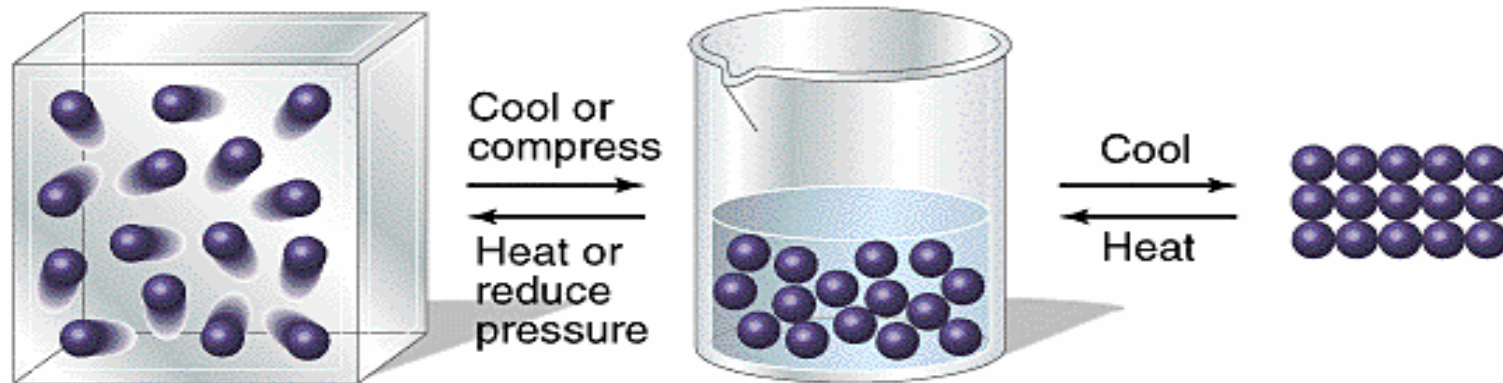


# Skupenské stavy



Gas

Total disorder; much empty space; particles have complete freedom of motion; particles far apart.

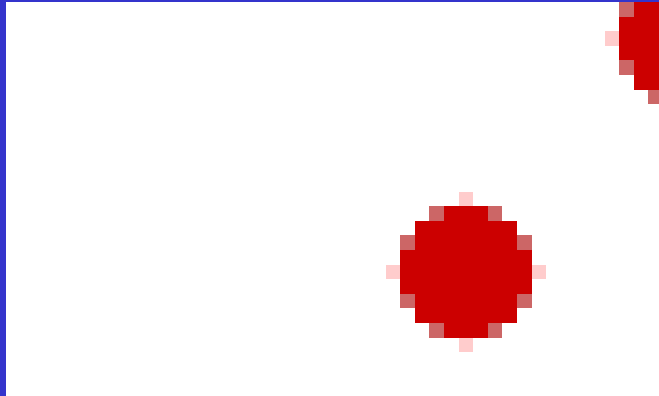
Liquid

Disorder; particles or clusters of particles are free to move relative to each other; particles close together.

Crystalline solid

Ordered arrangement; particles are essentially in fixed positions; particles close together.

# Skupenské stavy

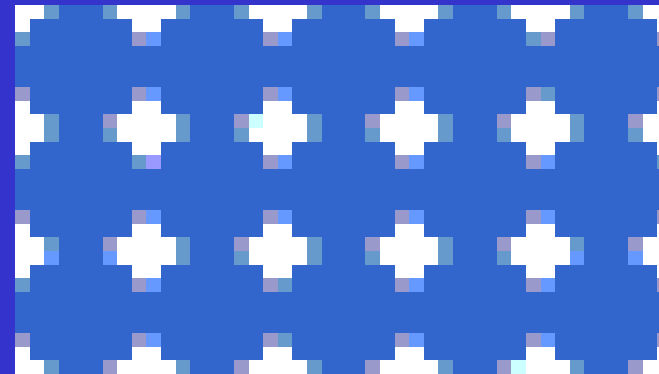


Plyn

Skupenství vody	Teplota, °C (tlak 1 bar)	Hustota, g cm <sup>-1</sup>
pevné	0	0.9168
kapalné	25	0.9971
plynné	400	3.26 10 <sup>-4</sup>

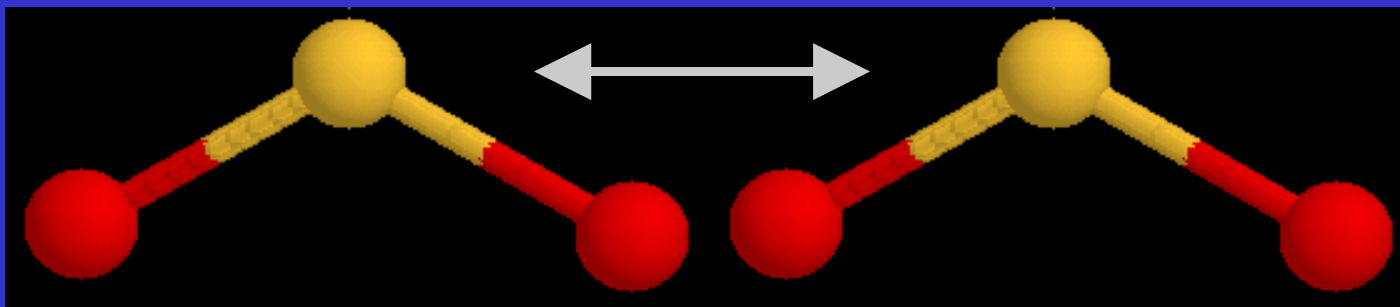
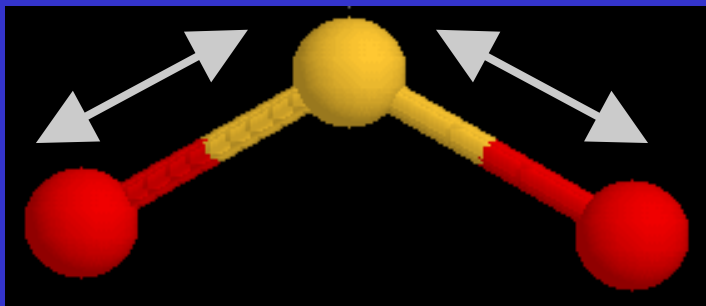


Kapalina

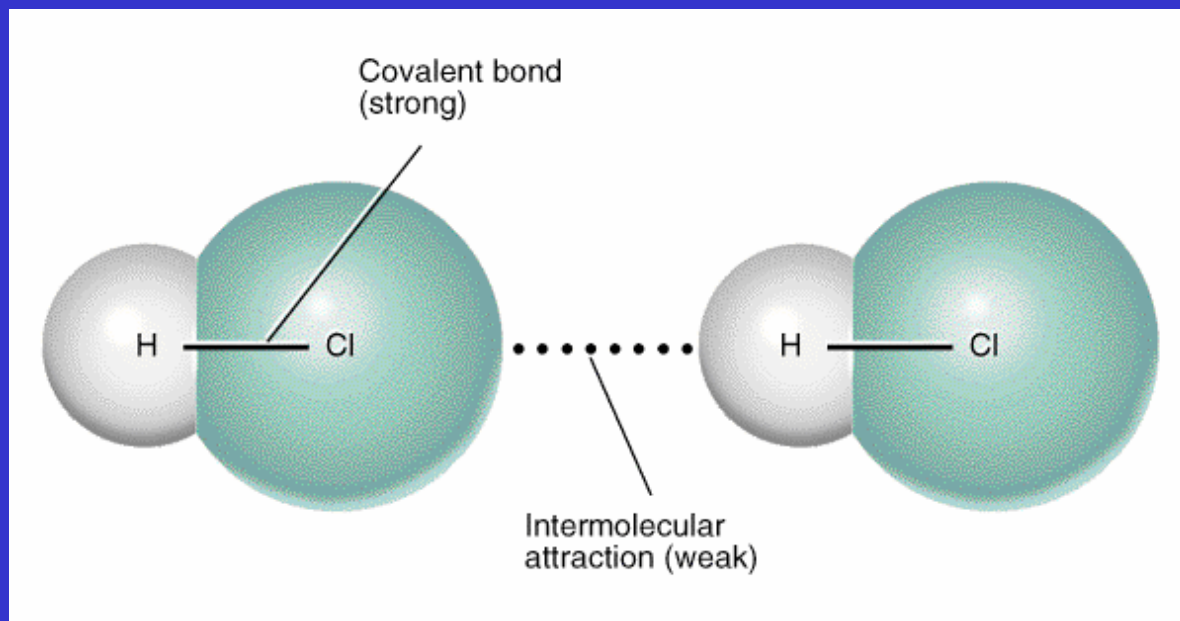


Molekulový krystal

## Rozdíl mezi kovalentní vazbou a mezimolekulovými silami



Typ vazby	Energie, kJ mol <sup>-1</sup>
Kovalentní	200 – 1000
Vodíková	10 – 50 (100)
Dipol-dipolová	2 – 10
Londonova disperzní	> 5



## Typy mezimolekulových vazeb (van der Waalsových interakcí)



ion – ion Coulombické interakce

ion – dipol

dipol – dipol → orientační, Keesom

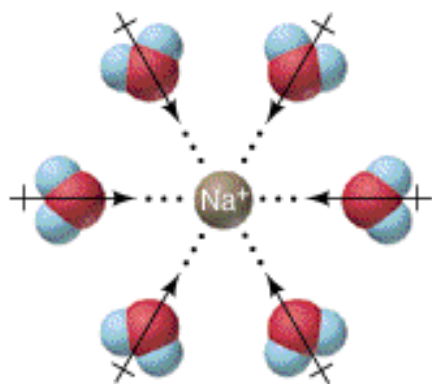
dipol – indukovaný dipol → indukční, Debye

ion – indukovaný dipol

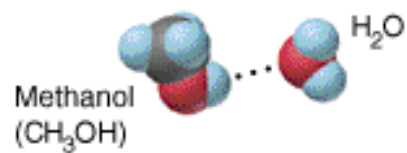
indukovaný dipol – indukovaný dipol → disperzní, London

van der Waalsova repulze (odpuzování)

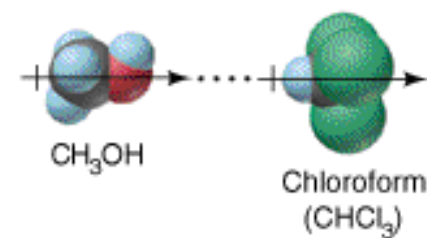
J. D. van der Waals  
(1837- 1923)  
NP za chemii 1910



