anomální vlastnosti polyvody
díky kontaminaci z kapilár
a z potu experimentátorů...*

Paměť vody



- Home
- Experiments
- Data
- Theory
- Implications
- Applications



1987:
Jacques Benveniste
@digibio.com

John Maddox
Editor Nature

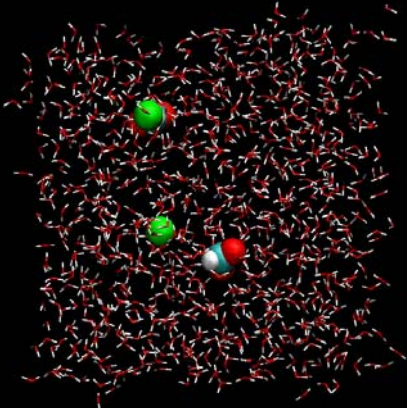
nature

NATURE VOL 338

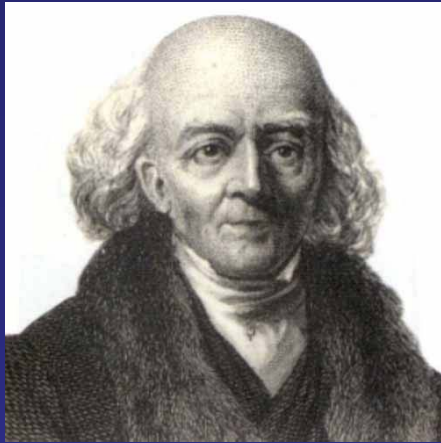
13 APRIL 1989

<1 ns

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.



Homeopatie



Samuel Hahneman (1755-1843)

+ *netoxické (ve své době revoluční)*
- *nejde za efekt placebo*



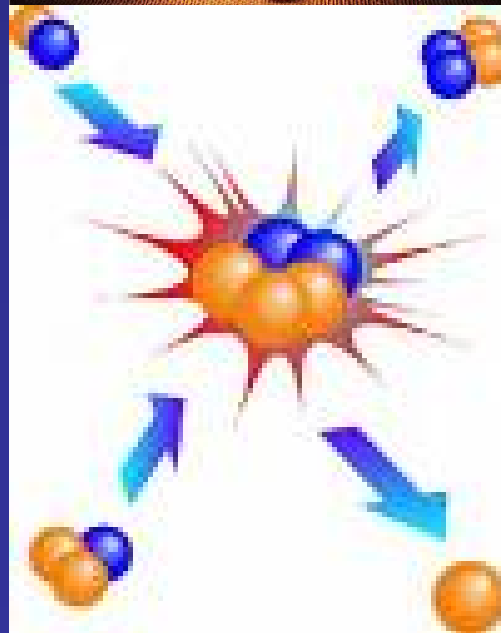
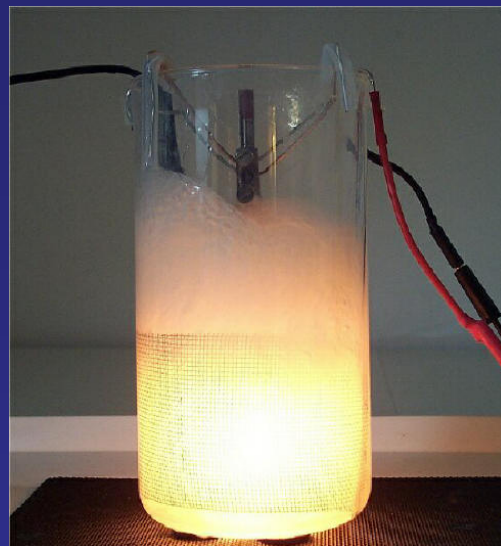
Studená fúze



