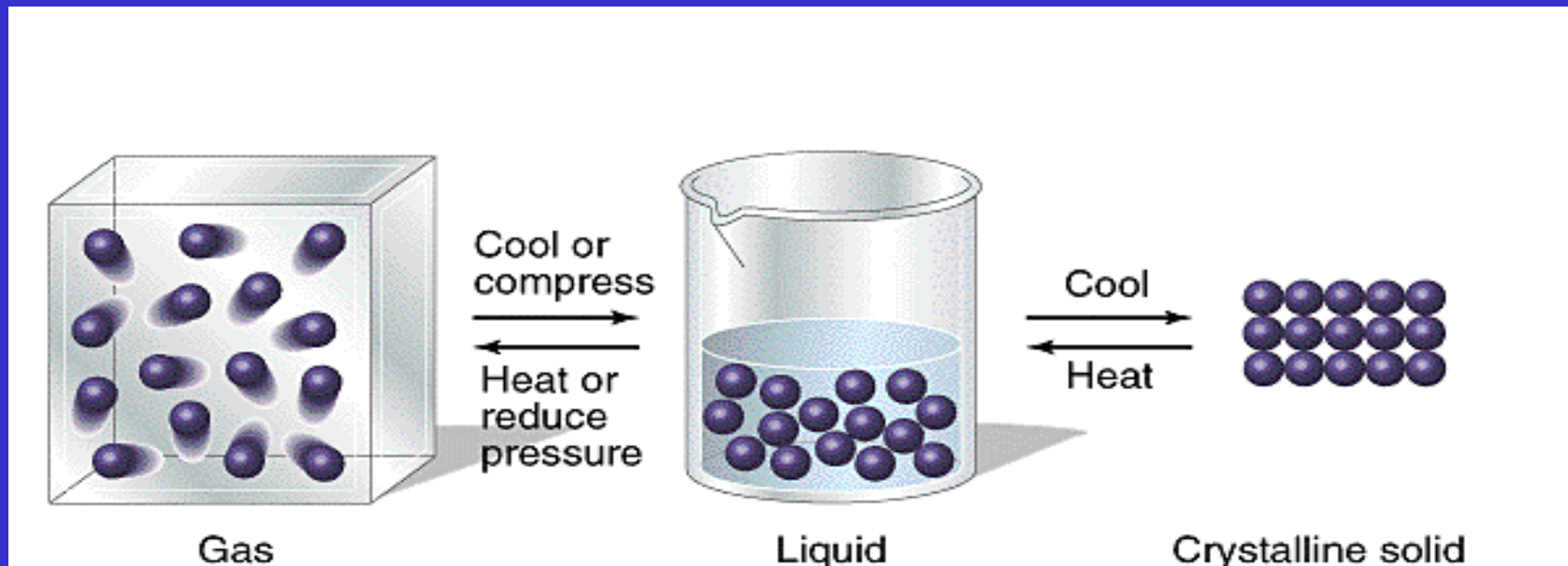


Skupenské stavy



Plyn

Zcela neuspořádané
Hodně volného prostoru
Zcela volný pohyb částic
Částice daleko od sebe

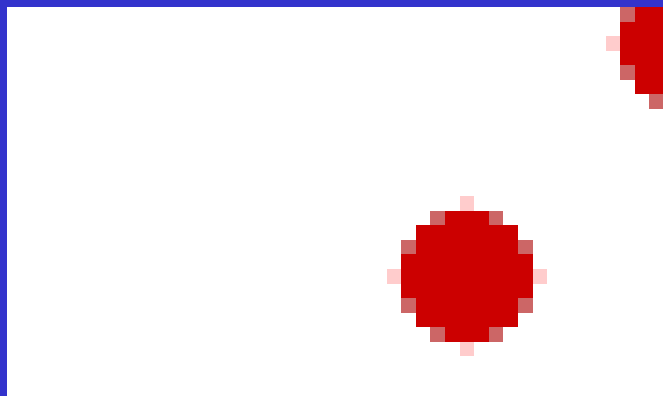
Kapalina

Částečně neuspořádané
Volný pohyb částic nebo skupin částic
Částice blíže u sebe

Pevná látka

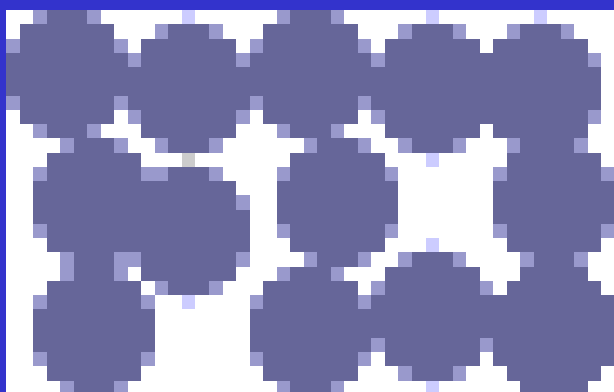
Pravidelně uspořádané
Částice na stálých pozicích
Částice blízko u sebe

Skupenské stavy

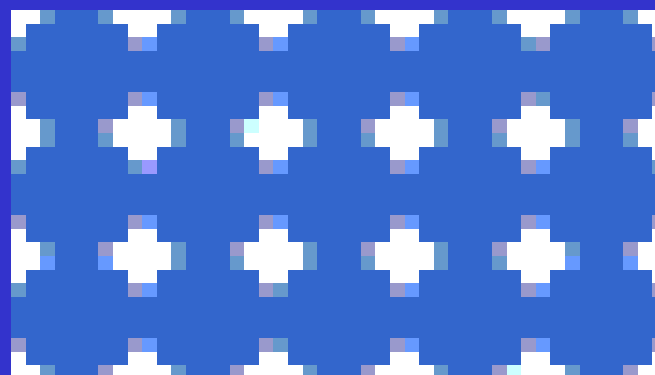


Plyn

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

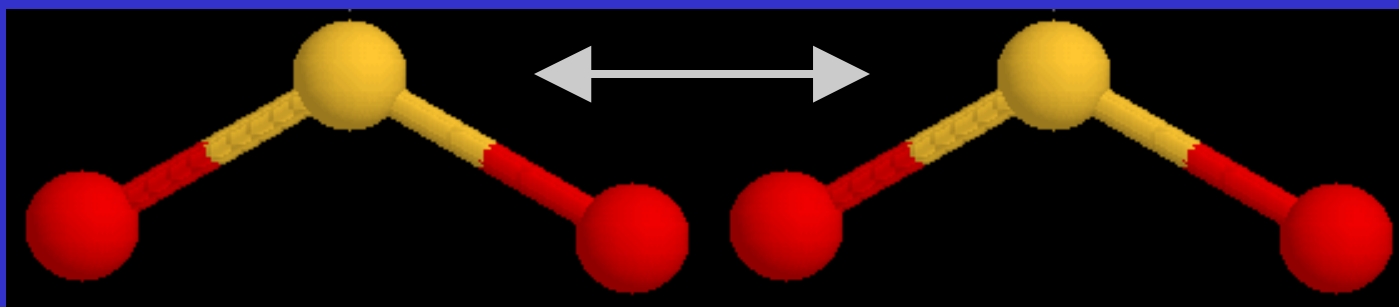
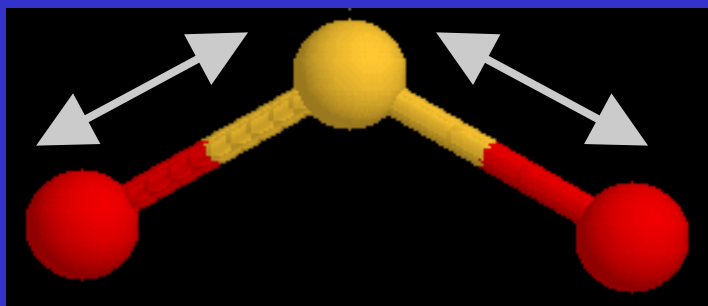


Kapalina

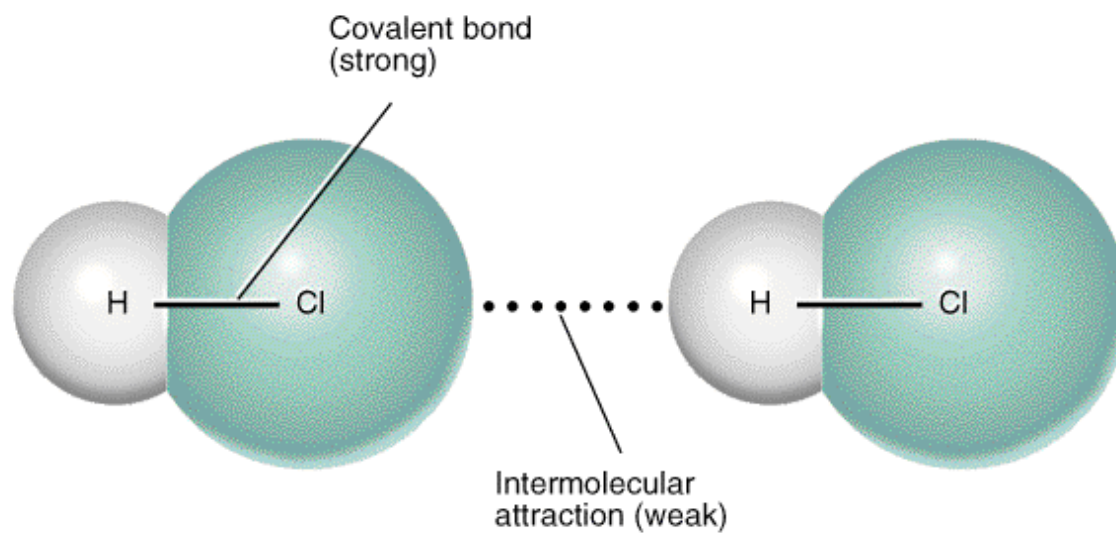


Molekulový krystal

Rozdíl mezi kovalentní vazbou a mezimolekulovými silami



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



Typy mezimolekulových vazeb (van der Waalsových interakcí)



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

ion – ion Coulombické interakce

ion – dipol

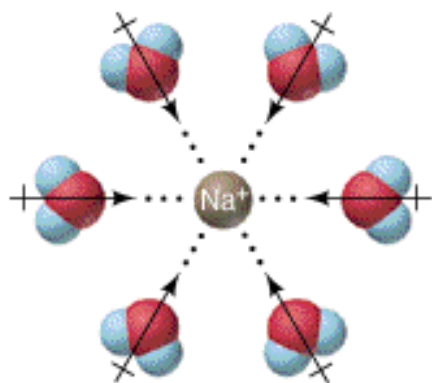
dipol – dipol → orientační, Keesom

dipol – indukovaný dipol → indukční, Debye

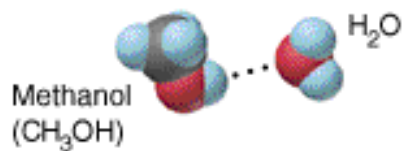
ion – indukovaný dipol

indukovaný dipol – indukovaný dipol → disperzní, London

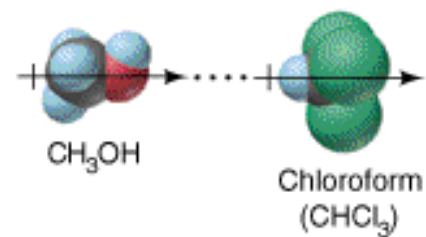
van der Waalsova repulze (odpuzování)