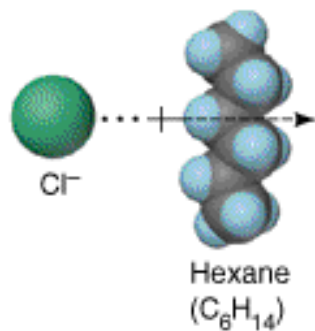
Ion-dipole



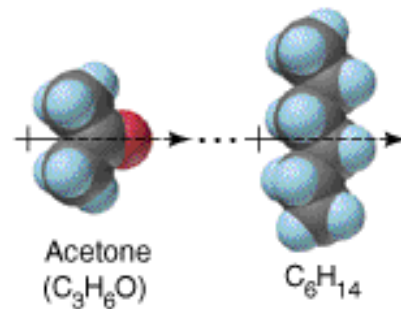
H bond



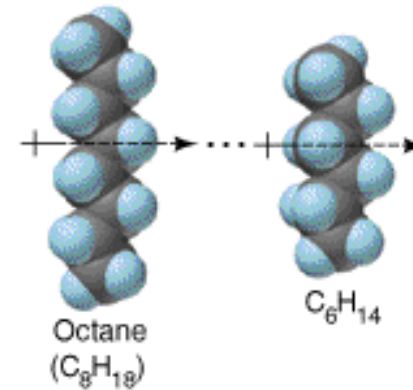
Dipole-dipole



Ion-induced dipole



Dipole-induced dipole



Dispersion

# Interakce ion - ion

Coulombův zákon

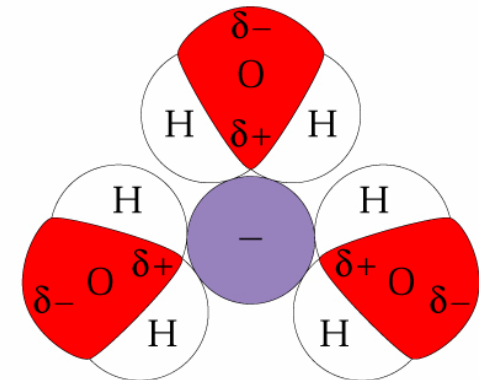
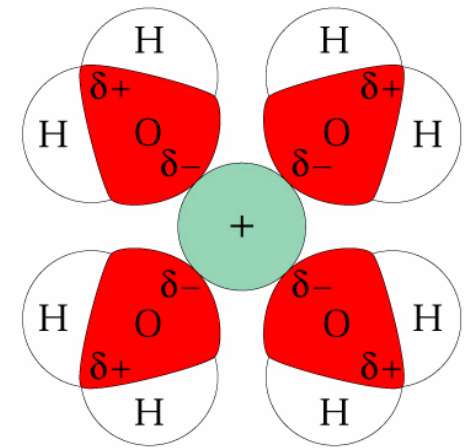
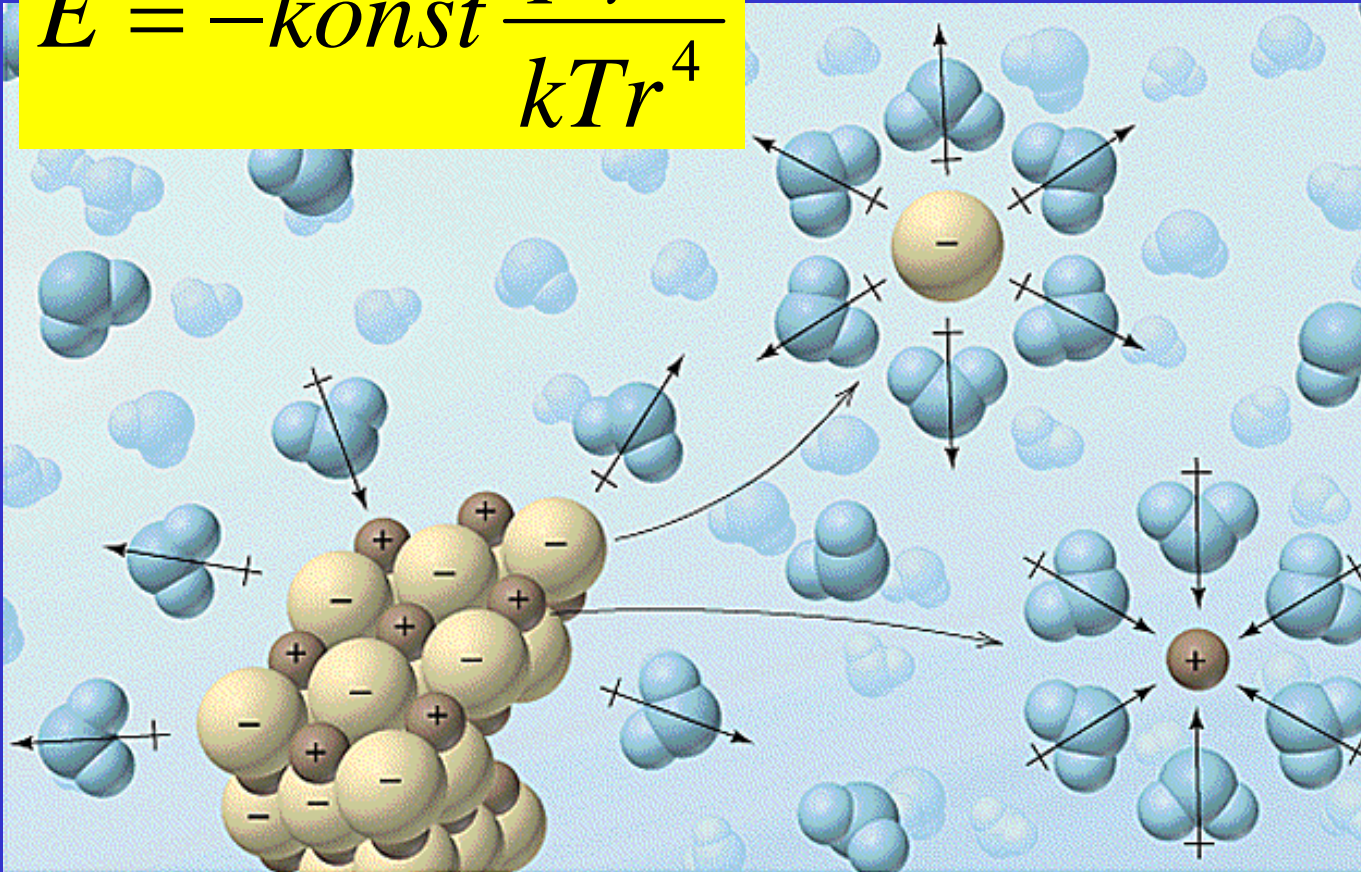
$$E = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r}$$





# Interakce ion - dipol

$$E = -konst \frac{q^2 \mu^2}{kTr^4}$$



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## Dipolový moment - $\mu$

proton a elektron, vzdáleny 1 Å

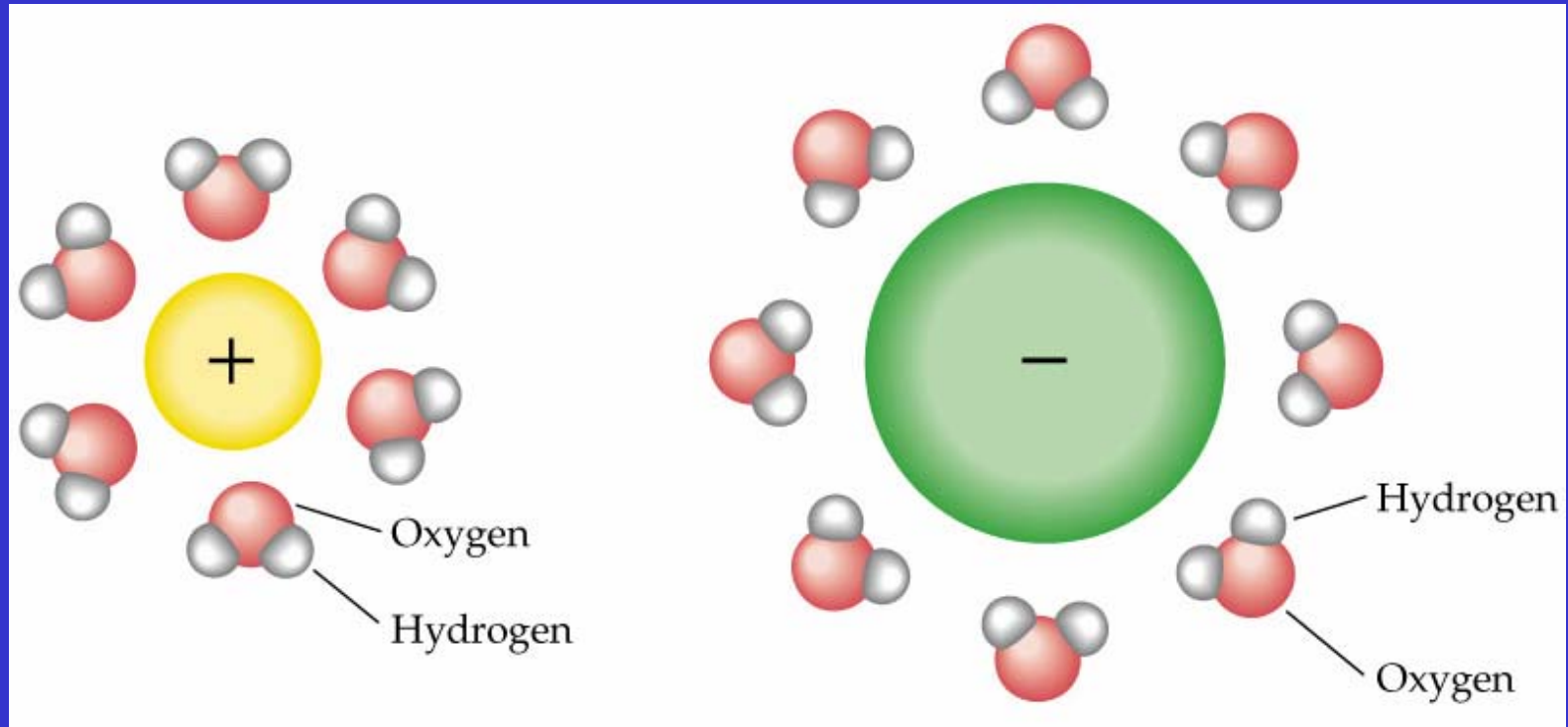
$$\mu = q L = (1.60 \cdot 10^{-19} \text{ C})(1.00 \cdot 10^{-10} \text{ m})$$

$$= 1.60 \cdot 10^{-29} \text{ C m} = \mathbf{4.80 \text{ D}}$$

dipolový moment **4.80 D**

je referenční hodnota, čisté +1 a -1 náboje vzdálené 100 pm, vazba mezi nimi je 100% iontová

# Interakce ion - dipol



## Hydratace/solvatace iontů

Interakce klesá s rostoucí velikostí iontu



K slabá

Rb nulová

Cs negativní



Interakce klesá

Interakce roste s rostoucím nábojem iontu



Ion-dipol



Polární koord. vazba



Interakce roste

# Solvatace elektronů

Na rozpuštěný v kapalném amoniaku



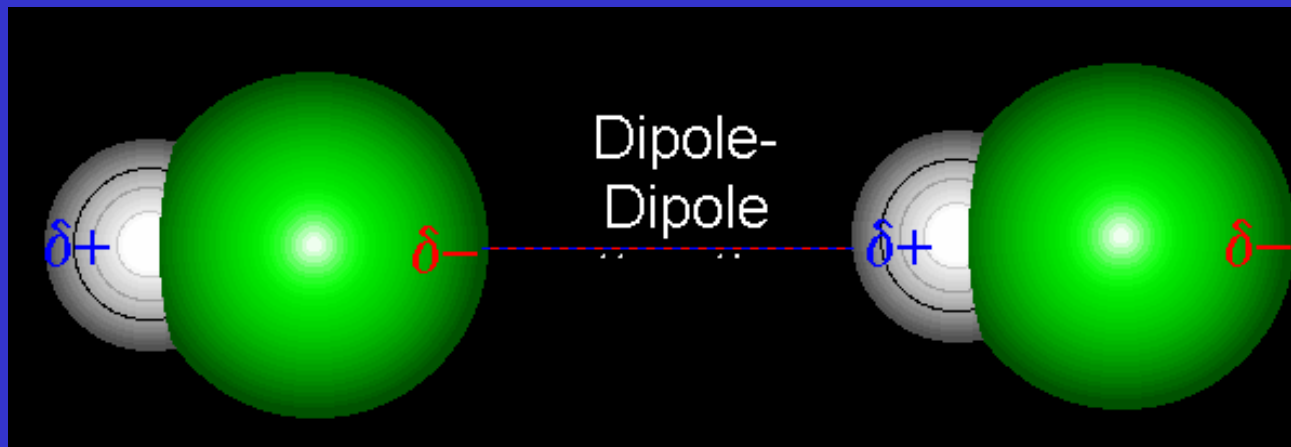
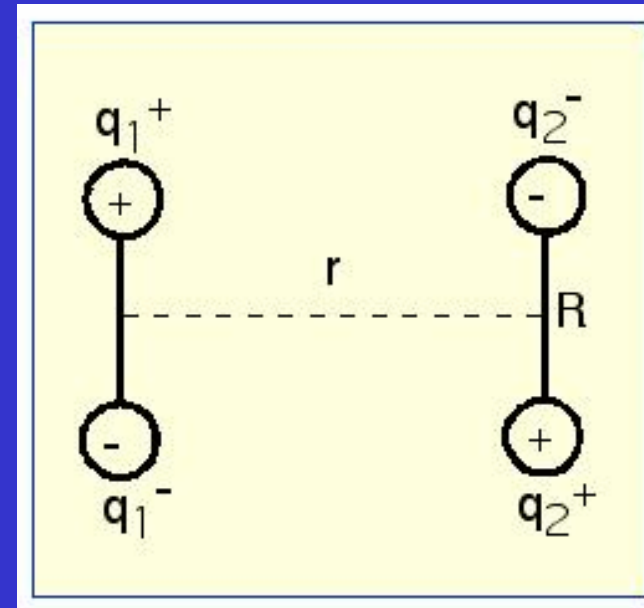
Modrý elektricky vodivý roztok

Silné redukční činidlo

# Interakce dipole - dipole

Keesom

$$E = -konst \frac{\mu_A^2 \mu_B^2}{kTr^6}$$



## Interakce dipol - dipol

Sloučenina	Butan	Aceton
$M_r$	58	58
Teplota varu, °C	- 0.5	57
Dipolový moment, C m	0	$9.3 \cdot 10^{-30}$