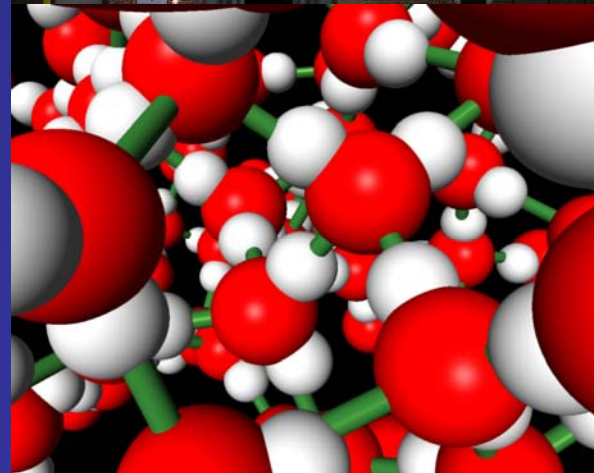
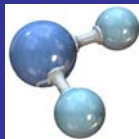
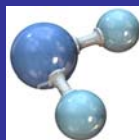
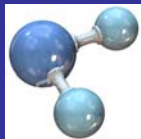
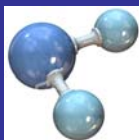
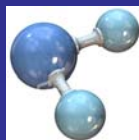
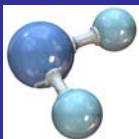
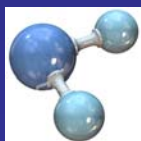
1989:

S. Pons & M. Fleischmann

„Vodíková bomba ve sklenici vody“

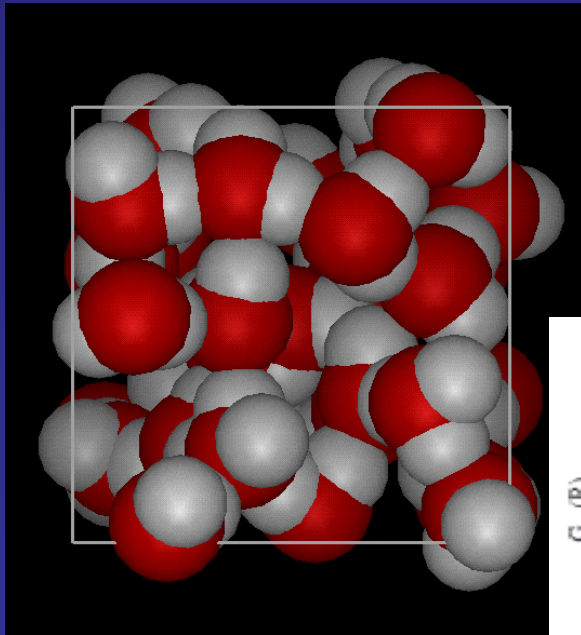


Rozumíme vodě?

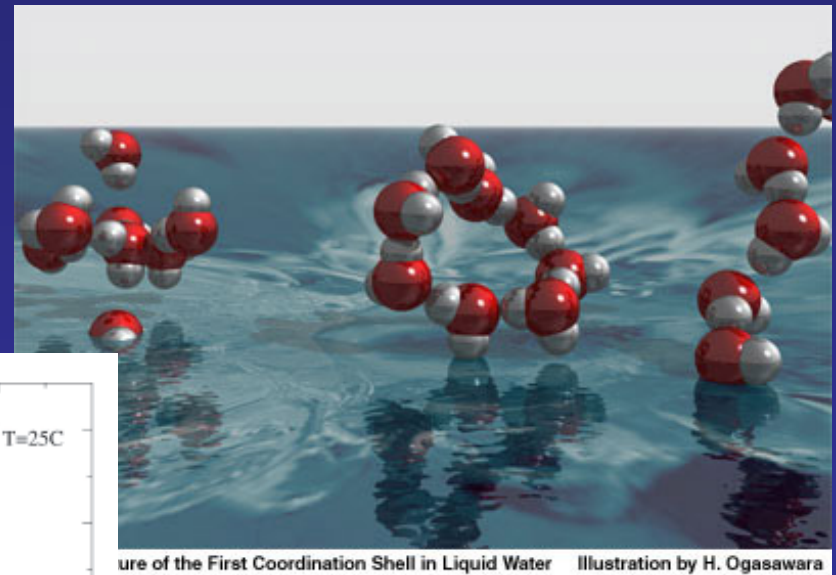
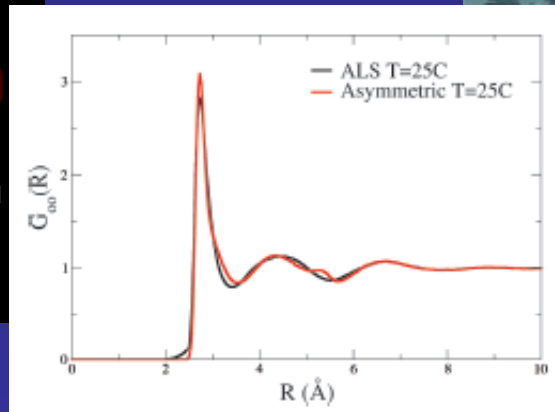


Vodní otazníky

Kolik vodíkových vazeb připadá na molekulu H_2O v kapalně vodě?