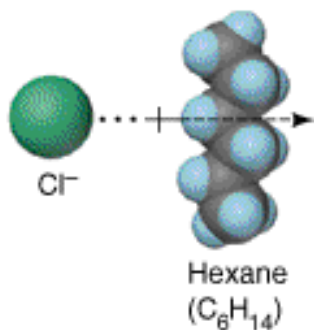
Ion-dipole



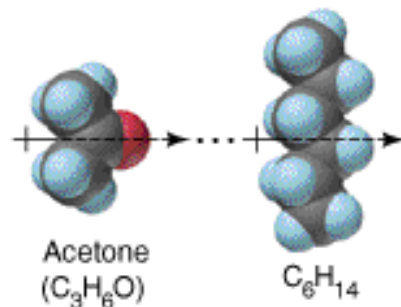
H bond



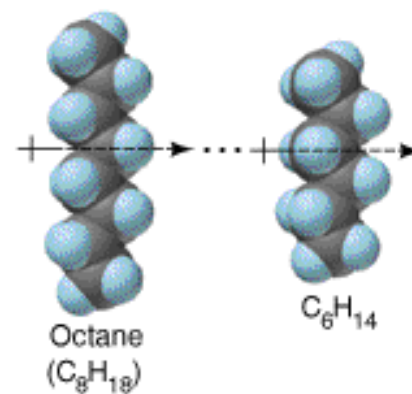
Dipole-dipole



Ion-induced dipole



Dipole-induced dipole



Dispersion

Interakce ion - ion

Coulombův zákon

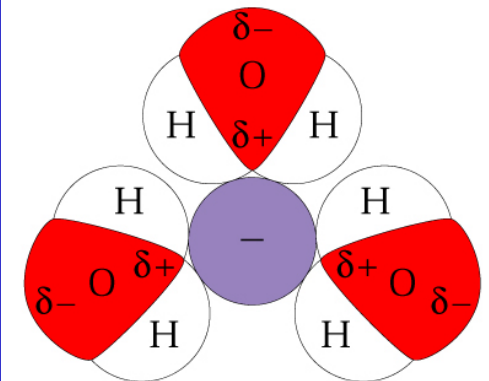
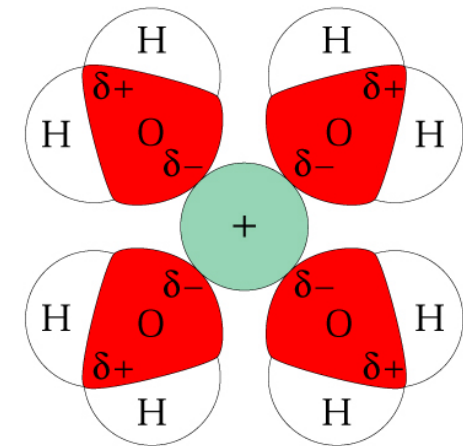
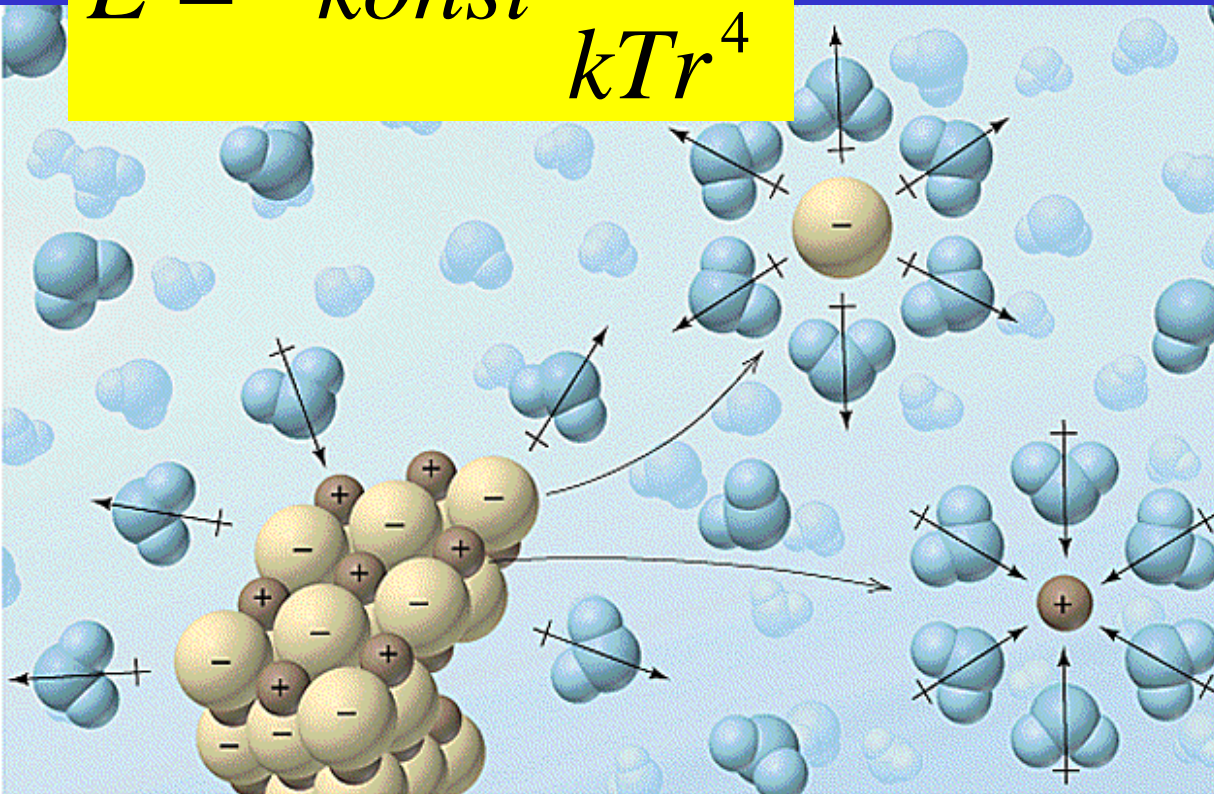
$$E = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r}$$

E = energie interakce
q = náboj iontu
r = meziiontová vzdálenost



Interakce ion - dipol

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



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E = energie interakce

q = náboj iontu

μ = dipolový moment

r = vzdálenost

T = teplota

k = Boltzmannova konstanta

Dipolový moment - μ

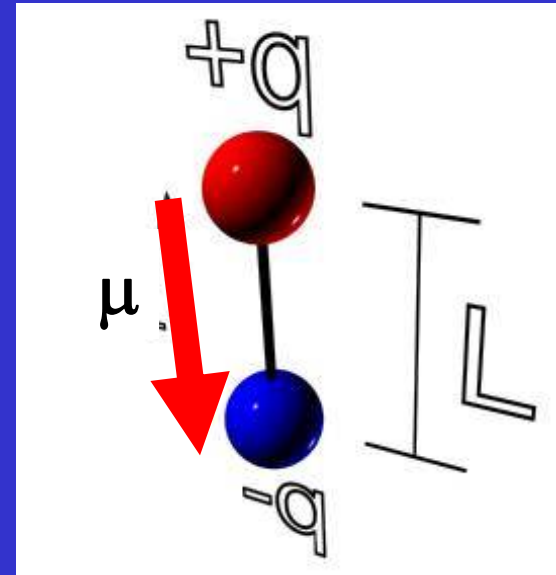
proton a elektron, vzdáleny 1 Å

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

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

dipolový moment **4.80 D**

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



Hydratace/solvatace iontů

Interakce klesá s rostoucí velikostí iontu

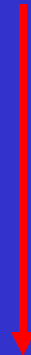


K^+ slabá

Rb^+ nulová

Cs^+ negativní

Interakce klesá



Interakce roste s rostoucím nábojem iontu



Ion-dipol



Polární koord. vazba



Interakce roste

Solvatace elektronů

Sodík rozpuštěný v kapalném amoniaku



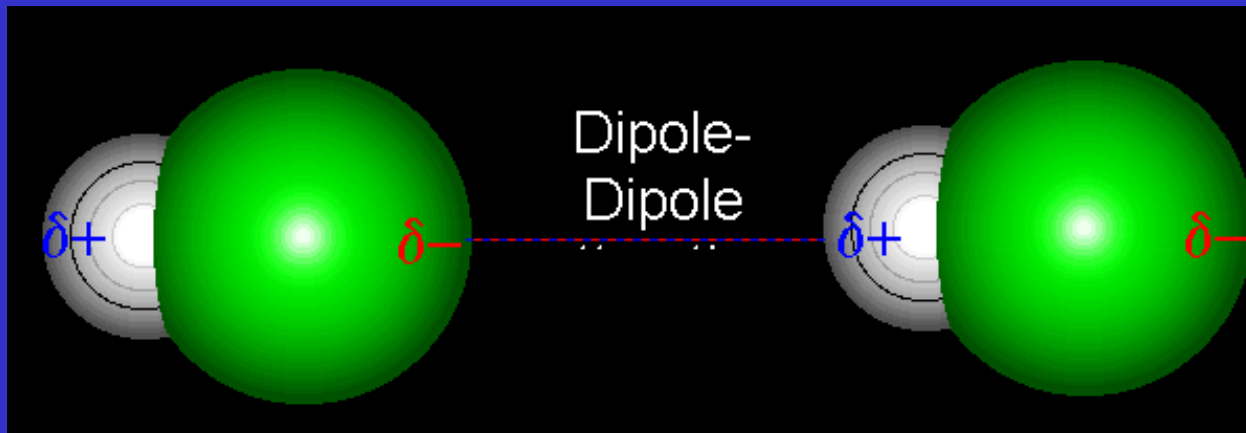
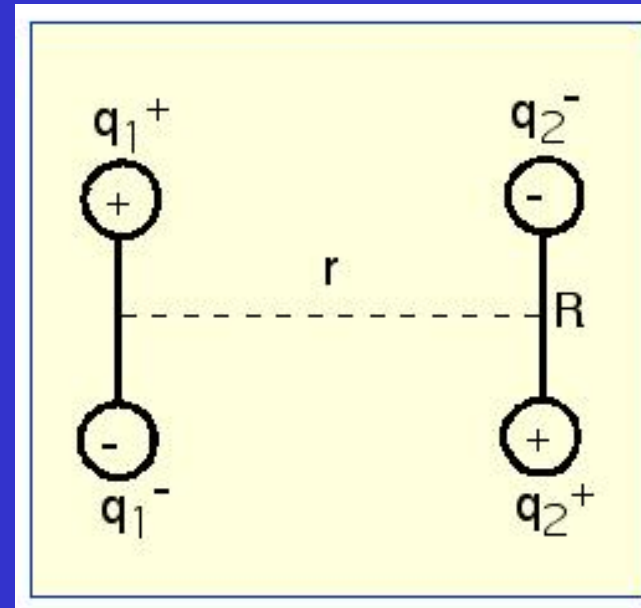
Modrý elektricky vodivý roztok