# Interakce ion – indukovaný dipol a dipol – indukovaný dipol

$$\mu(\text{indukovaný}) = \alpha E$$

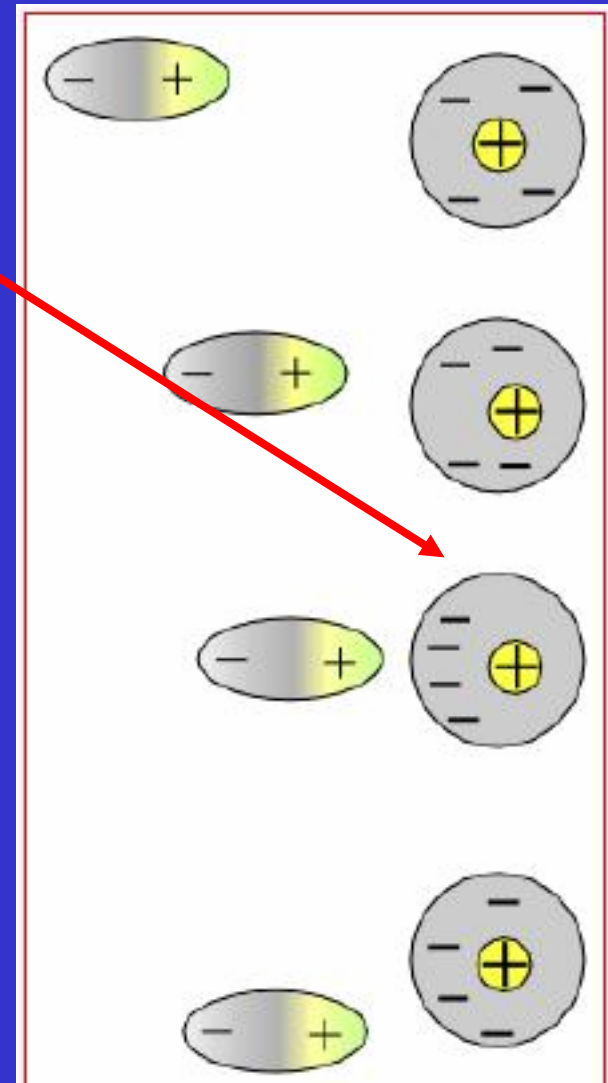
$\alpha$  = polarizovatelnost

ion – indukovaný dipol

$$E = -\textit{konst} \frac{q^2 \alpha}{r^4}$$

dipol – indukovaný dipol, Debye

$$E = -\textit{konst} \frac{\mu^2 \alpha}{r^6}$$

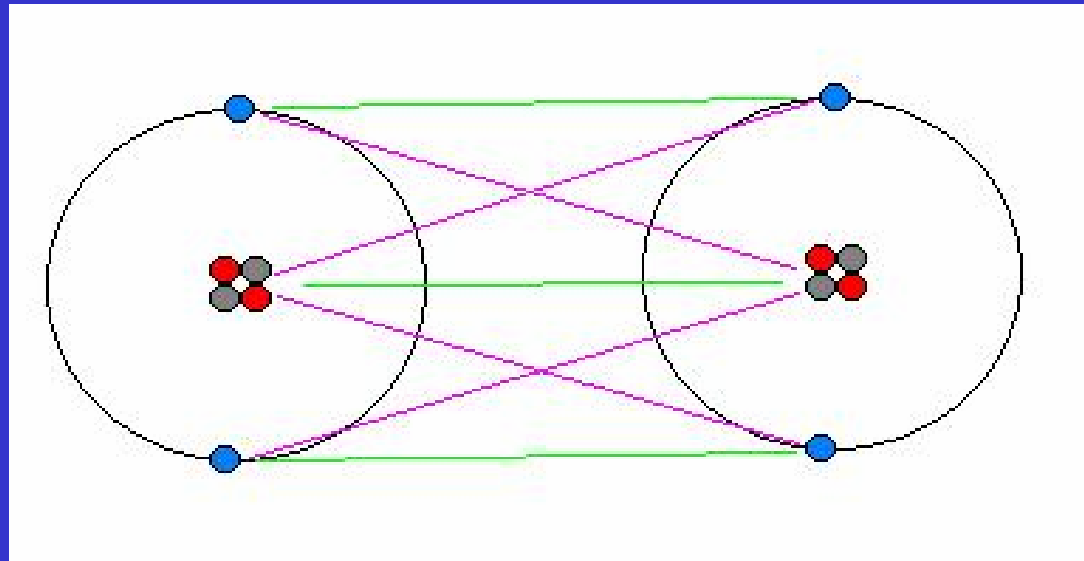


## Polarizovatelnost, $\alpha$ , m<sup>3</sup>

Skupina	Polarizovatelnost cm <sup>3</sup> 10 <sup>24</sup>	v.d.W poloměr Å
O	0.63	1.5
CH <sub>2</sub>	1.80	2.0
S	3.00	1.8

Molekula	Polarizovatelnost (Å <sup>3</sup> )	T <sub>varu</sub> (K)	Dipolový moment (D)
He	0.20	4.216	0
Ne	0.39	27.3	0
Ar	1.62	87.3	0
Kr	2.46	119.9	0
H <sub>2</sub> O	1.48	373.15	1.85
H <sub>2</sub> S	3.64	212.82	1.10
CCl <sub>4</sub>	10.5	349.85	0
C <sub>6</sub> H <sub>6</sub>	25.1	353.25	0
CH <sub>3</sub> OH	3.0	338	1.71
CH <sub>3</sub> F	3.84	195	1.81
CHCl <sub>3</sub>	8.50	334.85	1.01

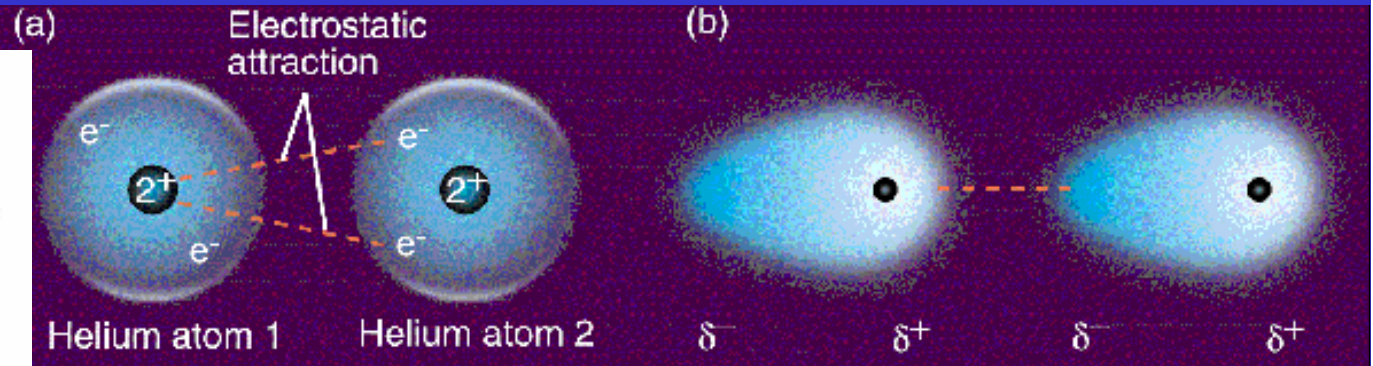
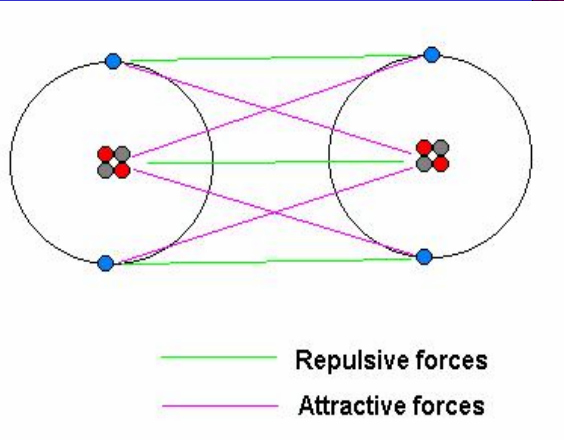
# Interakce indukovaný dipol – indukovaný dipol



**Odpudivé síly**

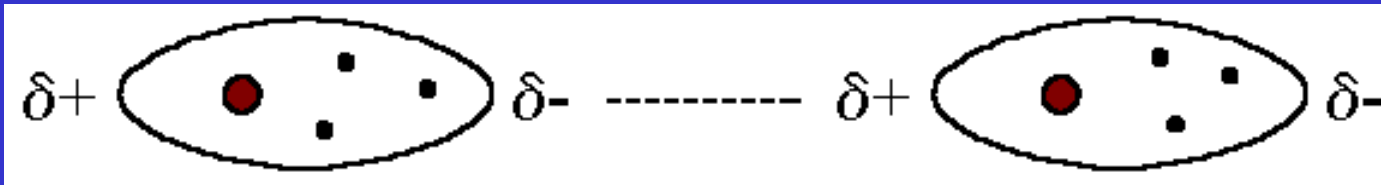
**Přitažlivé síly**

# Londonovy disperzní síly



$$E = -konst \frac{IE\alpha^2}{r^6}$$

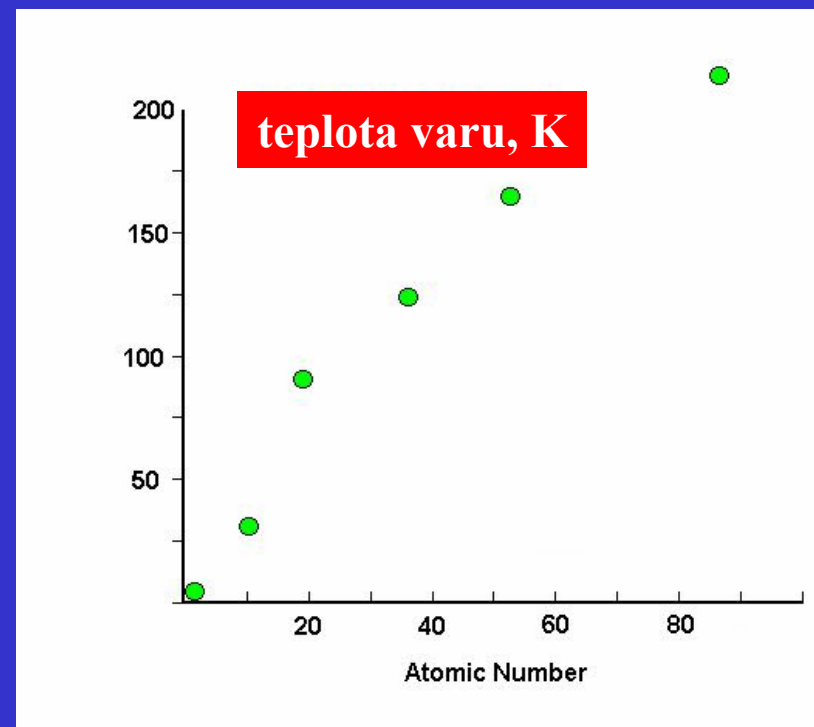
IE = ionizační energie  
 $\alpha$  = polarizovatelnost  
 r = vzdálenost