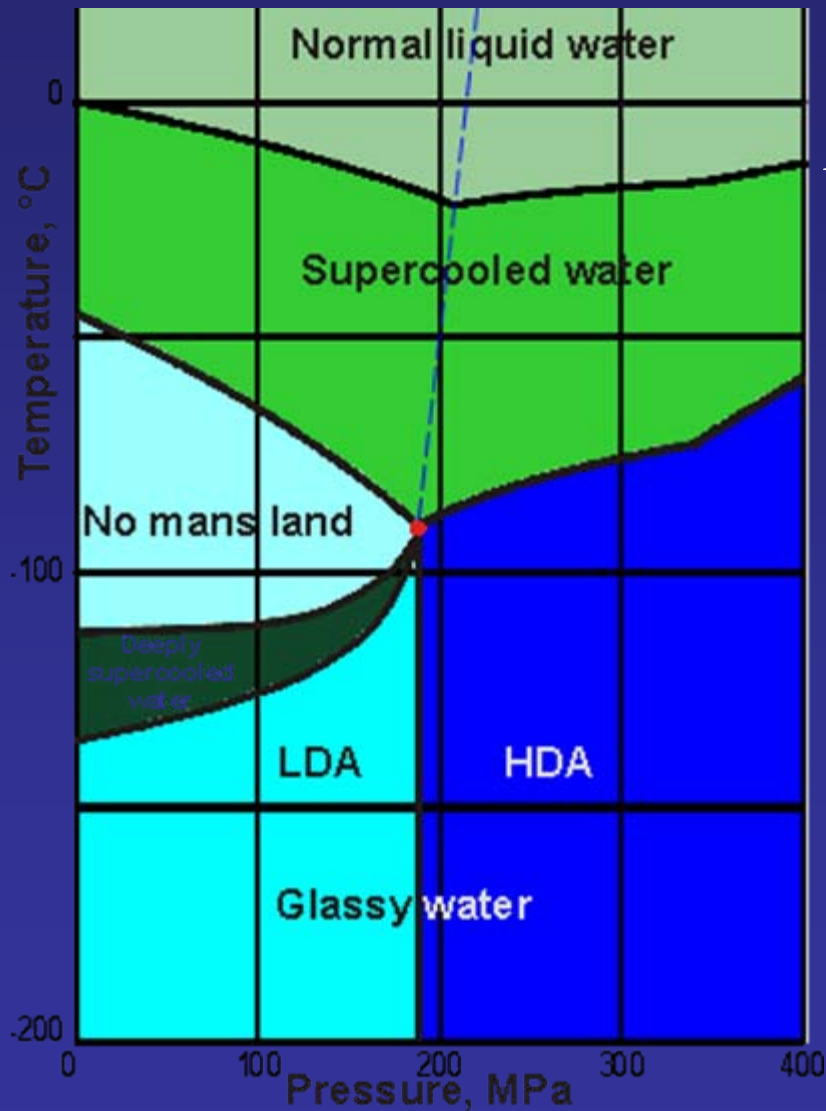
~3.5?



~2.5?

Strukturní experimenty potvrzují kanonický model...

Vodní otazníky



Je možný přechod od podchlazené kapaliny ke amorfnímu sklu bez krystalické fáze?