Silné redukční činidlo

Interakce dipol - dipol

Keesom

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



E = energie interakce
 μ = dipolový moment
r = vzdálenost
T = teplota
k = Boltzmannova konstanta

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

$$\mu(\text{indukovaný}) = \alpha E$$

α = polarizovatelnost

E = intenzita elektr. pole

ion – indukovaný dipol

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

dipol – indukovaný dipol, Debye

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

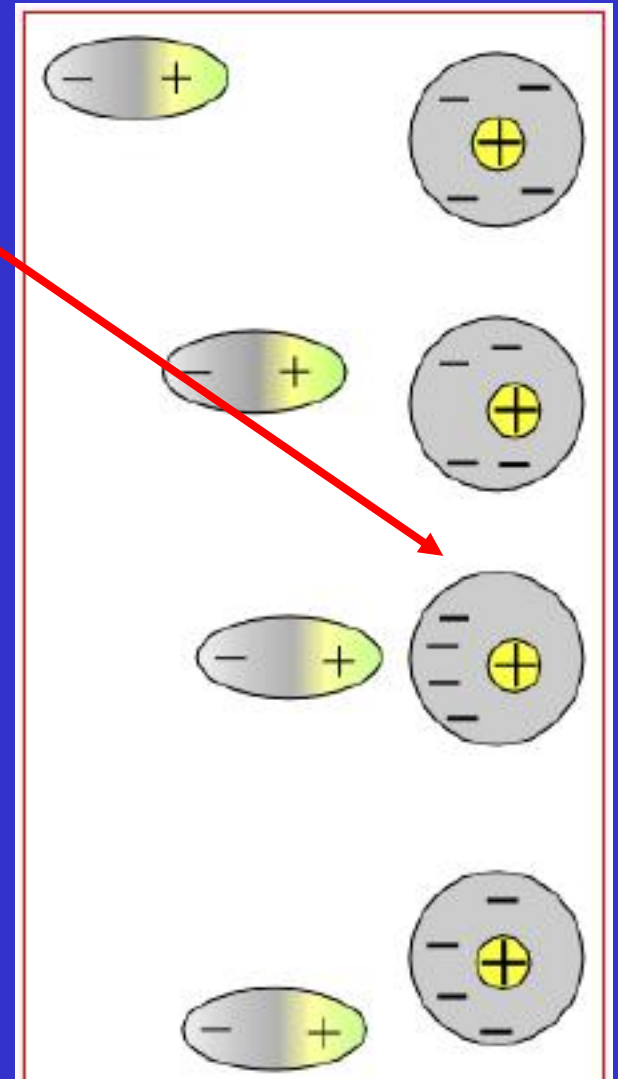
E = energie interakce

q = náboj

α = polarizovatelnost

μ = dipolový moment

r = vzdálenost

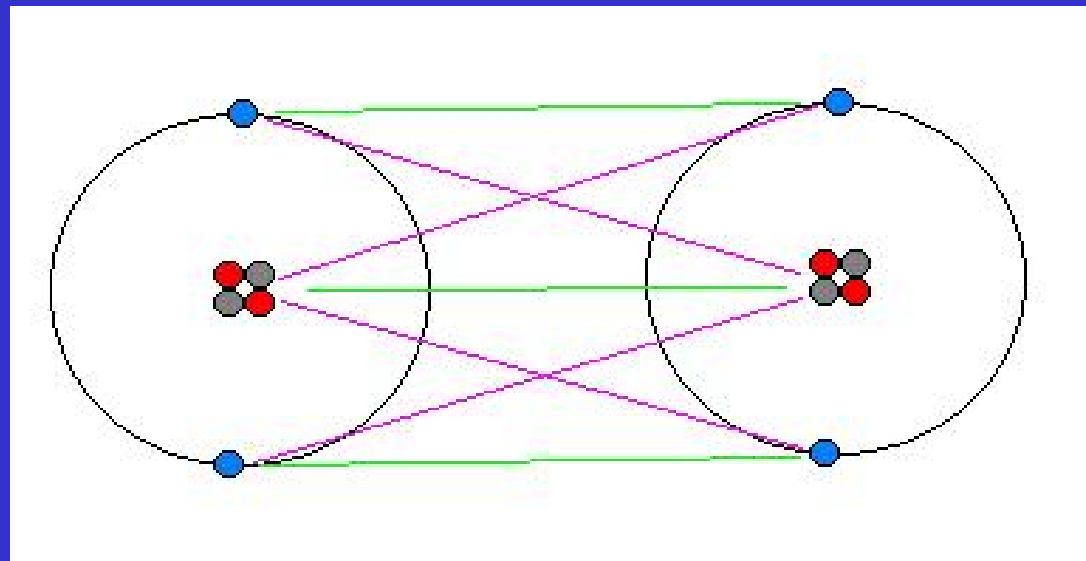


Polarizovatelnost, α , m³

Skupina	Polarizovatelnost, cm ³ 10 ²⁴	v.d.W poloměr, Å	Atomový poloměr, Å
O	0.63	1.5	0.66
CH ₂	1.80	2.0	-
S	3.00	1.8	1.04

Molekula	Polarizovatelnost (Å ³)	T _{varu} (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 ₂ O	1.48	373.15	1.85
H ₂ S	3.64	212.82	1.10
CCl ₄	10.5	349.85	0
C ₆ H ₆	25.1	353.25	0
CH ₃ OH	3.0	338	1.71
CH ₃ F	3.84	195	1.81
CHCl ₃	8.50	334.85	1.01

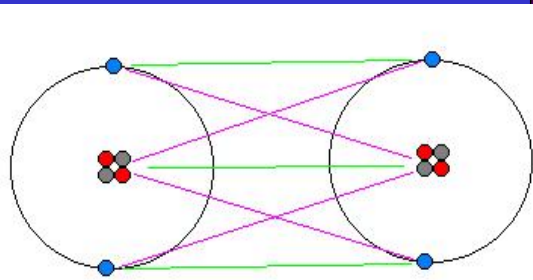
Interakce indukovaný dipol – indukovaný dipol



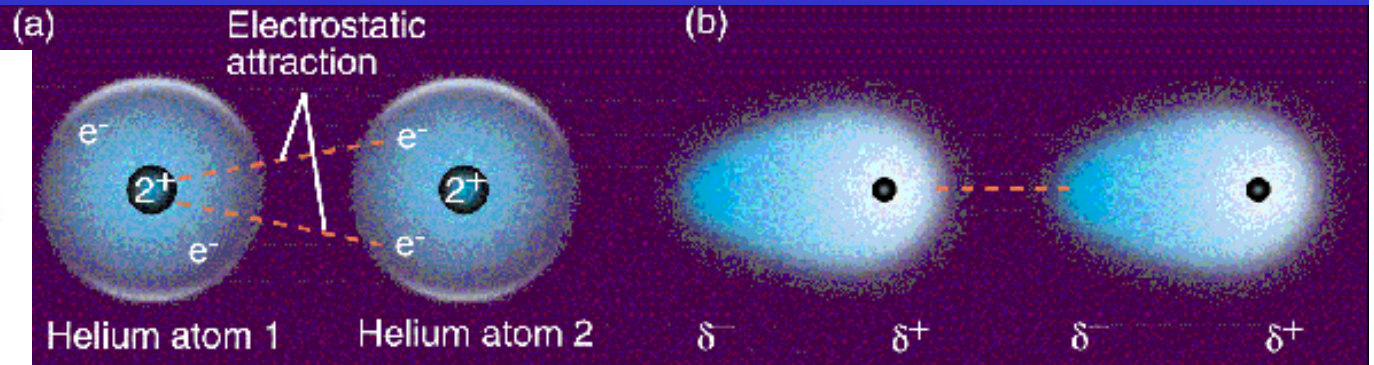
Odpudivé síly

Přitažlivé síly

Londonovy disperzní síly



— Repulsive forces
— Attractive forces



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

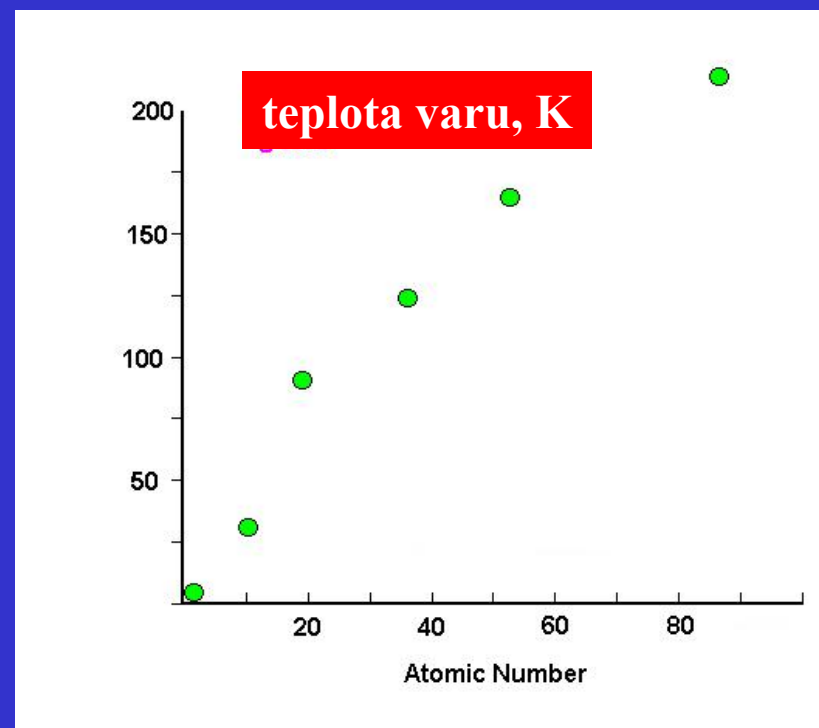
IE = ionizační energie
 α = polarizovatelnost
 r = vzdálenost