# Vliv polarizovatelnosti molekuly na velikost Londonových sil

Vliv Londonových sil na skupenství halogenů a vzácných plynů

S velikostí molekul roste polarizovatelnost

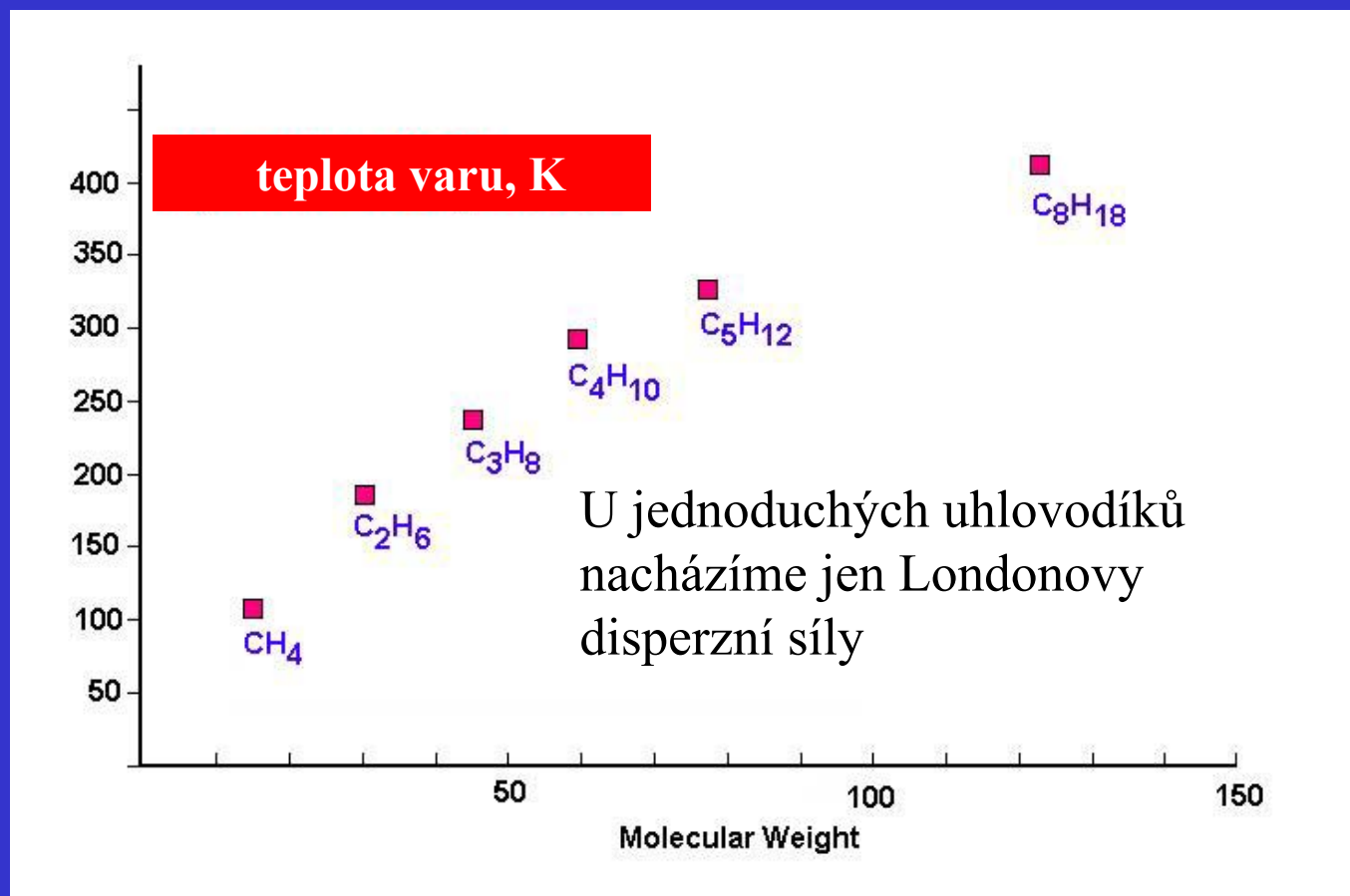


	teplota varu, K
F <sub>2</sub>	85.1
Cl <sub>2</sub>	238.6
Br <sub>2</sub>	332.0
I <sub>2</sub>	457.6

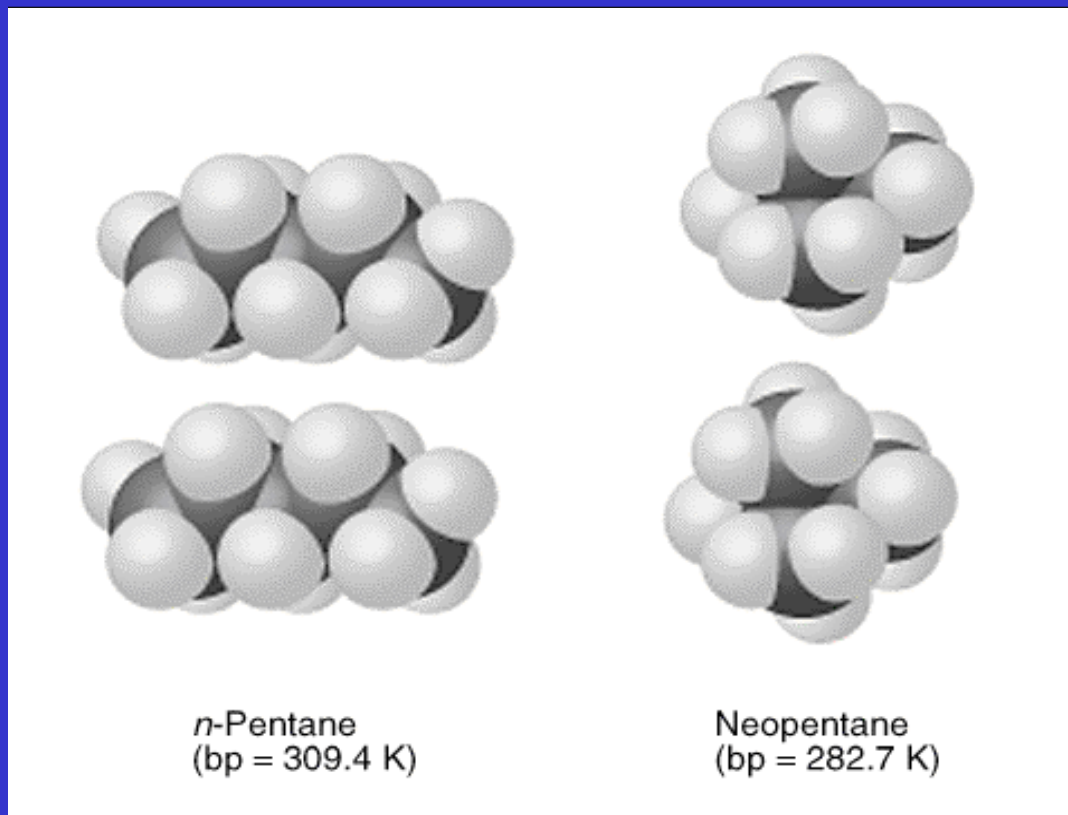
	teplota varu, K
He	4.6
Ne	27.3
Ar	87.5
Kr	120.9



# Vliv velikosti molekuly na velikost Londonových sil



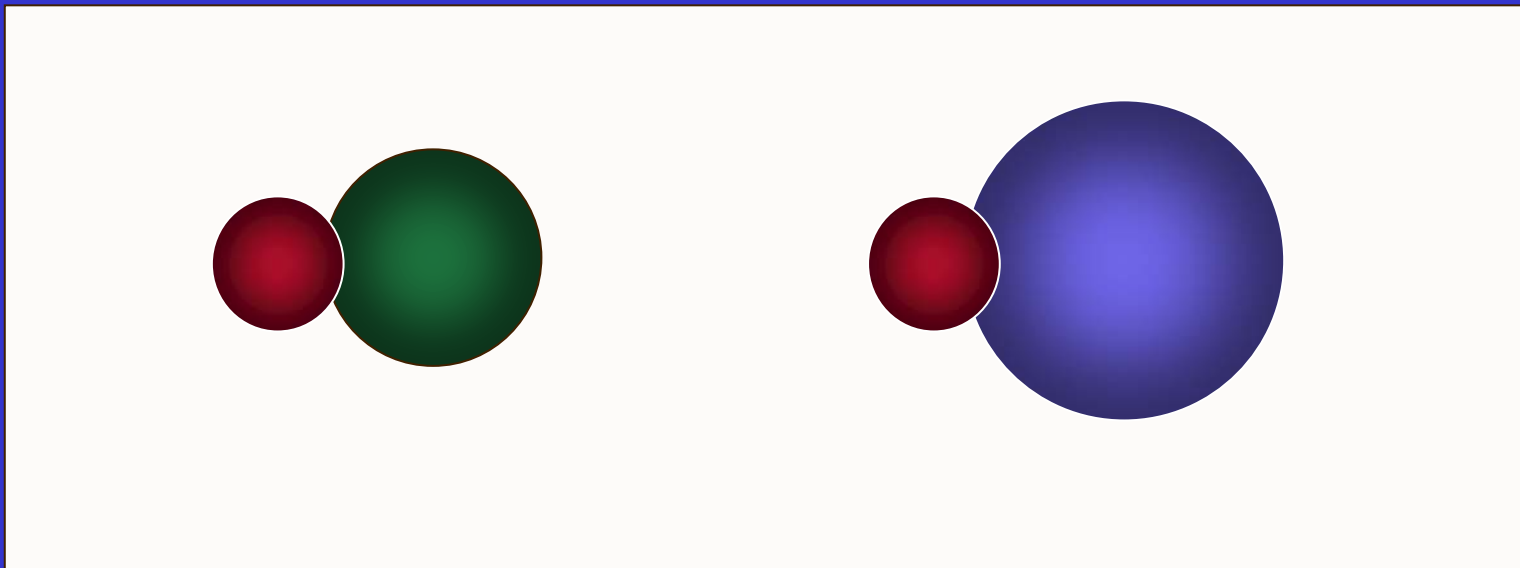
# Vliv tvaru molekuly na velikost Londonových sil



Stejná  $M_r$

Větší plocha dotyku

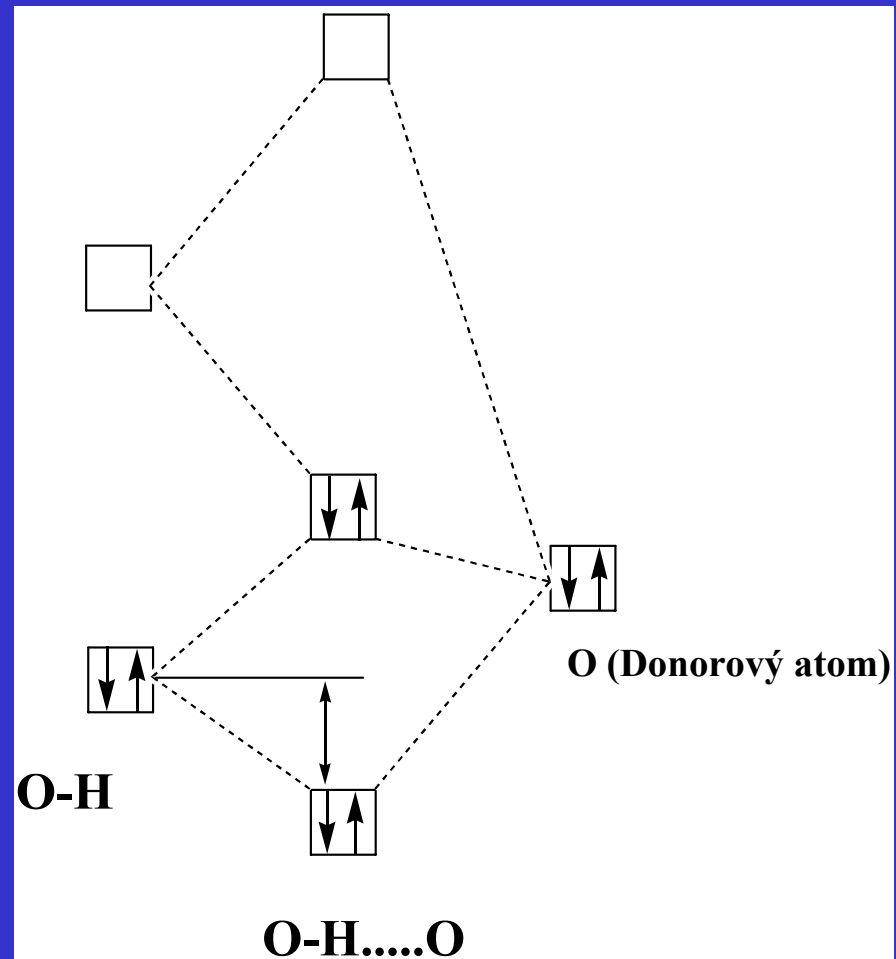
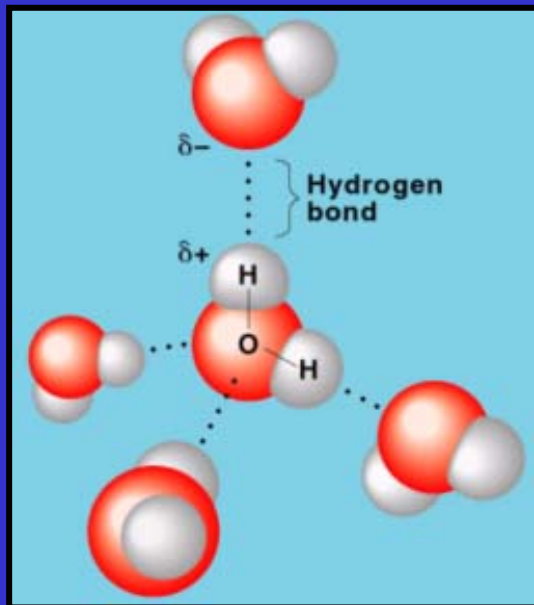
# Londonovy disperzní síly a dipol-dipolové interakce