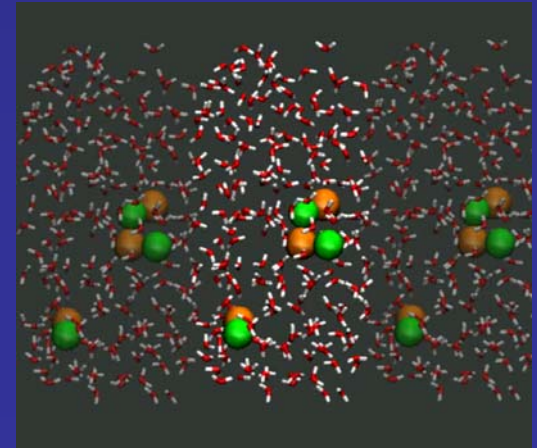
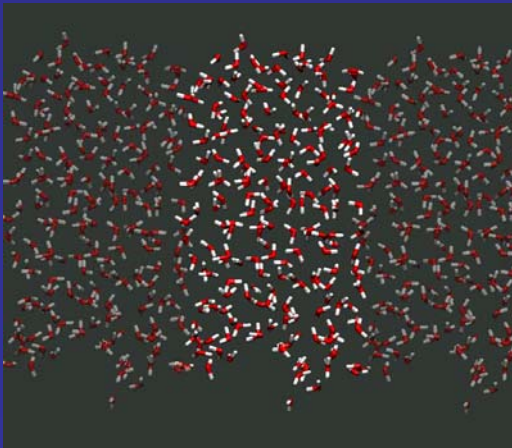
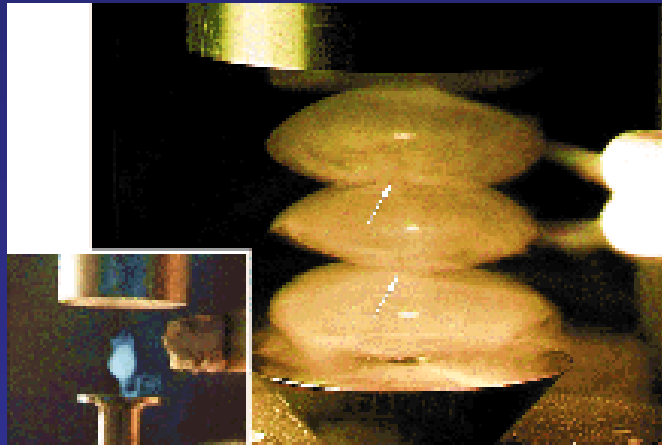
U oxidu křemičitého je možný přímý přechod z taveniny ke sklu...



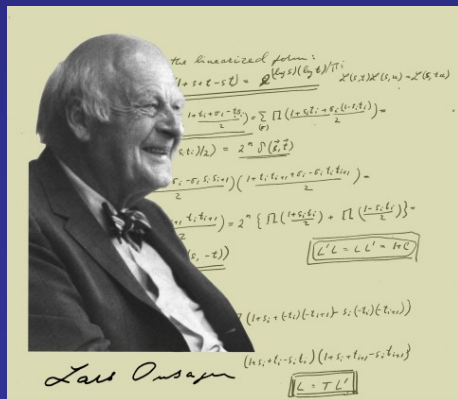
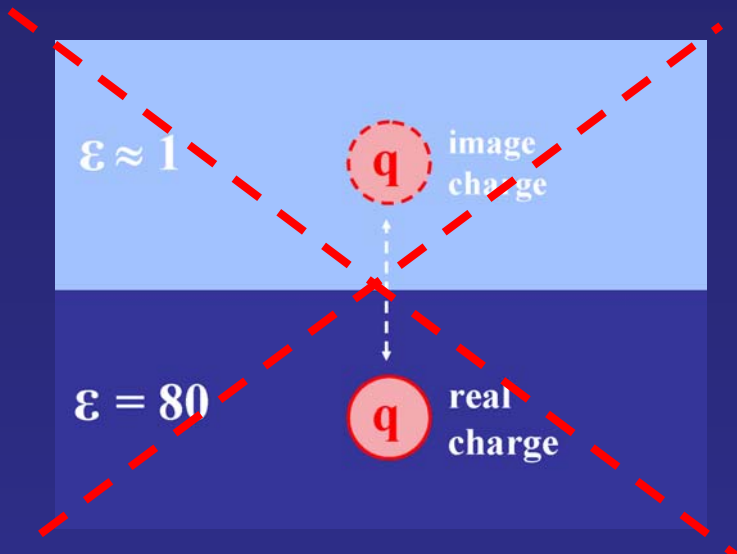
...u vody se to zatím nedaří (možná v „nanosvětě“).