Vliv polarizovatelnosti molekuly na velikost Londonových sil

Vliv Londonových sil na
skupenství halogenů a
vzácných plynů

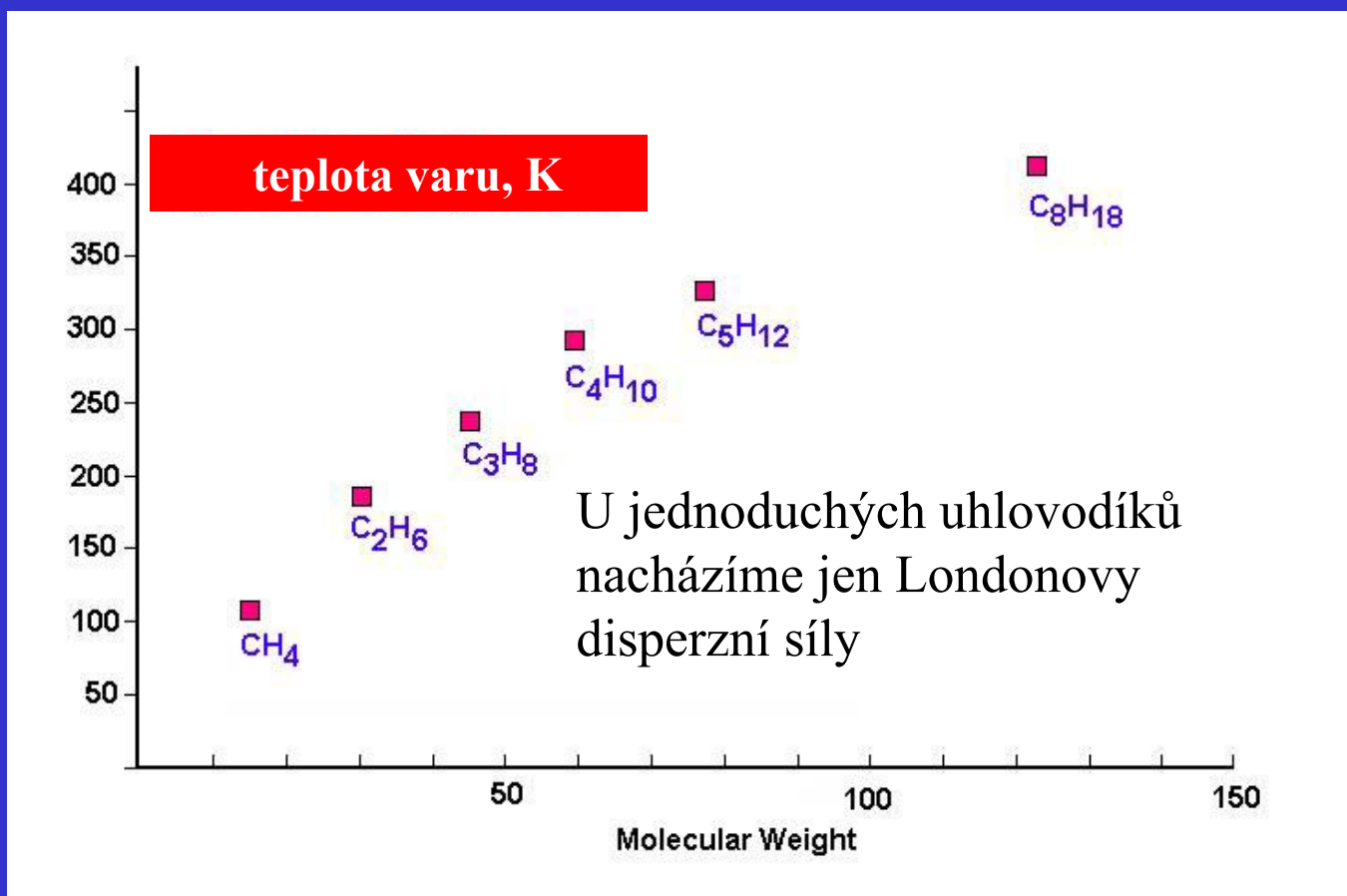
S velikostí molekul roste
polarizovatelnost



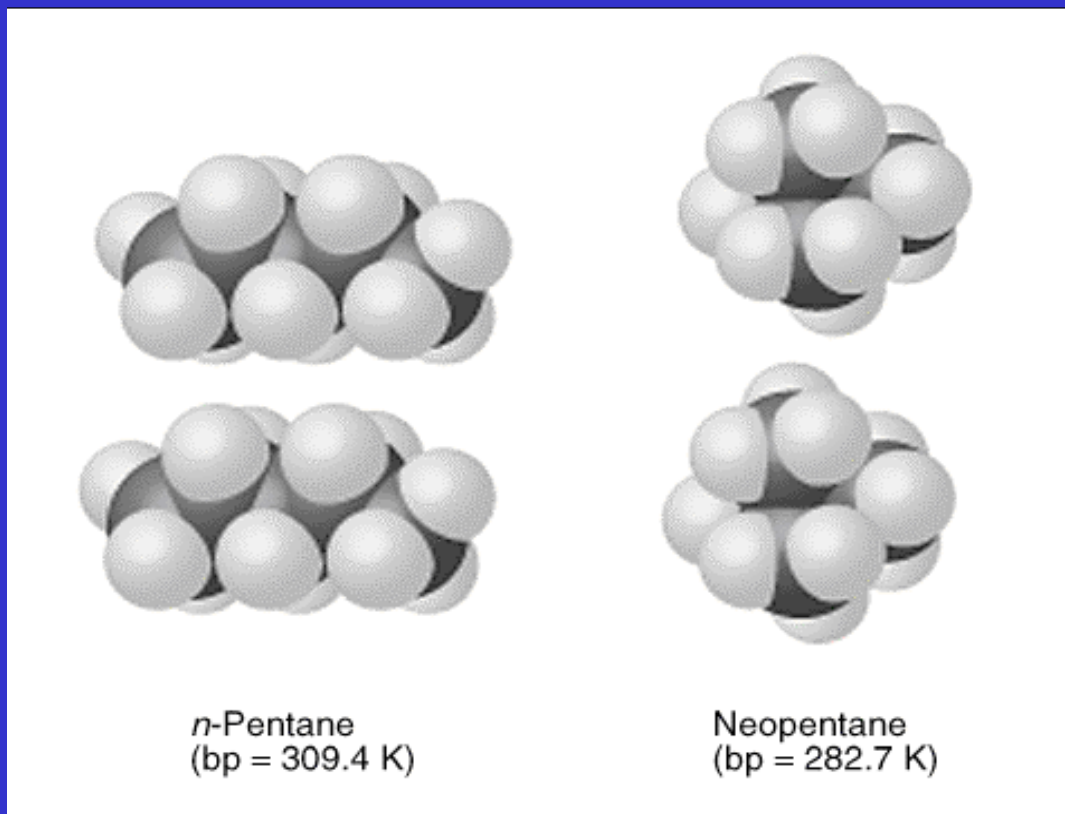
	teplota varu, K
F_2	85.1
Cl_2	238.6
Br_2	332.0
I_2	457.6

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

Vliv velikosti molekuly na velikost Londonových sil



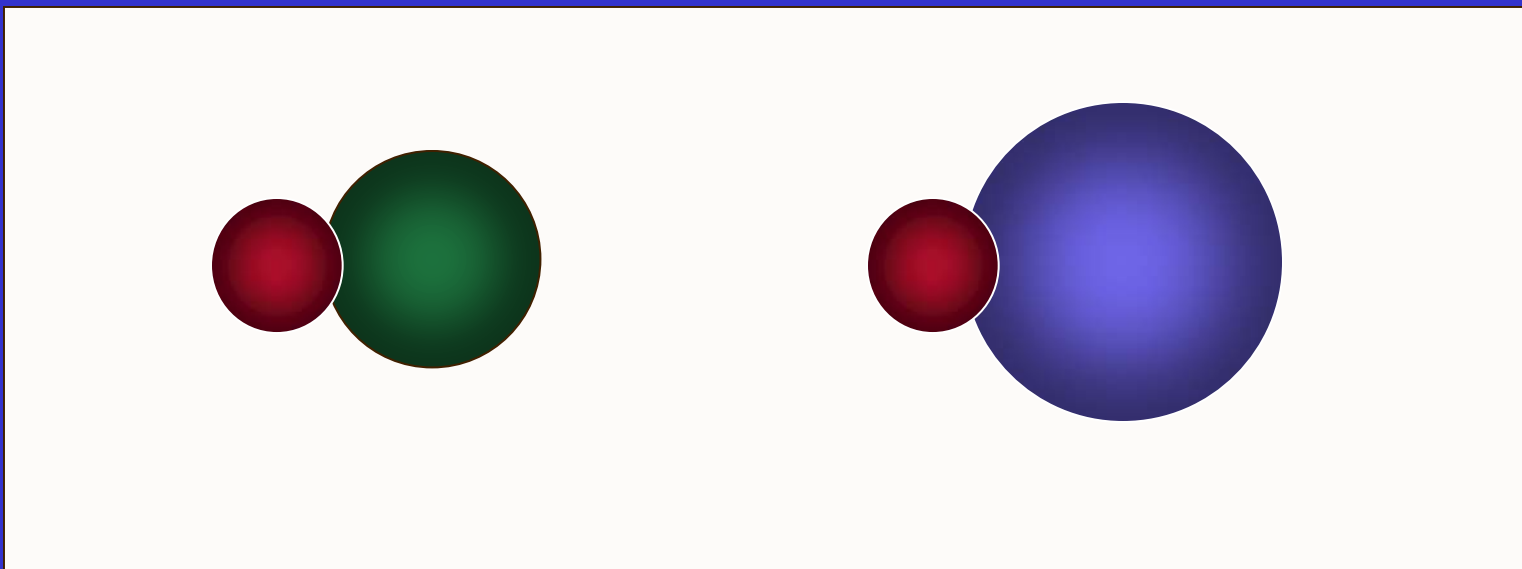
Vliv tvaru molekuly na velikost Londonových sil