**HCl:  $b_v = 189.5$  K**  
**Dipolový moment = 1.03 D**

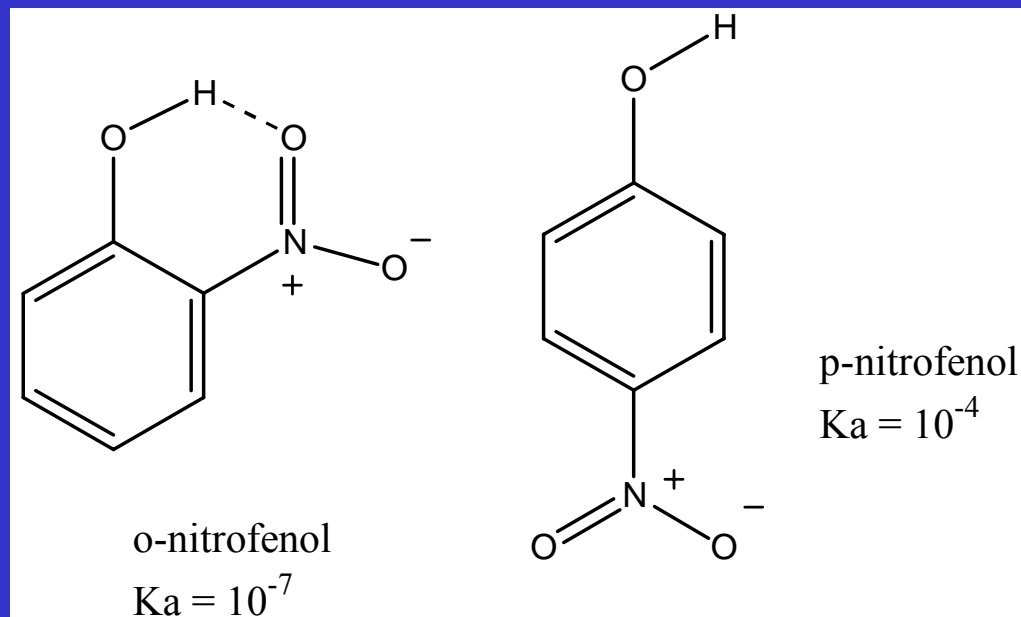
**HBr:  $b_v = 206.2$  K**  
**Dipolový moment = 0.79 D**

# Vodíková vazba



# Vodíková vazba

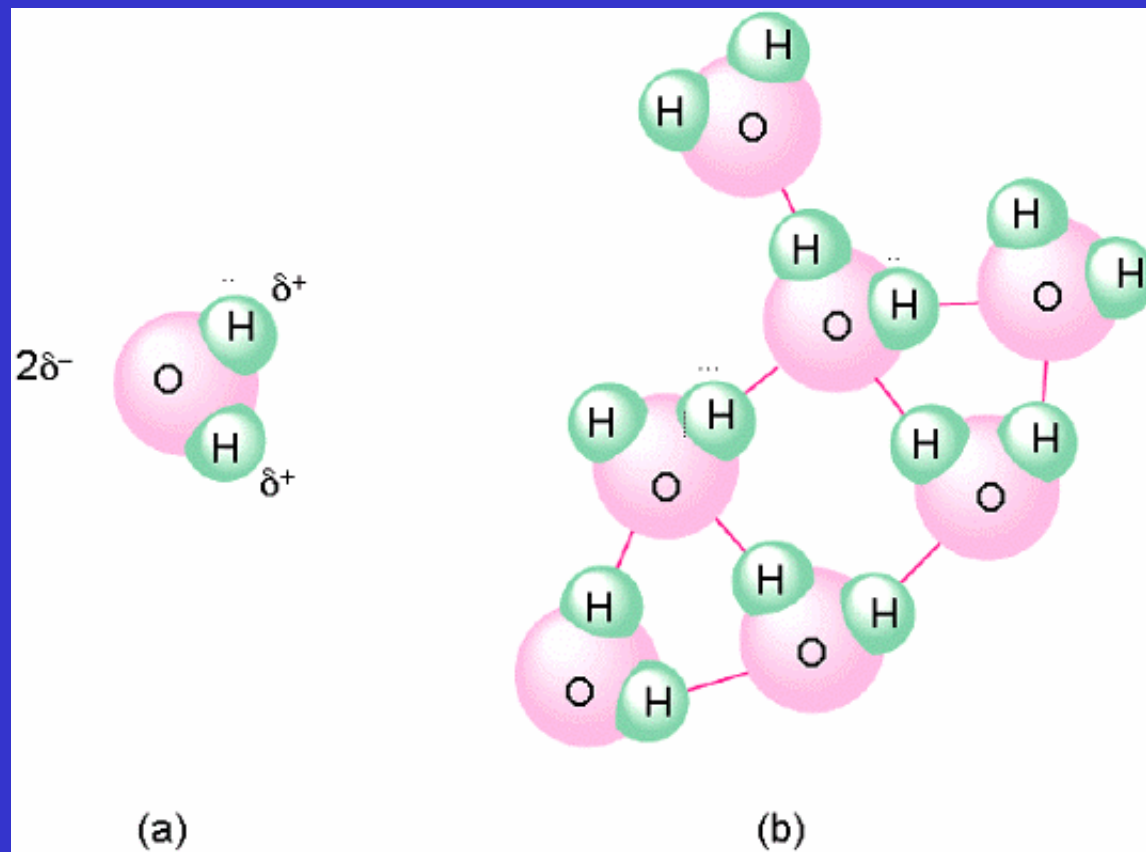
## Intramolekulární vodíková vazba



Snížená kyselost OH skupiny  
v důsledku tvorby vodíkové vazby

# Vodíková vazba

Intermolekulární

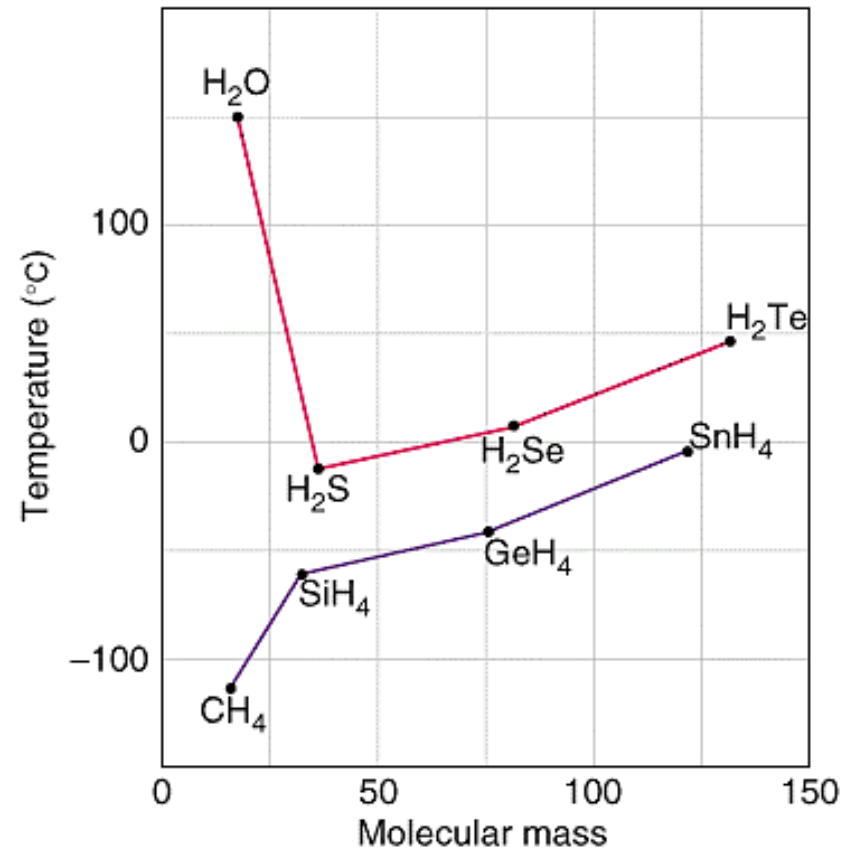




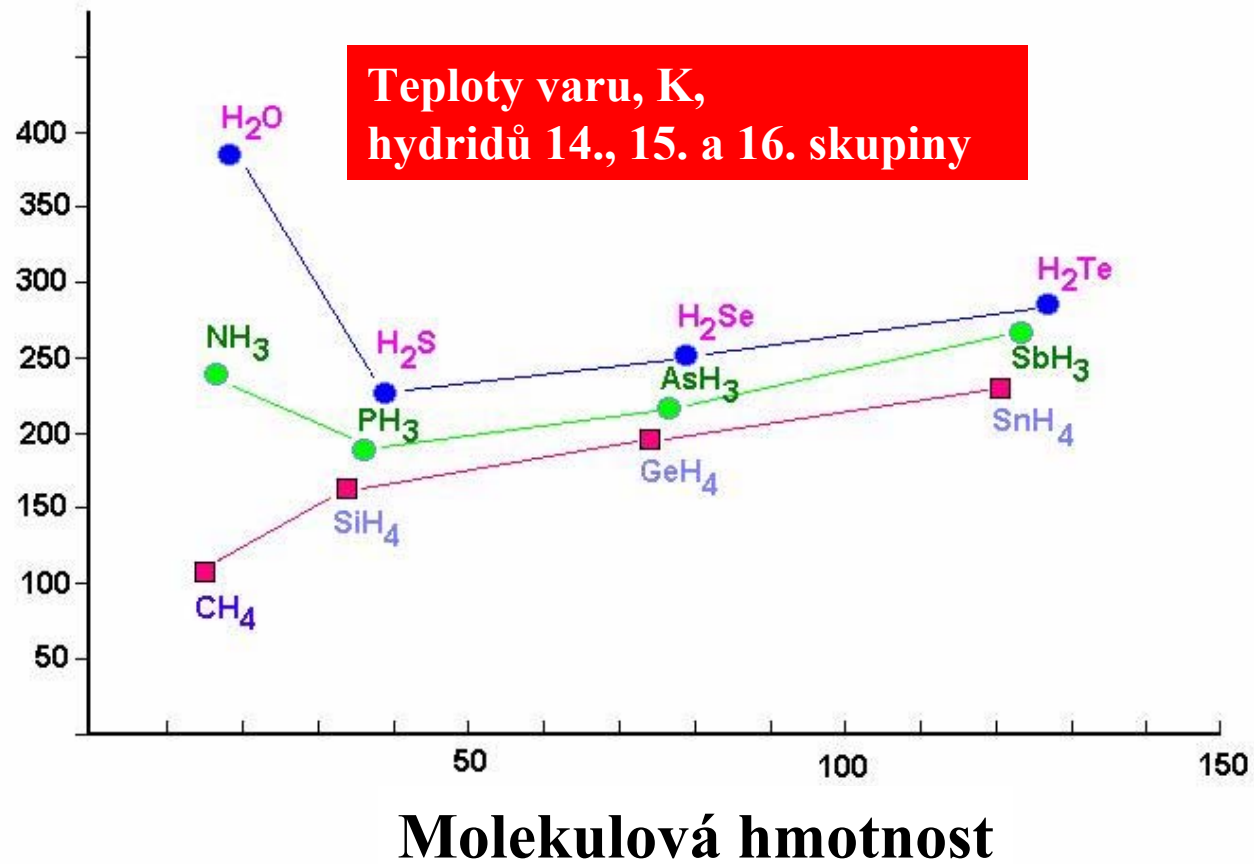
## Vodíková vazba

Vazba	Vzdálenost (Å)	Rozmezí (Å)
<b>N-H...N</b>	<b>3.10</b>	<b>2.88-3.38</b>
<b>N-H...O</b>		
- Amid NH	2.93	2.55-3.04
- Amino NH	3.04	2.57-3.22
<b>N-H...F</b>	<b>2.78</b>	<b>2.62-3.01</b>
<b>N-H...Cl</b>	<b>3.21</b>	<b>2.91-3.52</b>
<b>O-H...N</b>	<b>2.80</b>	<b>2.62-2.93</b>
<b>O-H...O</b>		
- Alkohol OH	2.74	2.55-2.96
- Voda OH	2.80	2.65-2.93
<b>O-H...Cl</b>	<b>3.07</b>	<b>2.86-3.21</b>