Naše vodní otazníky

*Rozdílné chování vody uvnitř a na povrchu kapaliny:
i) Kde a jak začíná čistá či slaná voda mrznout?*

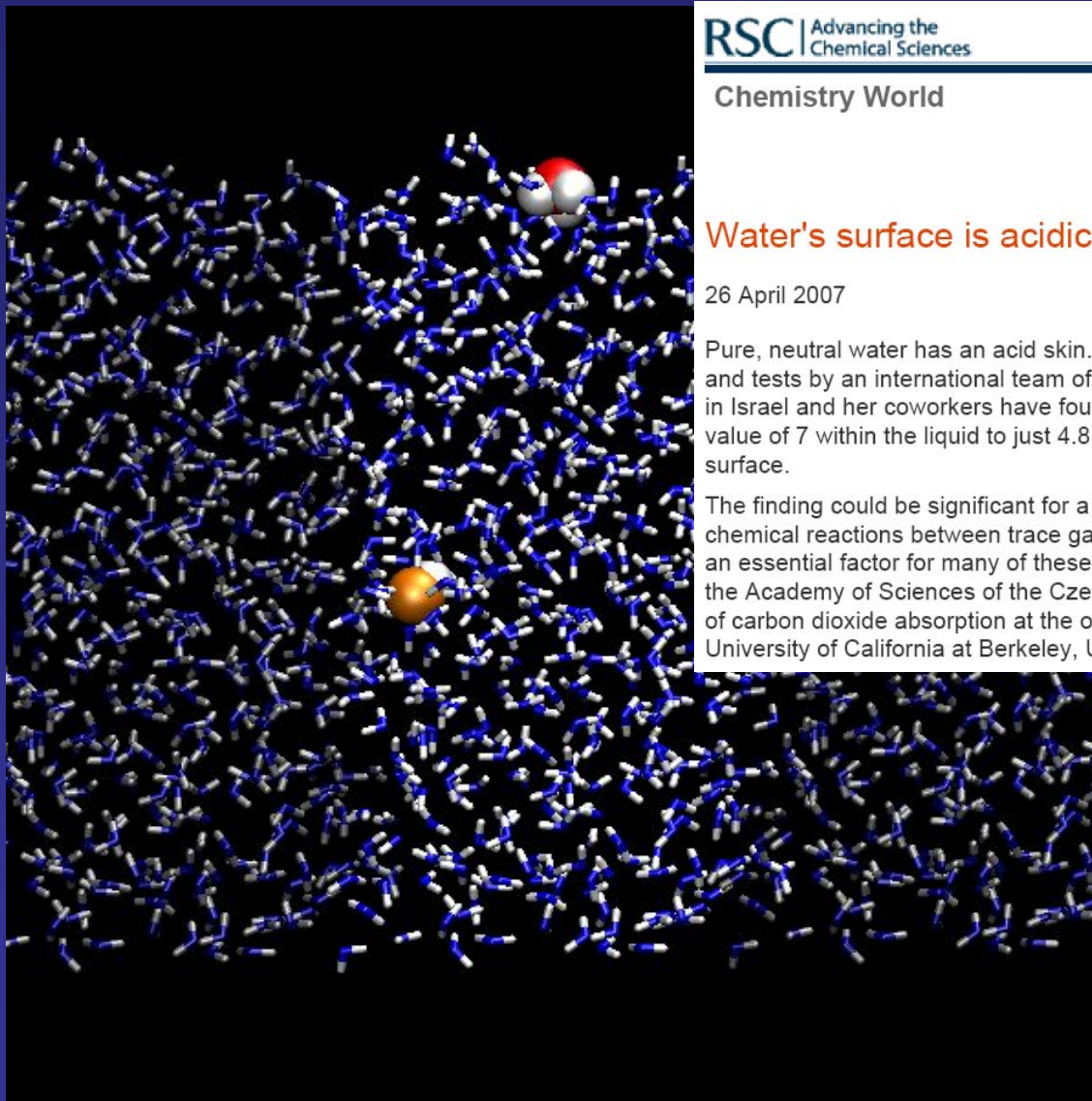


ii) Jak se chovají ionty na vodním povrchu?