Stejná M_r

Větší plocha dotyku

Londonovy disperzní síly a dipol-dipolové interakce

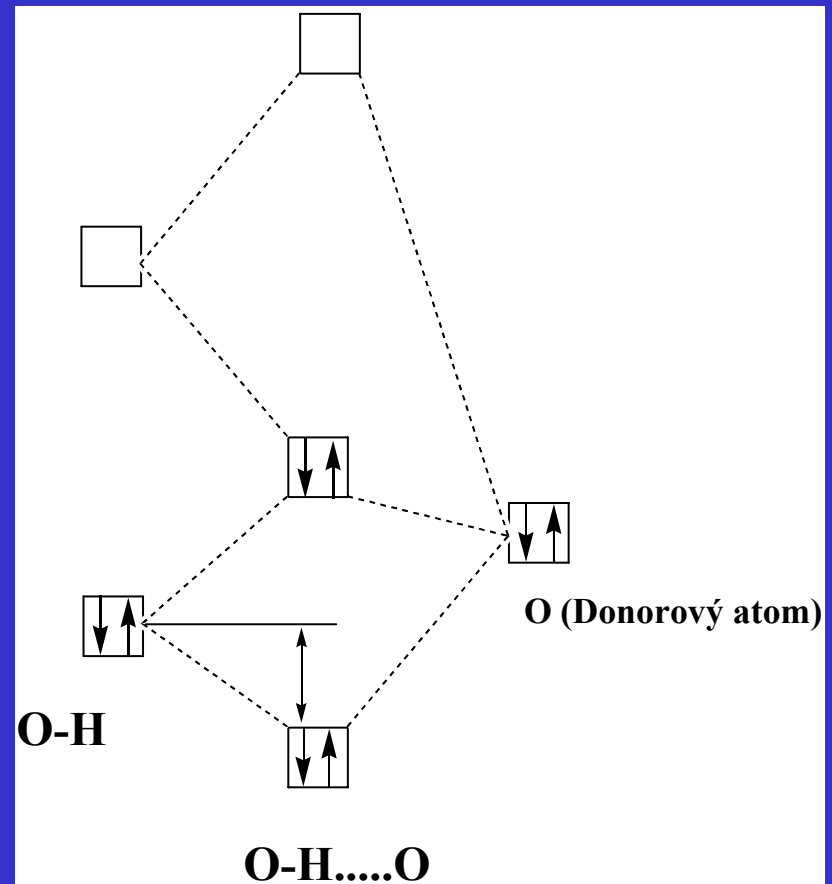
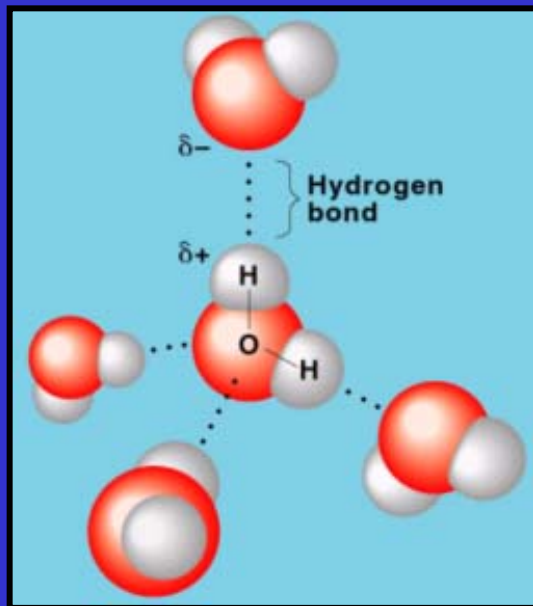


HCl: $b_v = 189.5 \text{ K}$
Dipolový moment = 1.03 D

HBr: $b_v = 206.2 \text{ K}$
Dipolový moment = 0.79 D

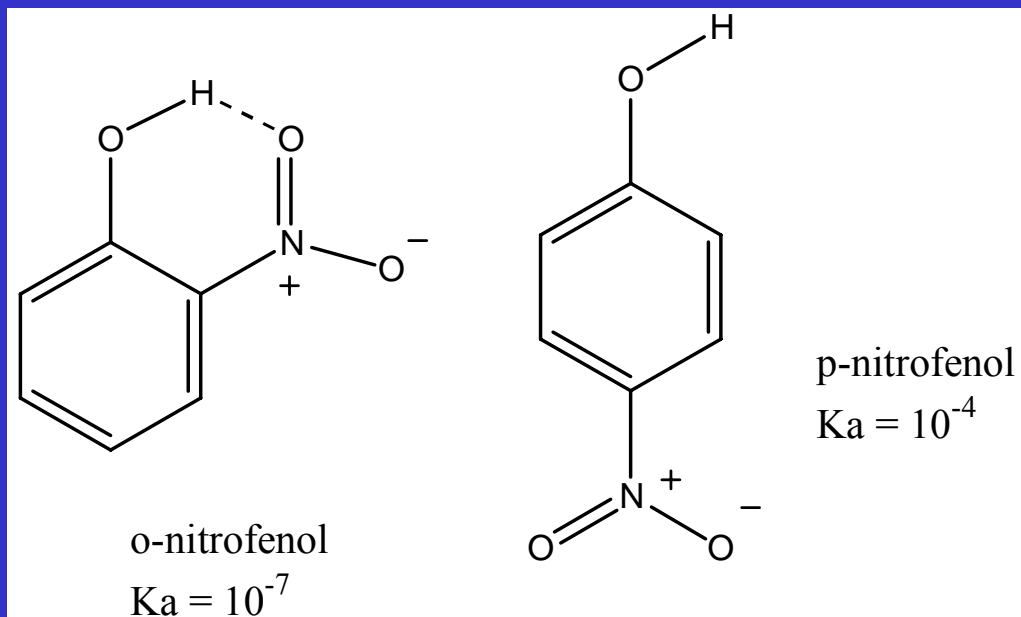
Vodíková vazba

H s elektronegativními atomy (F, O, N, C,...)