# Vodíková vazba

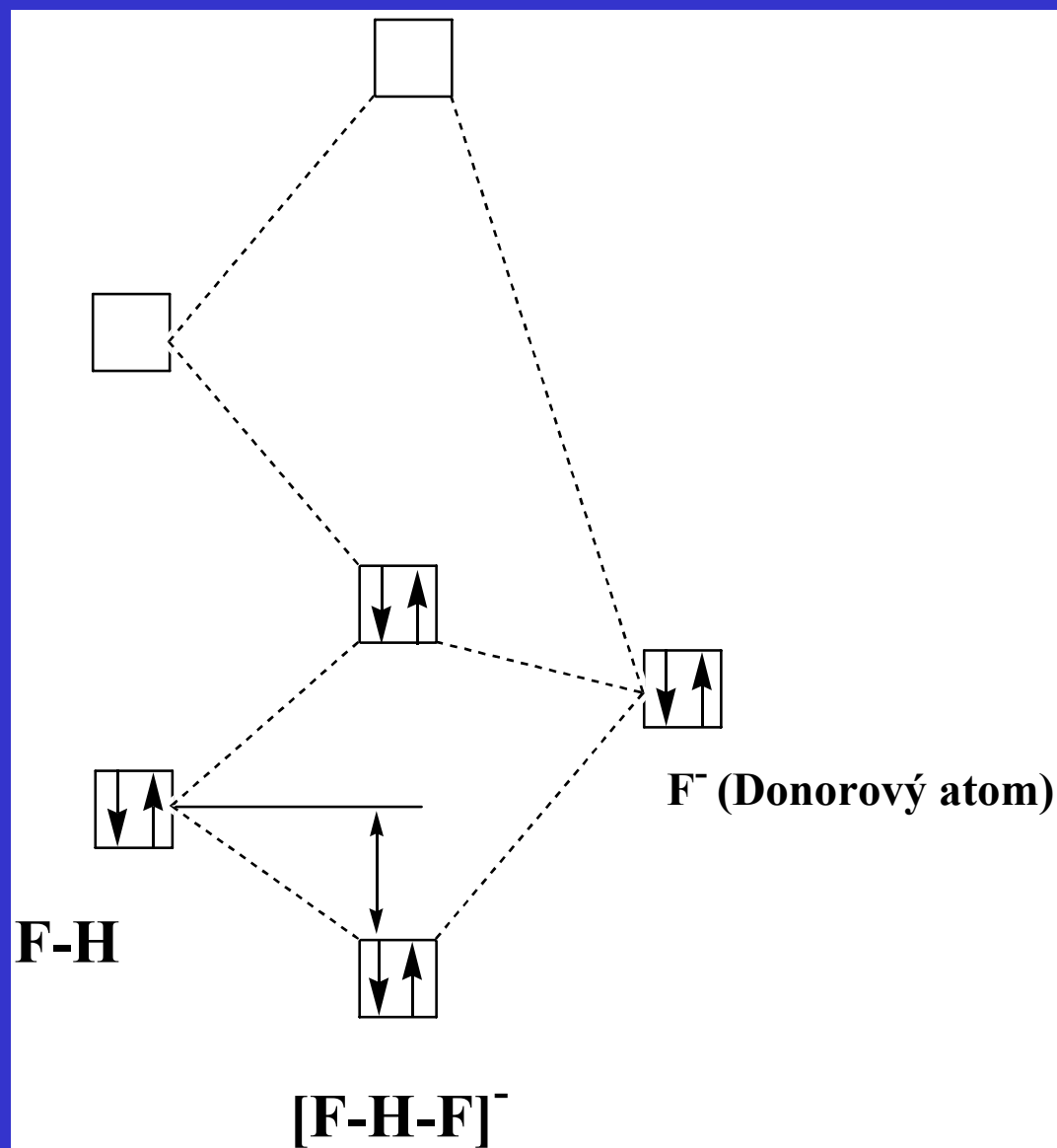


# Vodíková vazba

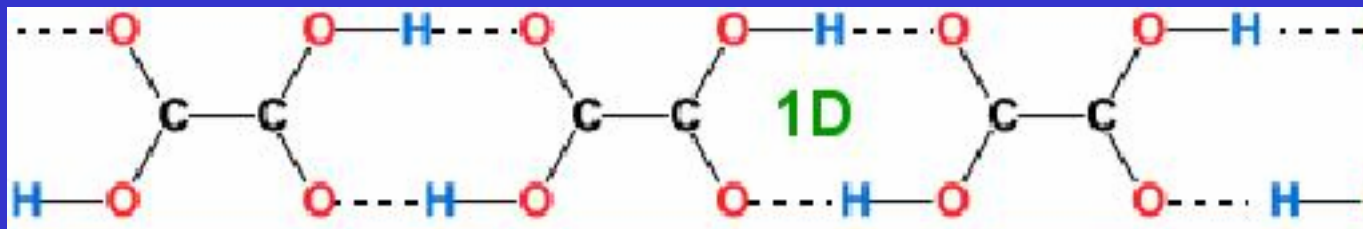
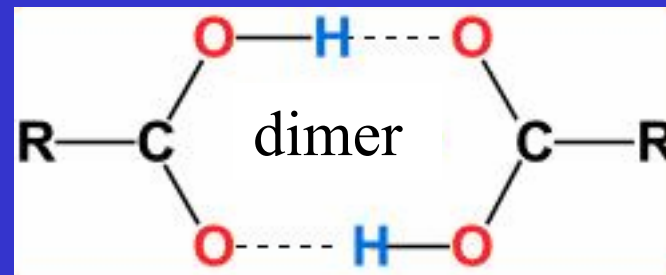




Velmi silná vazba  
Symetrické rozložení  
vazebných délek



# Vodíková vazba



Krystalové inženýrství

# Struktura HF

## 1D. HF

Ortorrómbico: B mmb

a (Å) 3.42

b (Å) 4.32

c (Å) 5.41

V (Å<sup>3</sup>) 79.9

Z 4

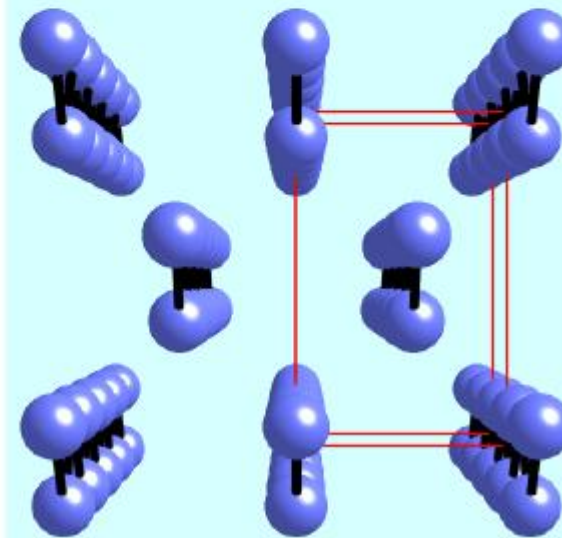
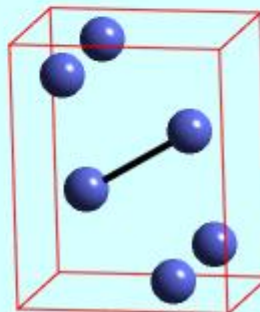
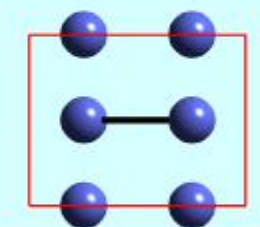
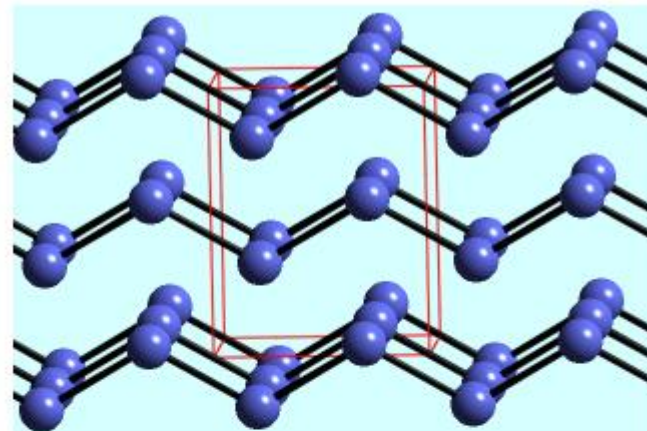
Dx (gcm<sup>-3</sup>) 1.66

F-H (Å) -

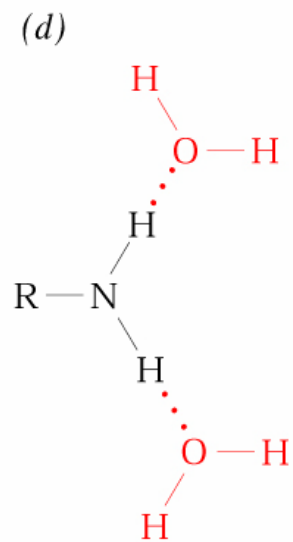
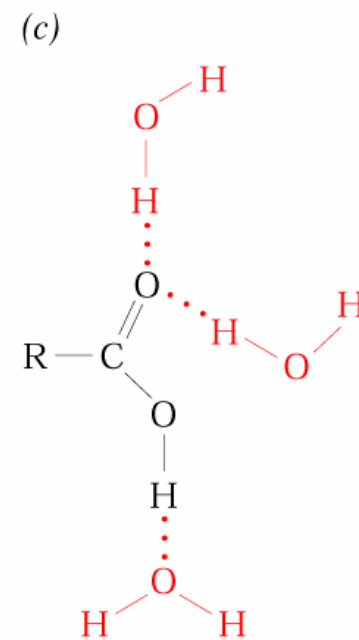
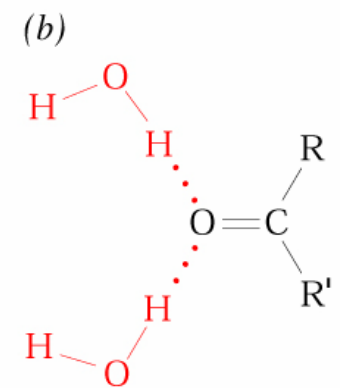
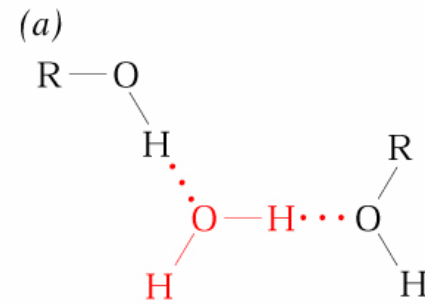
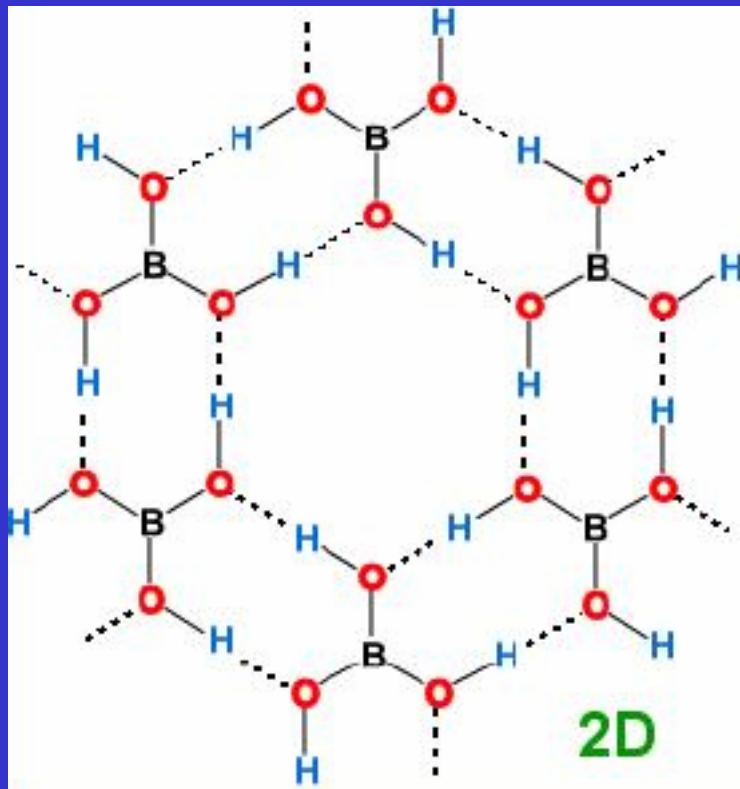
F...F (Å) 2.49