Měkké (polarizovatelné) ionty, např. bromid či iodid, se akumulují na vodním povrchu v rozporu s Onsagerovou teorií elektrolytů.

iii) Jak je to na povrchu čisté vody?



RSC | Advancing the
Chemical Sciences

Chemistry World

Water's surface is acidic

26 April 2007

Pure, neutral water has an acid skin. This striking notion has now been confirmed by calculations and tests by an international team of scientists. Victoria Buch of the Hebrew University of Jerusalem in Israel and her coworkers have found that the pH of pure water falls from the perfectly neutral value of 7 within the liquid to just 4.8 or less - about as acidic as beer - where water meets air at the surface.

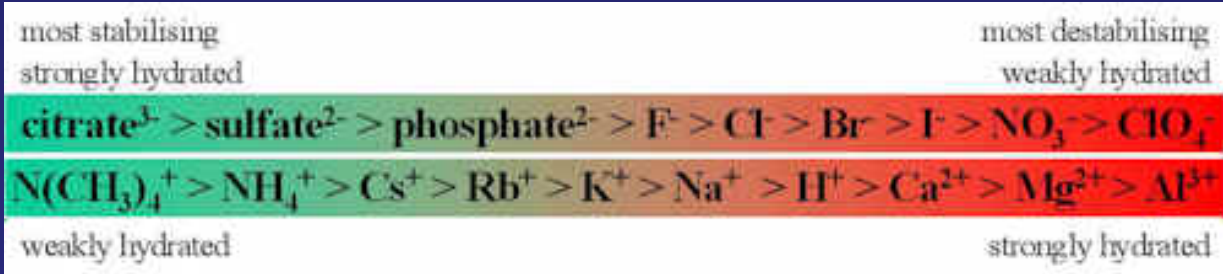
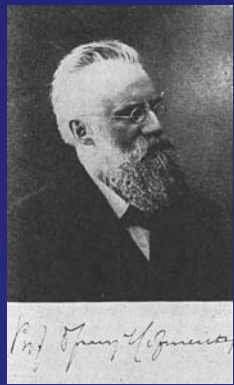
The finding could be significant for a number of disciplines. In the atmosphere, many important chemical reactions between trace gases take place at the surface of water droplets in clouds. 'pH is an essential factor for many of these reactions,' said Pavel Jungwirth, one of Buch's collaborators at the Academy of Sciences of the Czech Republic in Prague. 'The low pH could also affect the rates of carbon dioxide absorption at the ocean surface,' added water specialist Richard Saykally of the University of California at Berkeley, US.



Water has an acid sting at its surface

V souhlase se spektroskopií, ale v rozporu s elektroforetickými měřeními.

iv) Ionty na rozhraní mezi vodou a bílkovinou



(Franz Hofmeister Arch. Exp. Pathol. Pharmakol. 1888, 24, 247)

Chemical & Engineering News

Science & Technology

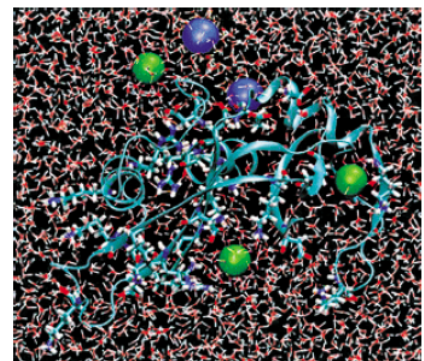
November 26, 2007
Volume 85, Number 48
pp. 47-49

A Renaissance For Hofmeister

Flurry of new research overturns long-held ideas about ions, water, and macromolecules

Elizabeth K. Wilson

IT STARTED in the late 1800s with egg whites. At the German Medical School, in Prague, the prolific research chemist Franz Hofmeister was dissolving gloopy egg-white proteins in solutions of different ions, duly noting that some, such as sulfate and fluoride, caused the proteins to precipitate readily, whereas others, such as iodide and isocyanate, did not.



Sodík se akumuluje více než draslík na povrchu bílkovin!

Courtesy Of P. Jungwirth, L. Vrbka, J. Vondrášek, B. Jagoda-Cwiklik, R. Vácha



Společenské vodní otazníky

30 n. l.:

Jak proměnit vodu ve víno?