Vodíková vazba

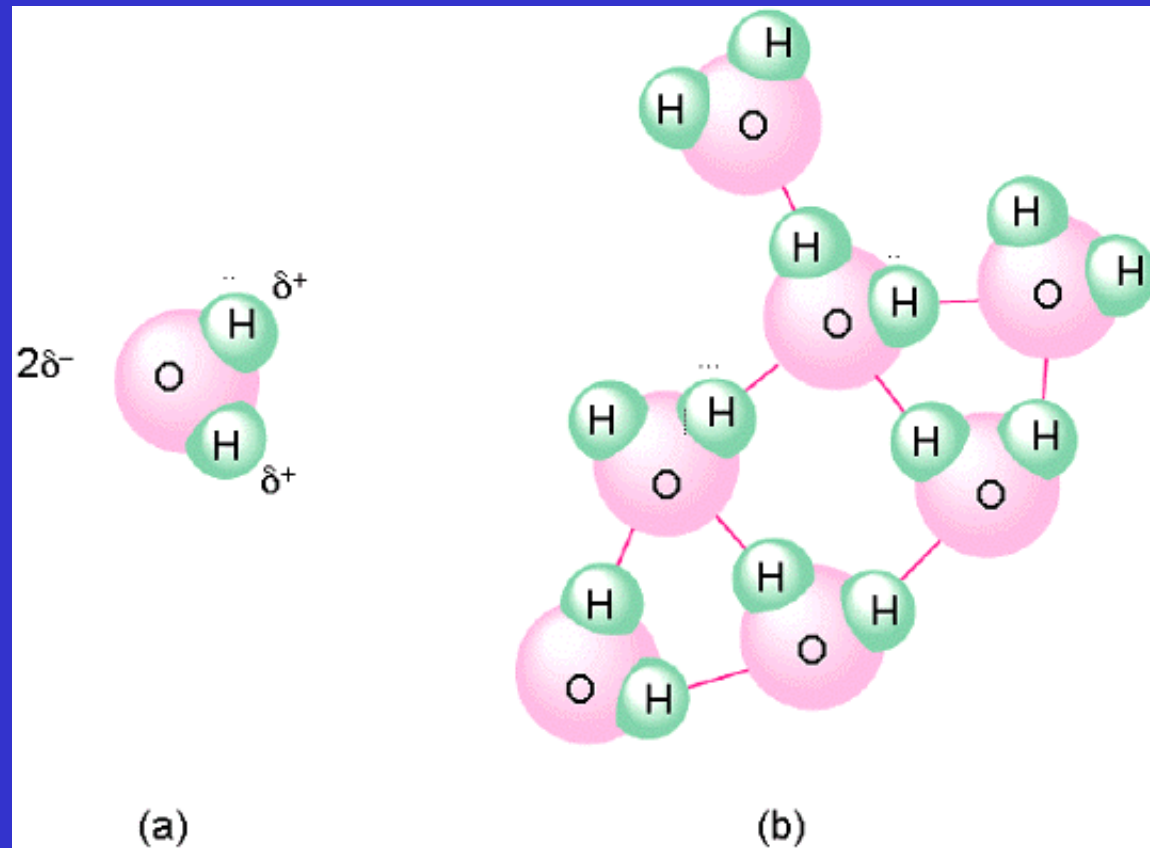
Intramolekulární vodíková vazba



Snížená kyselost OH skupiny
v důsledku tvorby vodíkové vazby

Vodíková vazba

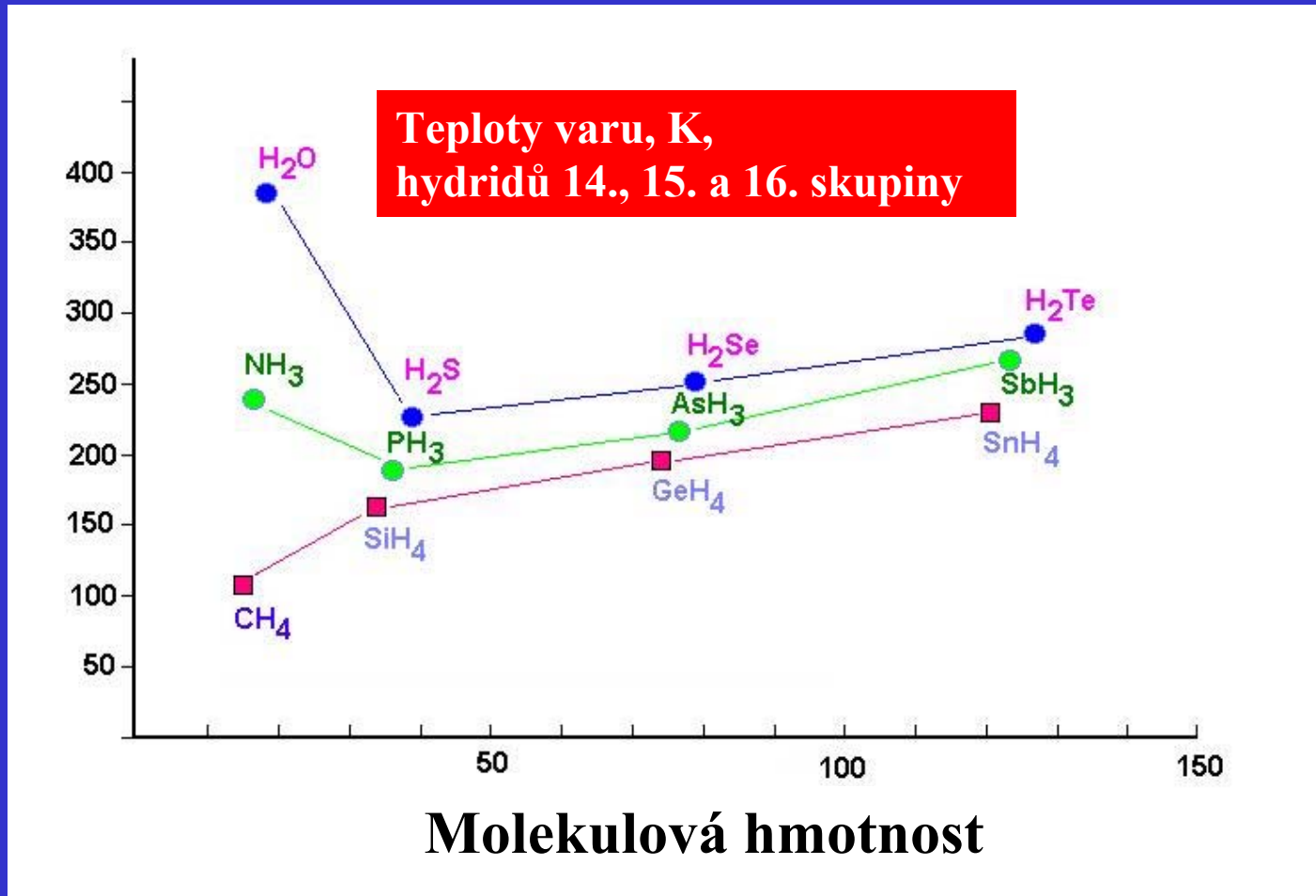
Intermolekulární



Vodíková vazba

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

Vodíková vazba



HF_2^- hydrogendifluorid

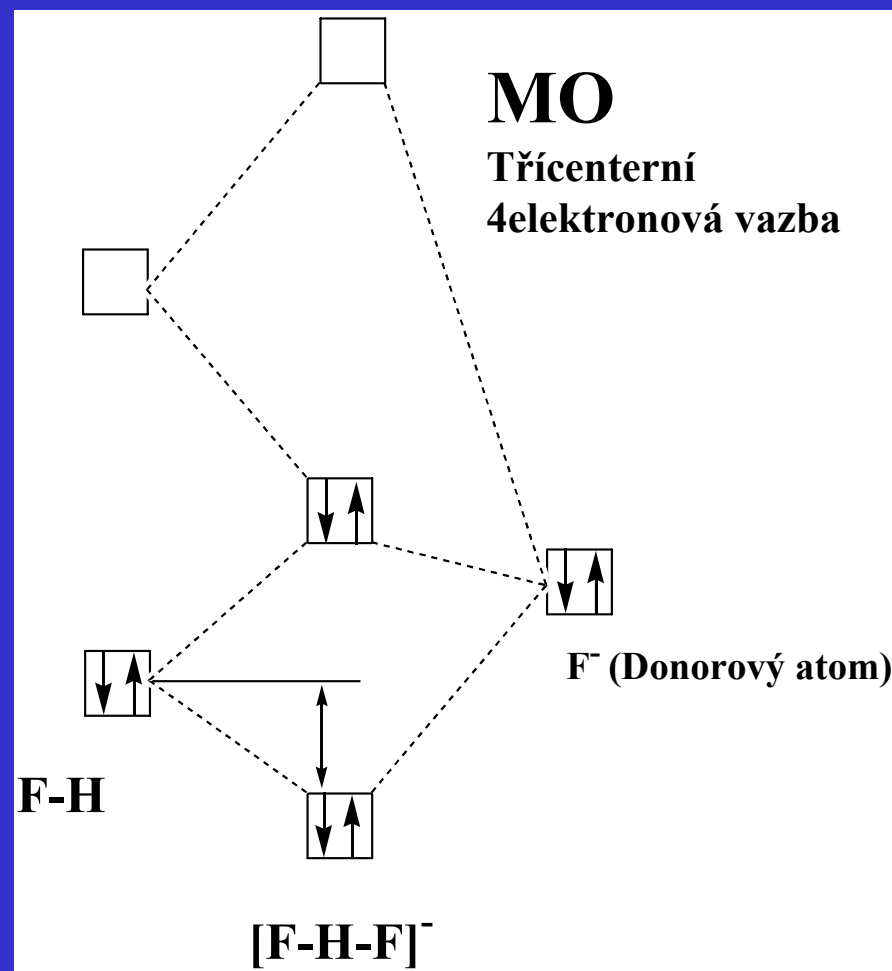
Nejsilnější známá H-vazba

155 kJ mol^{-1}

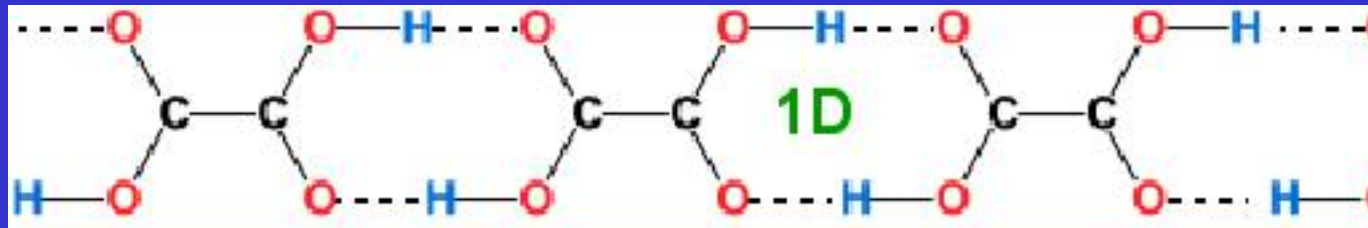
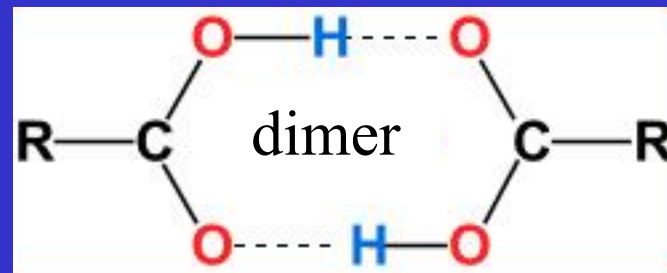
Symetrické rozložení
vazebných délek H-F 114 pm

Vazebný úhel
 $\text{F-H-F} = 180^\circ$

Autodisociace HF
 $2 \text{ HF} \leftrightarrow \text{H}_2\text{F}^+ + \text{HF}_2^-$



Vodíková vazba



Krystalové inženýrství
Samouspořádání

Struktura HF

1D. HF

Ortorrómbico: B mmb

a (Å) 3.42

b (Å) 4.32

c (Å) 5.41

V (Å³) 79.9

Z 4

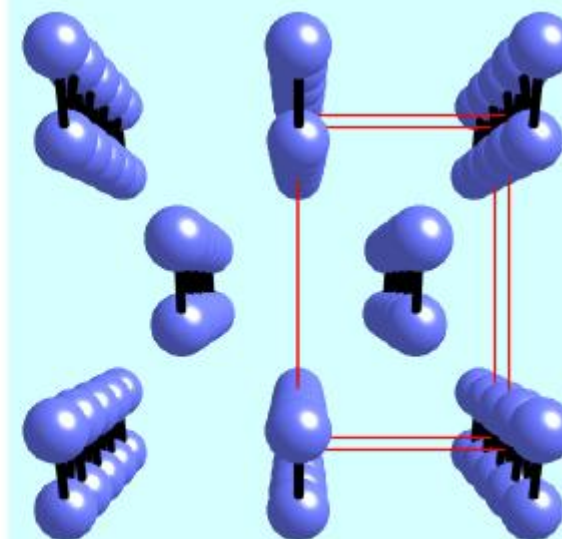
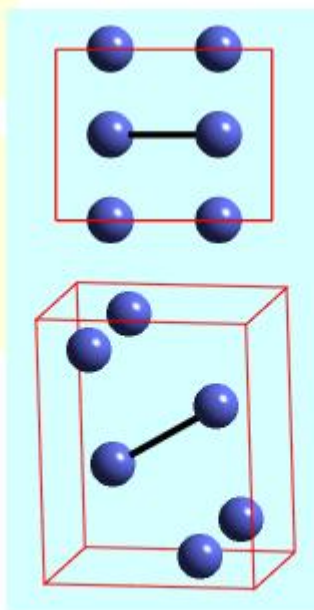
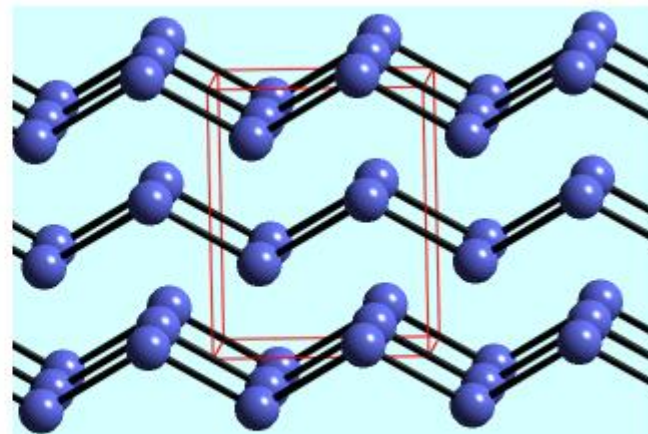
Dx (gcm⁻³) 1.66

F-H (Å) -

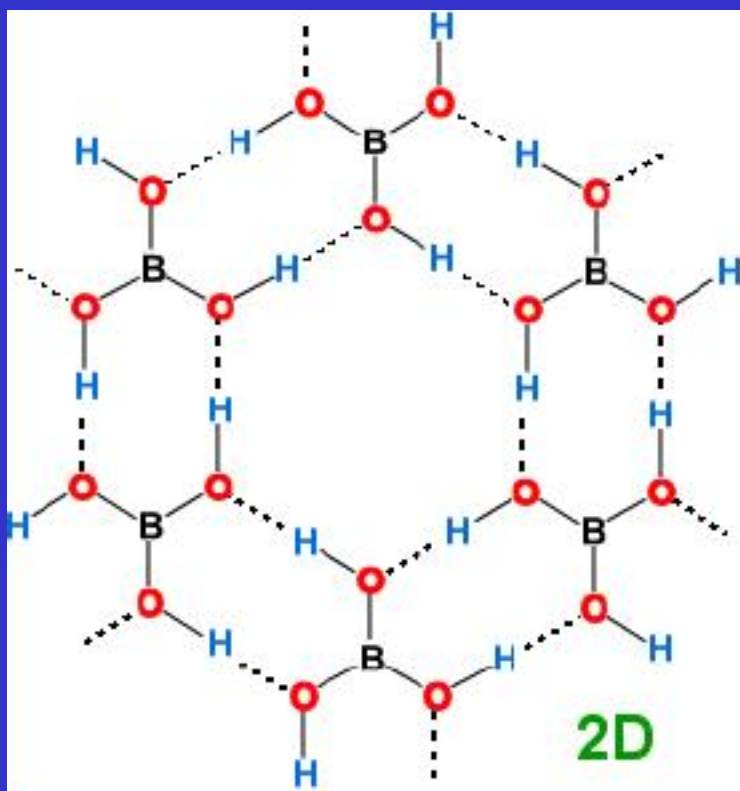
F...F (Å) 2.49

H...F (Å) -

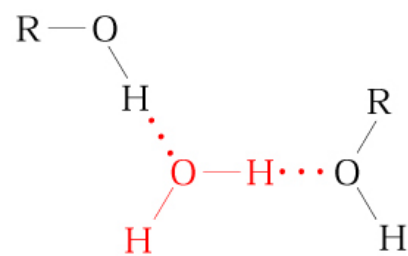
F-H...F (°) 180°



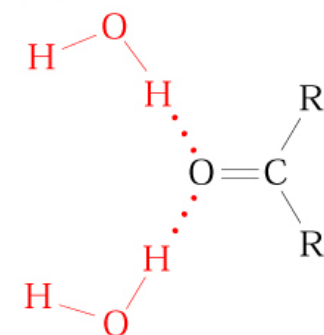
Kyselina boritá



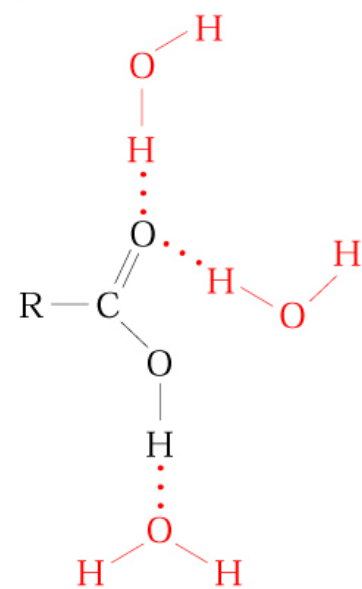
(a)