H...F (Å) -

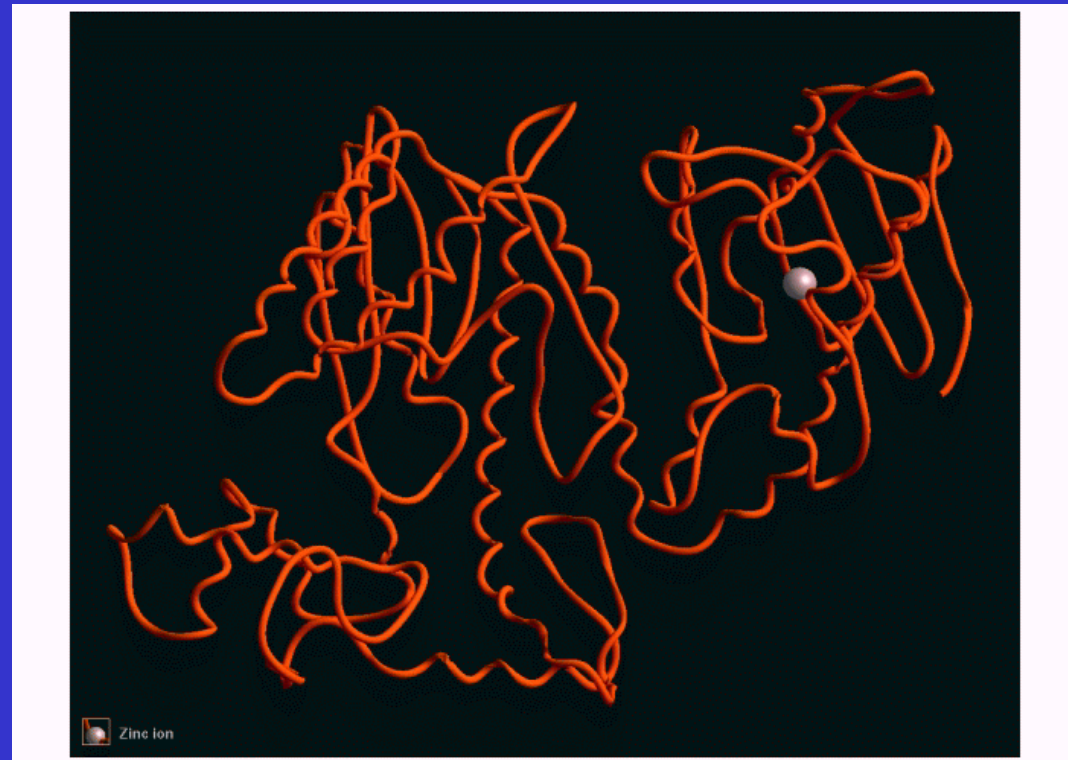
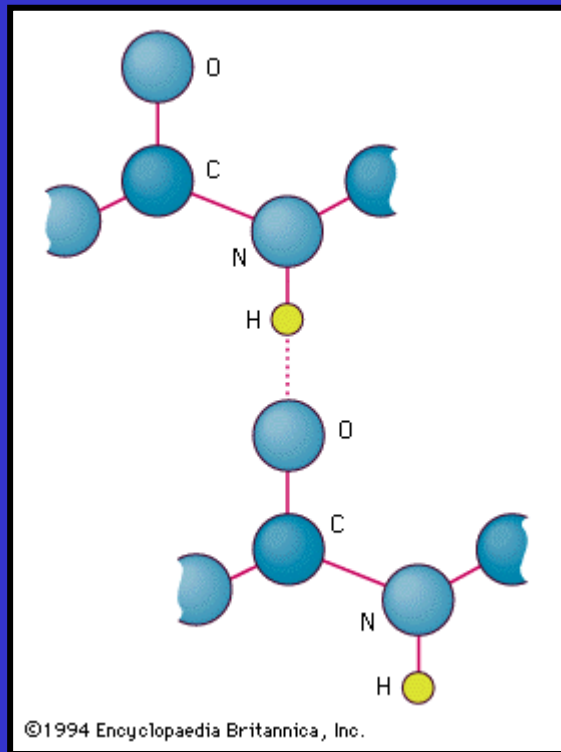
F-H...F (°) 180°



# Kyselina boritá

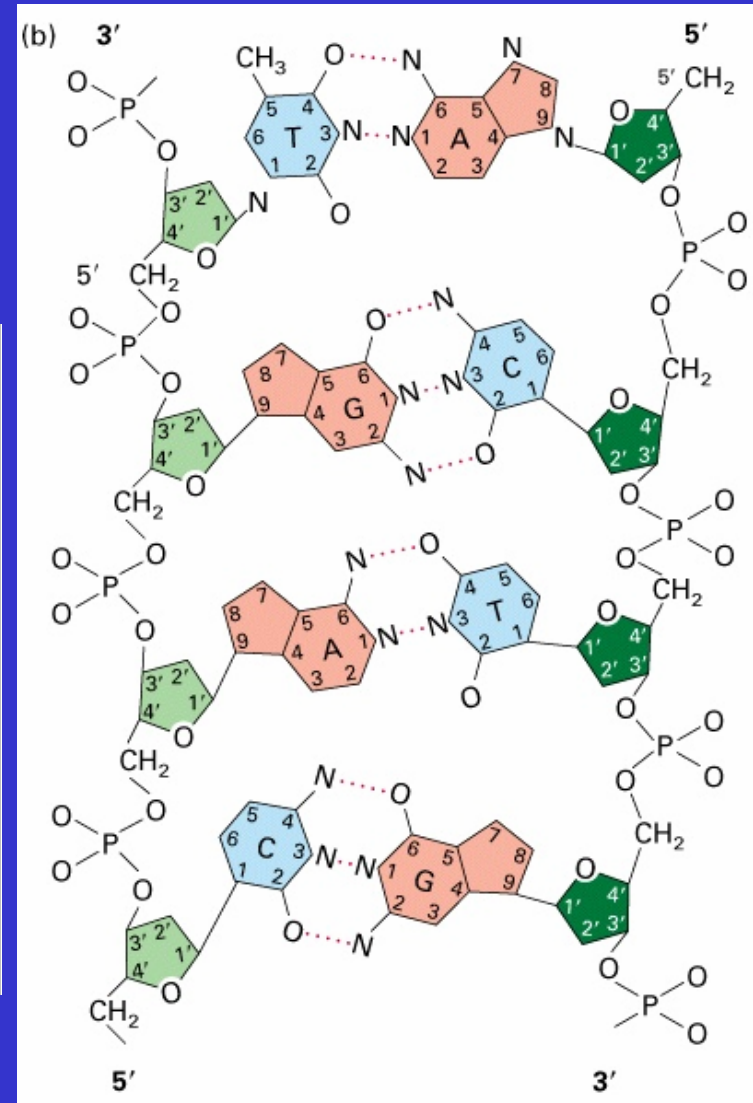
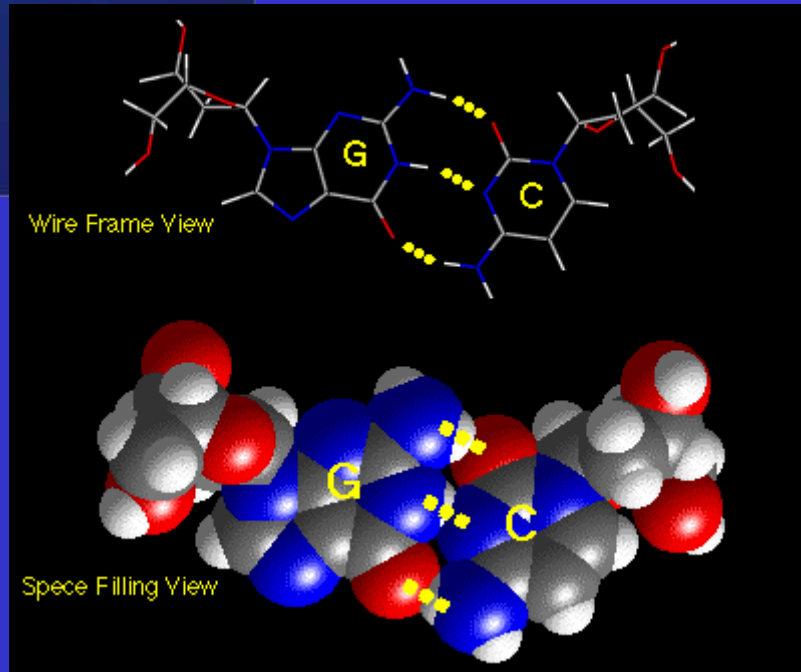


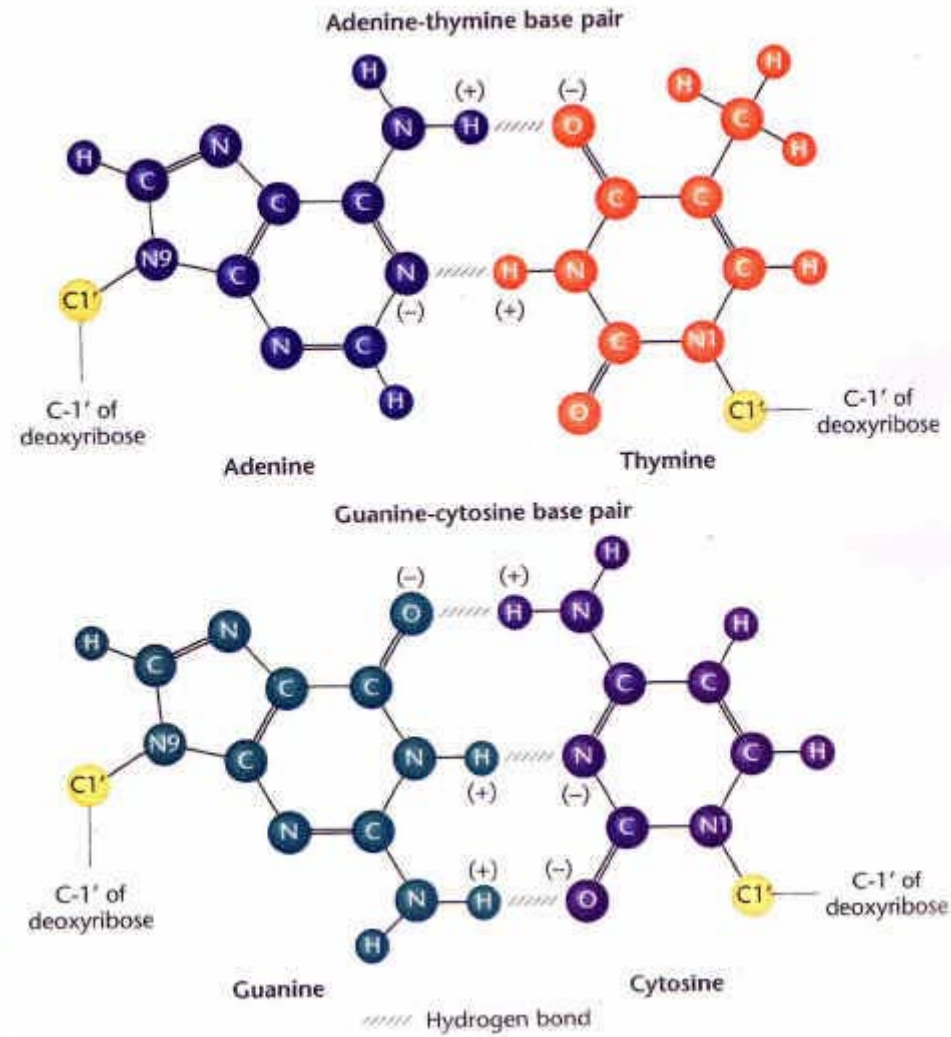
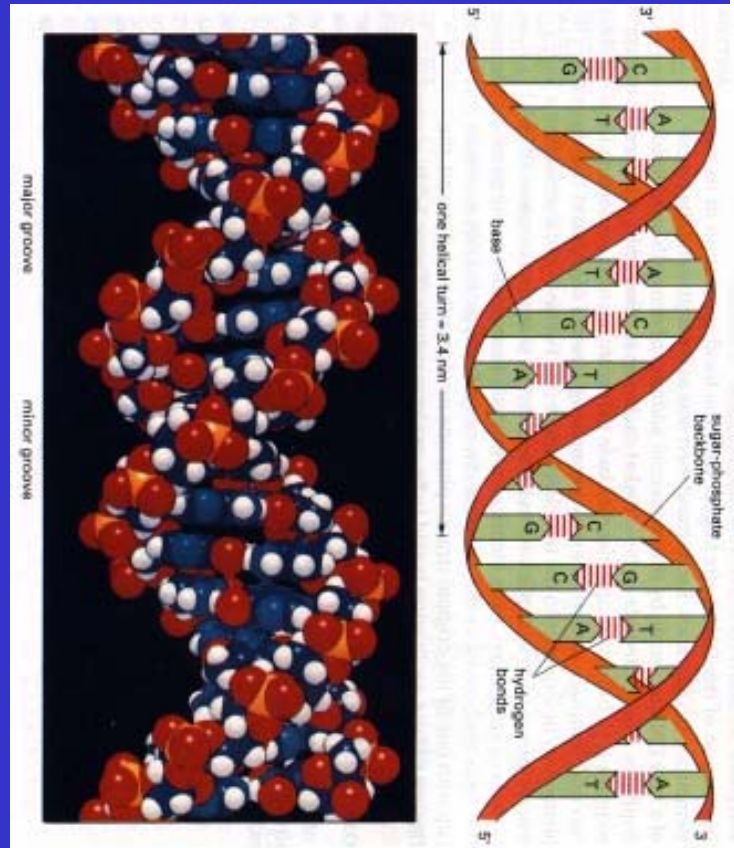
# Struktura proteinů