2000 n. l.:

*Jak proměnit slanou vodu
ve sladkou?*



Poděkování

*Studenti a postdoci: Luboš Vrbka, Martin Mucha, Martina Roeselová,
Robert Vácha, Eva Pluhařová, Jan Heyda,
Mikael Lund, Barbara Jagoda-Cwiklik, ...*

Experimentální a teoretičtí spolupracovníci

Philip Ball: H₂O A biography of water

www



Děkuji vám za pozornost!

pH tělních tekutin

Žaludeční šťávy	1.0 – 3.5
Moč	4.8 – 8.4
Sliny	6.5 – 7.5
Krev	7.3 – 7.4
Mozkomíšňní mok	7.3 – 7.5
Žluč	7.1 – 8.5
Slinivka	8.0 – 8.3

Vaginální pH = 3.8 – 4.5

*Mírně se mění během menstruačního cyklu.
Vyšší pH může signalizovat infekci.*



Nobelova nebo Ig-Nobelova cena?



???



Traditional explanation of salting-out



Kosmotropes vs Chaotropes



e.g., SO_4^{2-} : organize water layers, „steel water“, salt-out

e.g, I^- : disorganize water, salt-in

...but modern spectroscopies, diffraction, and simulations show that ions do not impose long-range ordering beyond the first solvent shell → *Search for alternative explanations!*

Chemical & Engineering News

A Renaissance For Hofmeister

Flurry of new research overturns long-held ideas about ions, water, and macromolecules

November 26, 2007

Volume 85, Number 48

pp. 47-49

CHEMISTRY Tobias & Hemminger

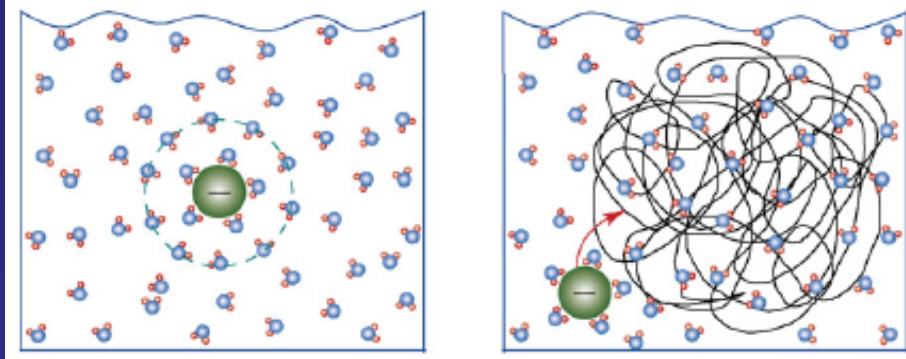
Getting Specific About Specific Ion Effects

Recent studies are shedding light on the mechanisms that drive the properties of salt solutions.

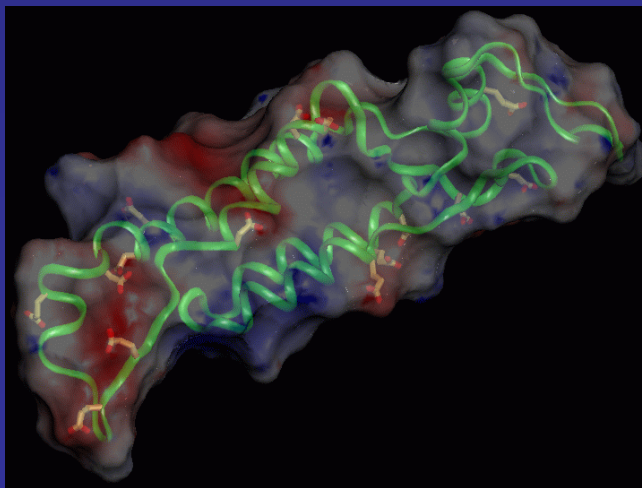
SCIENCE VOL 319 29 FEBRUARY 2008

Cherche la...interface

If not water “structure making” and “structure breaking”...



...then direct interactions of ions with surfaces of hydrated proteins shall be decisive for specific ion effects.



*Exploring ion specificity
at charged, polar, and
non-polar regions of
protein surface!*