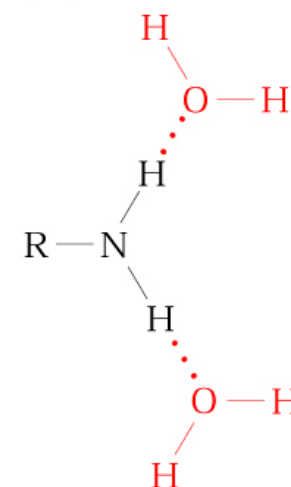
(b)



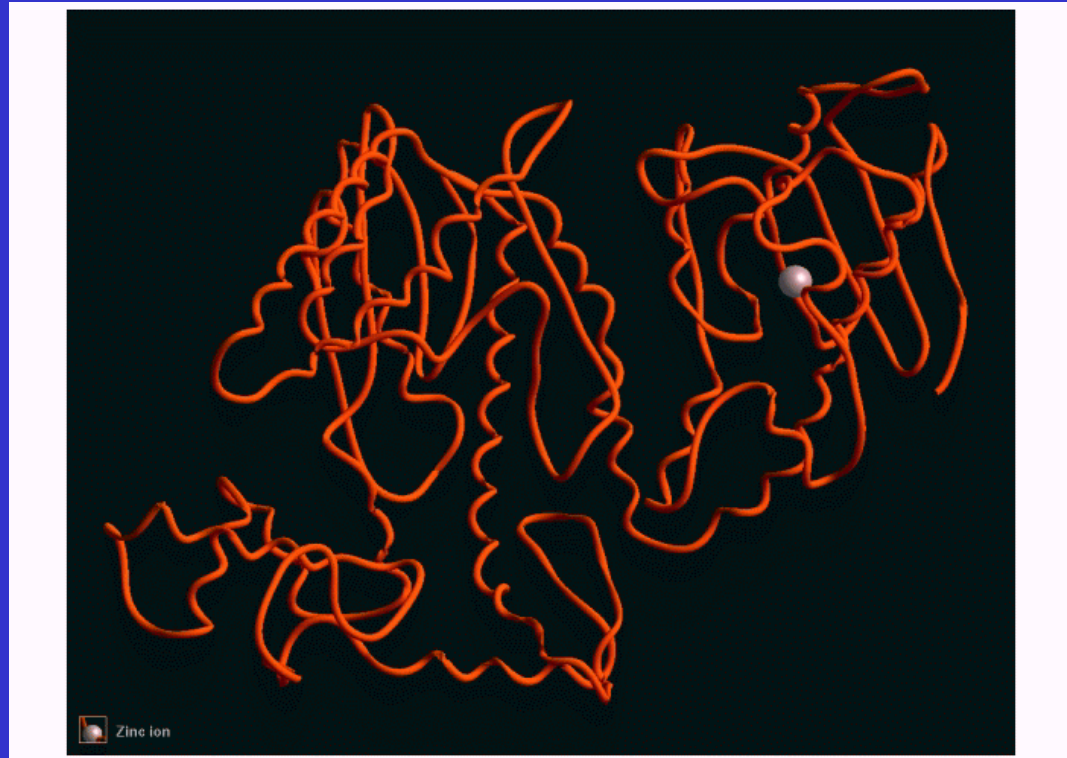
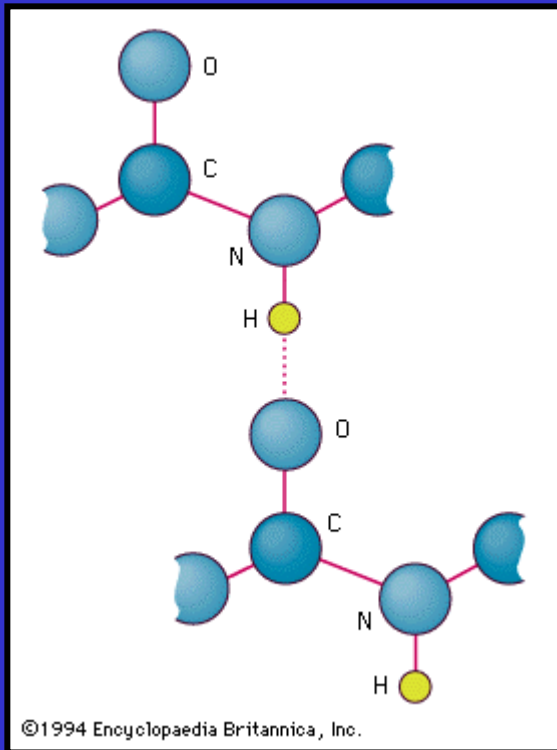
(c)



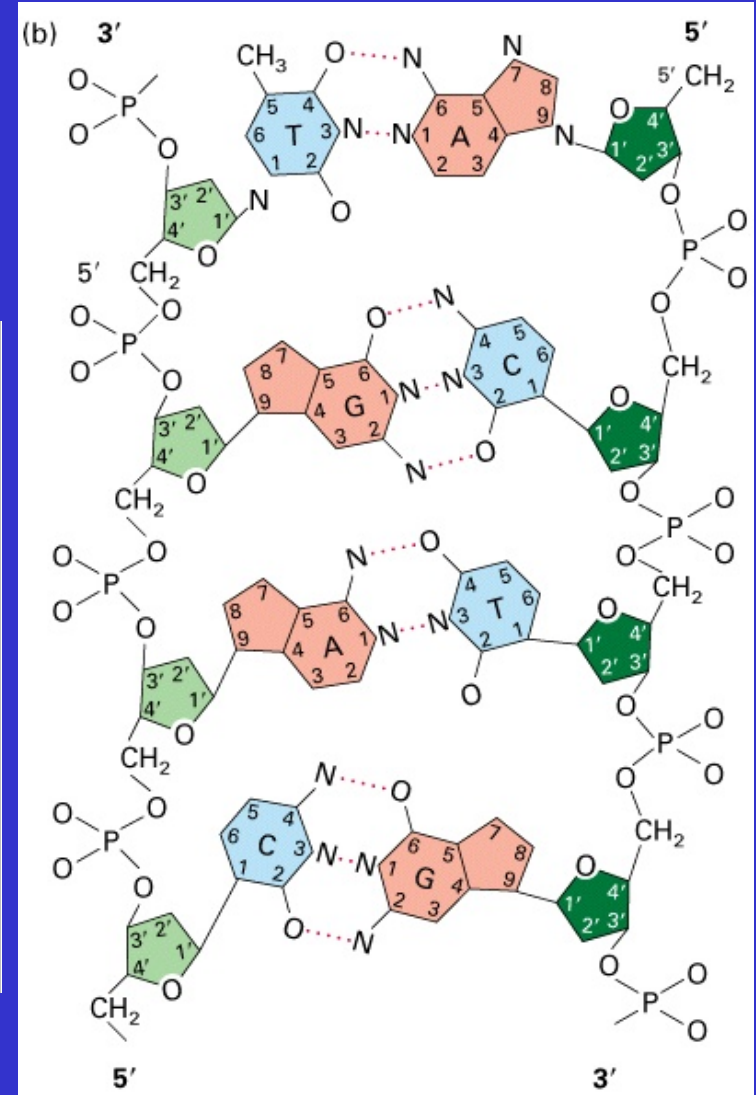
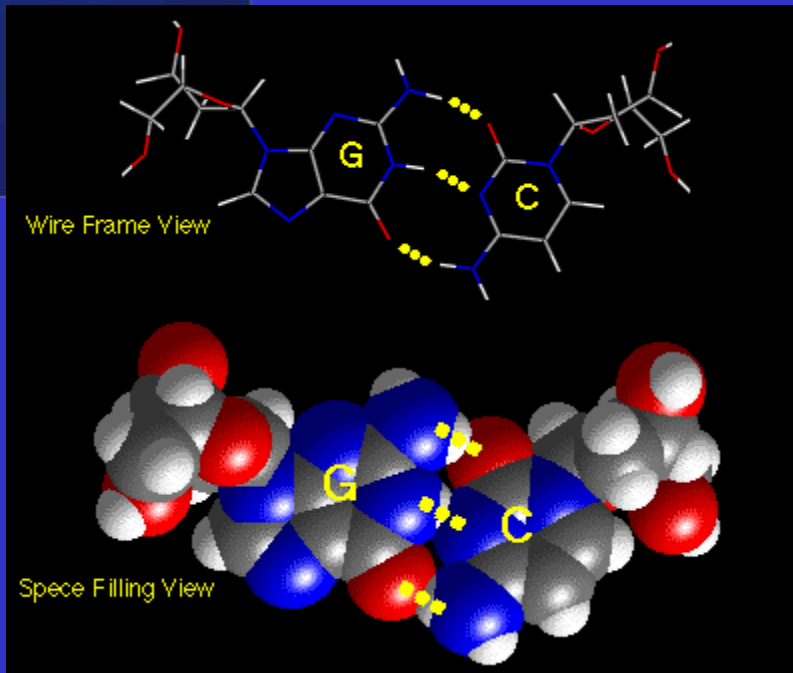
(d)