# Struktura DNA





# Struktura ledu

## 3D. H<sub>2</sub>O

Hexagonal: P6<sub>3</sub>/mmc

a (Å) 4.5227

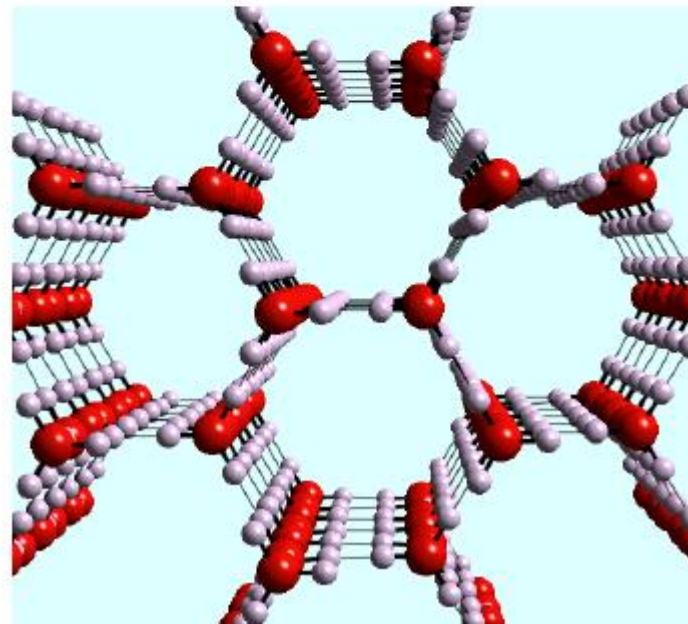
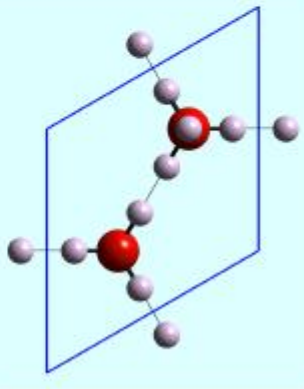
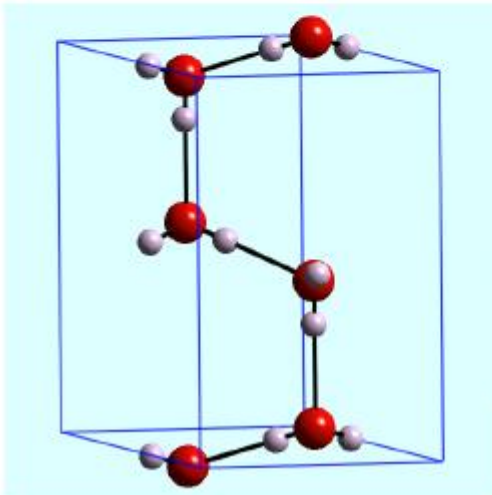
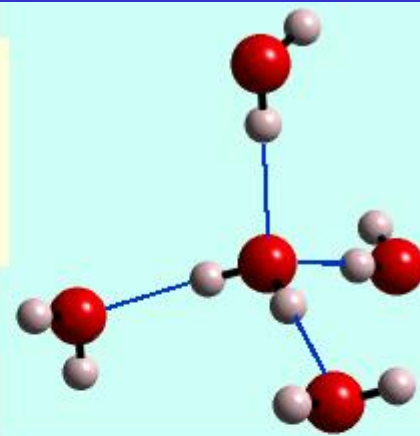
c (Å) 7.3671

V (Å<sup>3</sup>) 121.9

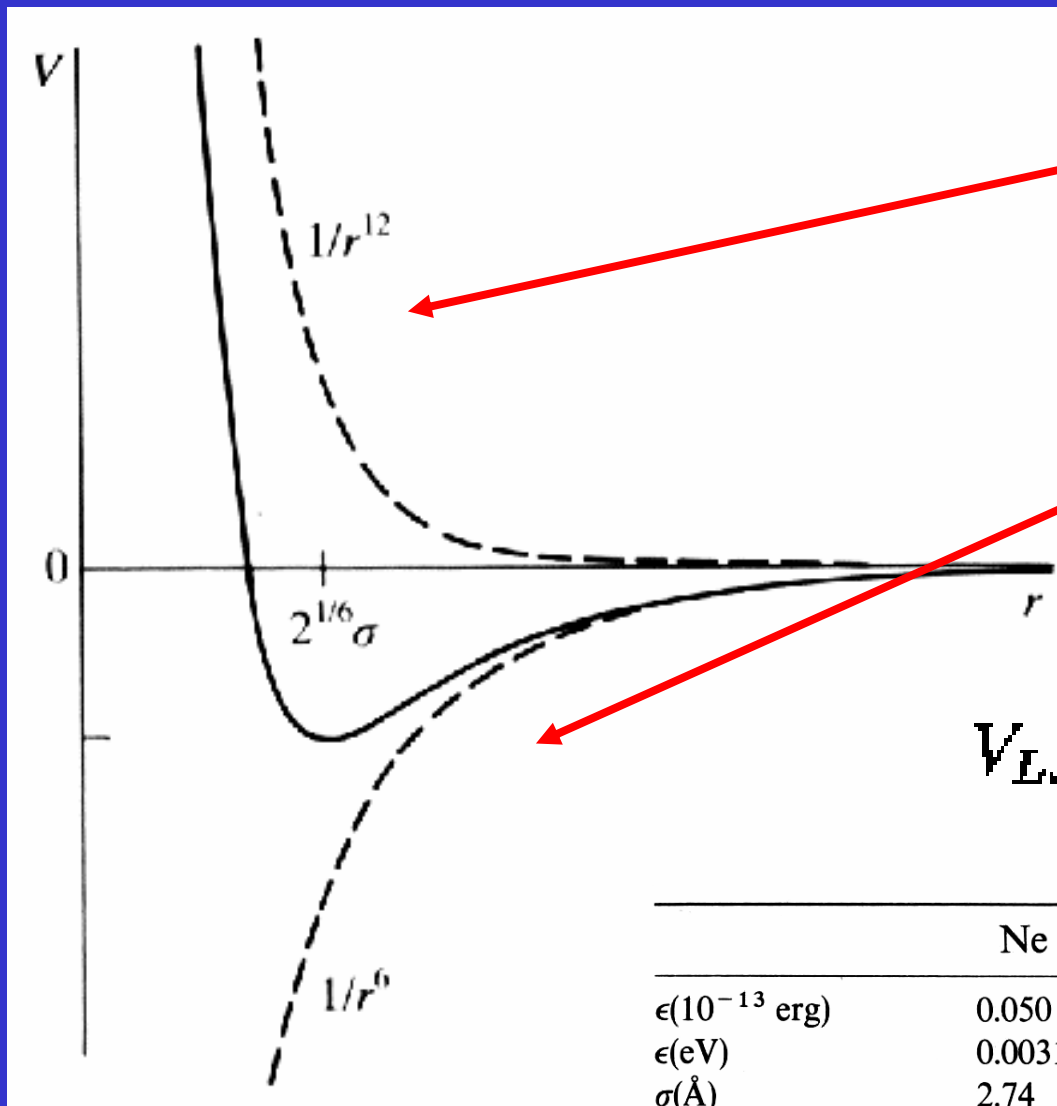
Z 3

Dx (gcm<sup>-3</sup>) 0.74

O-H (Å)	0.82, 0.86
O...O (Å)	2.765, 2.773
H...O (Å)	1.91, 1.95
O-H...O (°)	180°



## Rovnováha přitažlivých a odpudivých sil



Odpudivé síly  
v.d. Waalsova repulze  
 $E = 1/r^{12}$

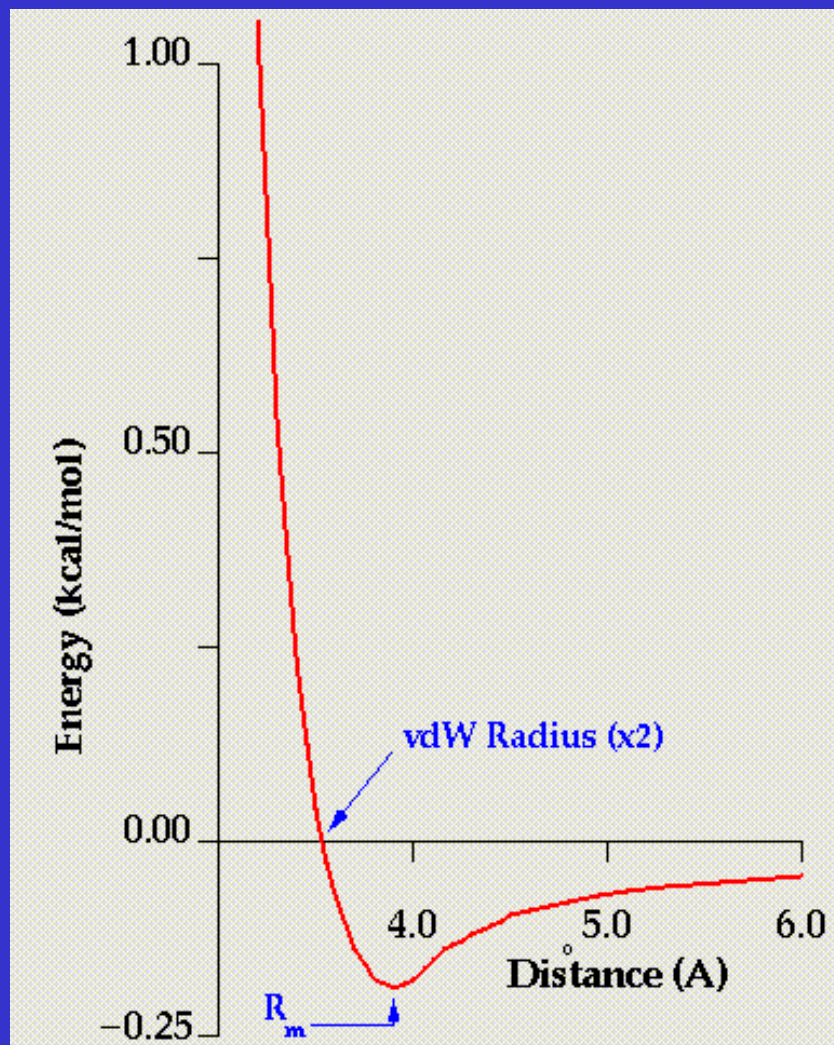
Přitažlivé síly  
 $E = 1/r^6$

**Lennard-Jones**

$$V_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

	Ne	Ar	Kr	Xe
$\epsilon(10^{-13} \text{ erg})$	0.050	0.167	0.225	0.320
$\epsilon(\text{eV})$	0.0031	0.0104	0.0140	0.0200
$\sigma(\text{\AA})$	2.74	3.40	3.65	3.98





Skupina	vdW	0.5 R <sub>m</sub>
<b>C atom</b>		
- alifat	1.7 Å	2.0 Å
- aromati	1.7 Å	
<b>O atom</b>		
- karbonyl	1.4 Å	1.9 Å
- alkohol	1.5 Å	
<b>N atom</b>		
- amid	1.52 Å	1.80 Å
- amin	1.65 Å	
- ammonium	1.50 Å	
<b>F atom</b>	1.35 Å	
<b>Cl atom</b>	1.80 Å	
<b>Br atom</b>	1.95 Å	
<b>I atom</b>	2.15 Å	
<b>S atom</b>	1.85 Å	

## Van der Waalsovy poloměry, Å

Ag 1.72	Ar 1.88	As 1.85	Au 1.66
Br 1.85	C 1.70	Cd 1.58	Cl 1.75
Cu 1.40	F 1.47	Ga 1.87	H 1.20
He 1.40	Hg 1.55	I 1.98	In 1.93
K 2.75	Kr 2.02	Li 1.82	Mg 1.73
N 1.55	Na 2.27	Ne 1.54	Ni 1.63
O 1.52	P 1.80	Pb 2.02	Pd 1.63
Pt 1.72	S 1.80	Se 1.90	Si 2.10
Sn 2.17	Te 2.06	Tl 1.96	U 1.86
Xe 2.16	Zn 1.39		