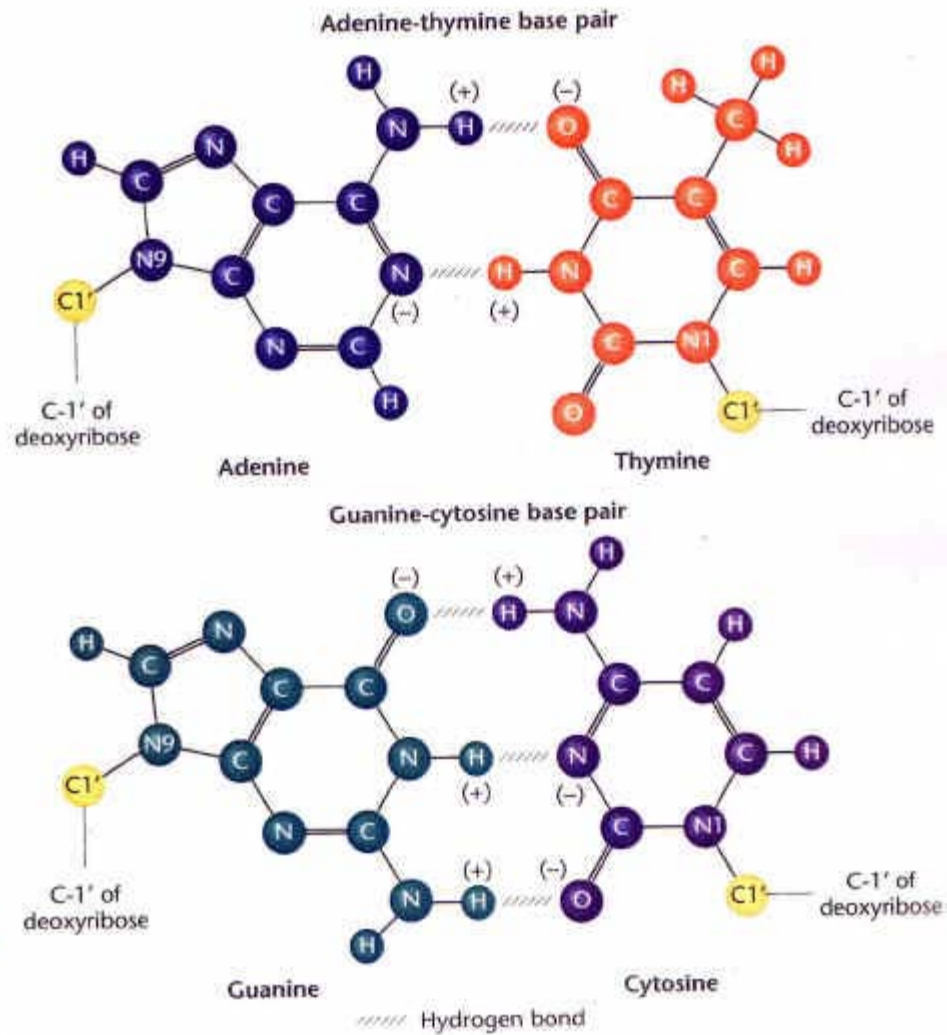
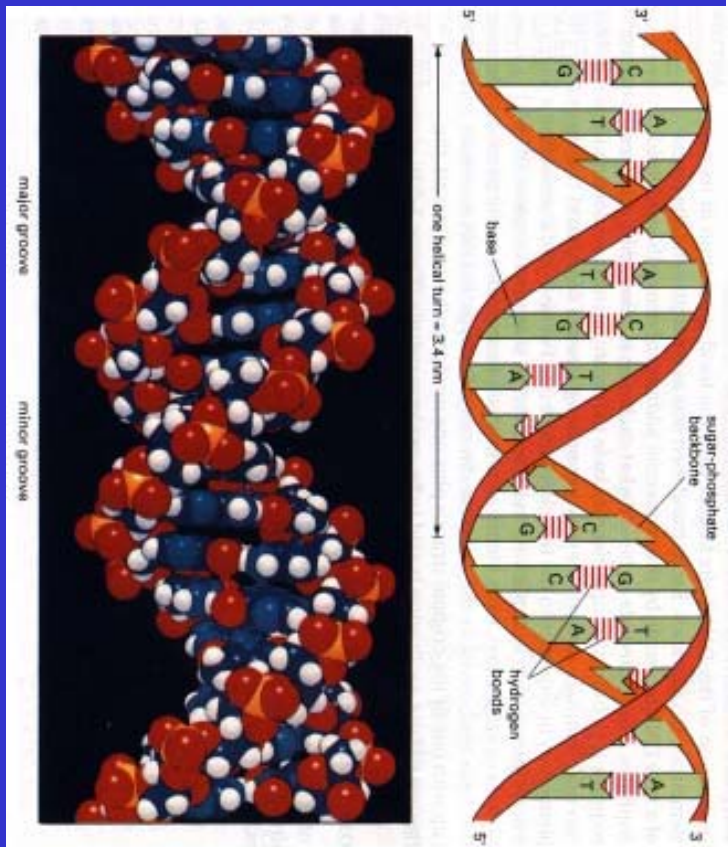


Struktura proteinů



Struktura DNA





Struktura ledu

3D. H₂O

Hexagonal: P6₃/mmc

a (Å) 4.5227

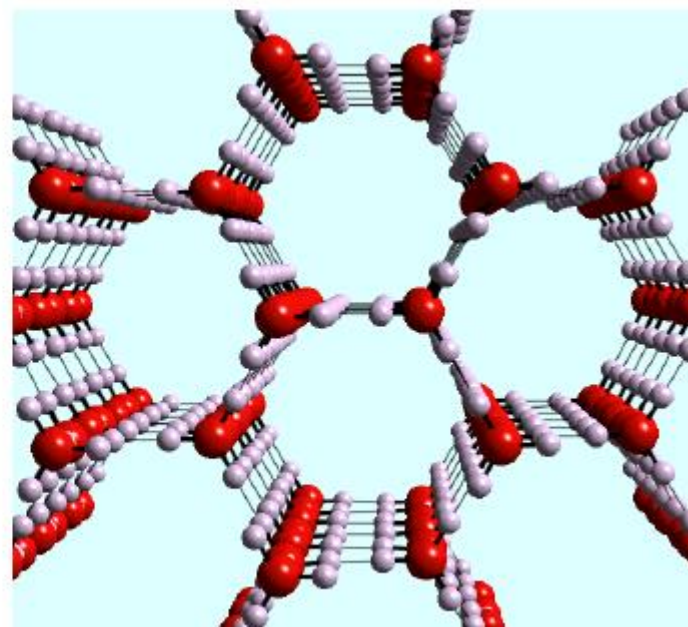
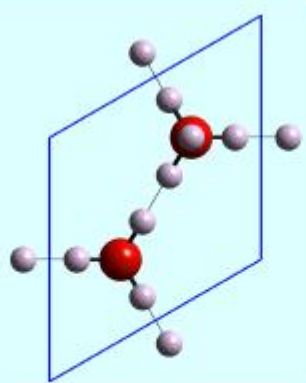
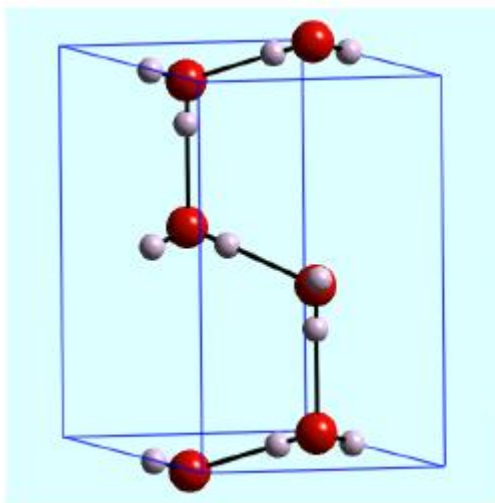
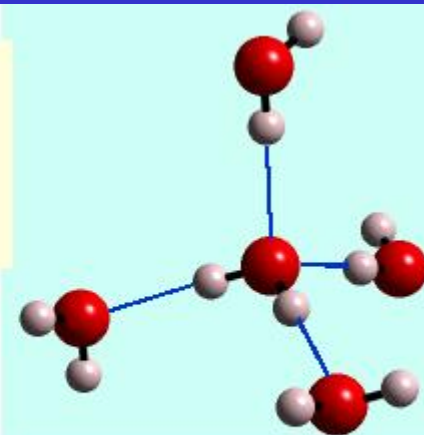
c (Å) 7.3671

V (Å³) 121.9

Z 3

Dx (gcm⁻³) 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°



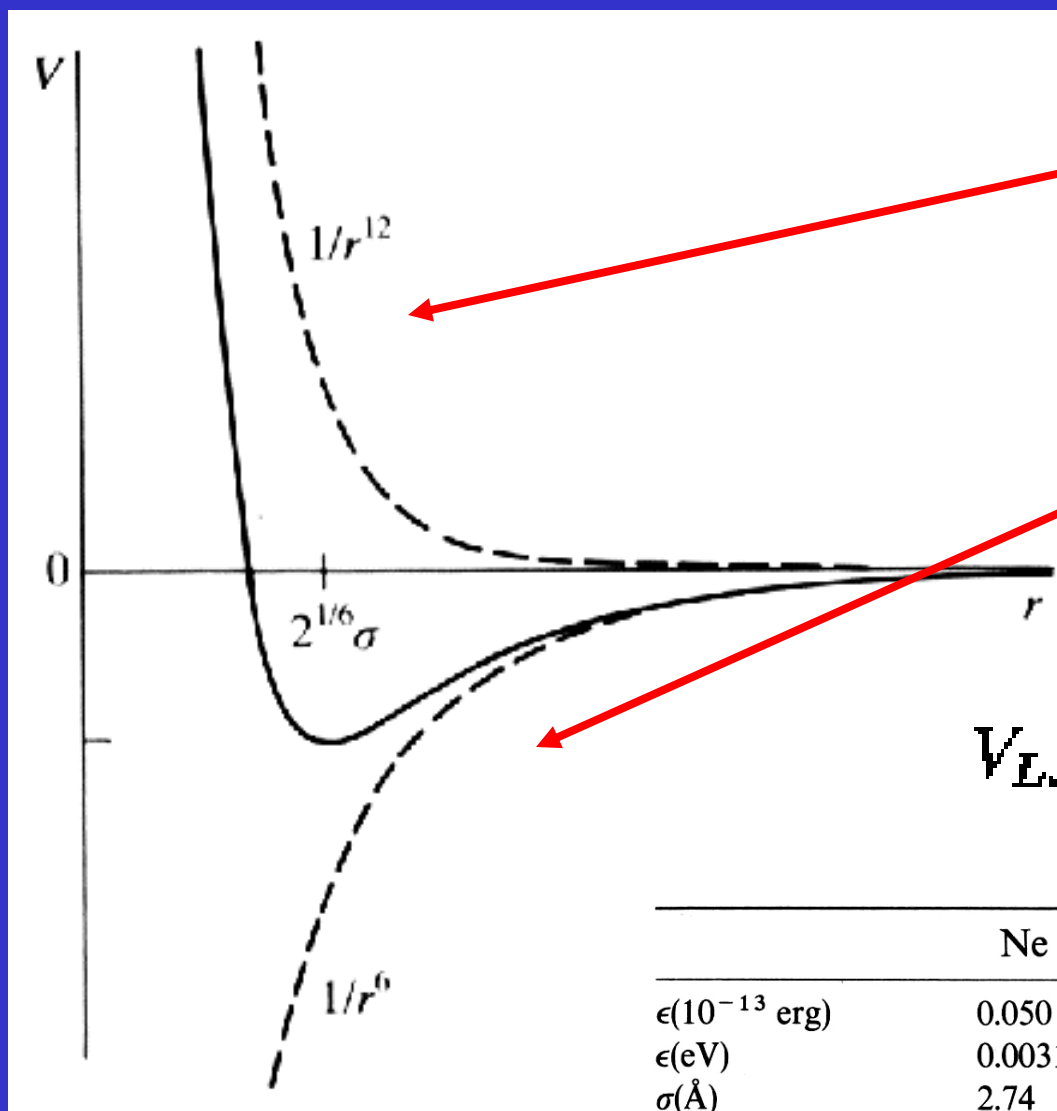
Rovnováha přitažlivých a odpuzivých sil

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

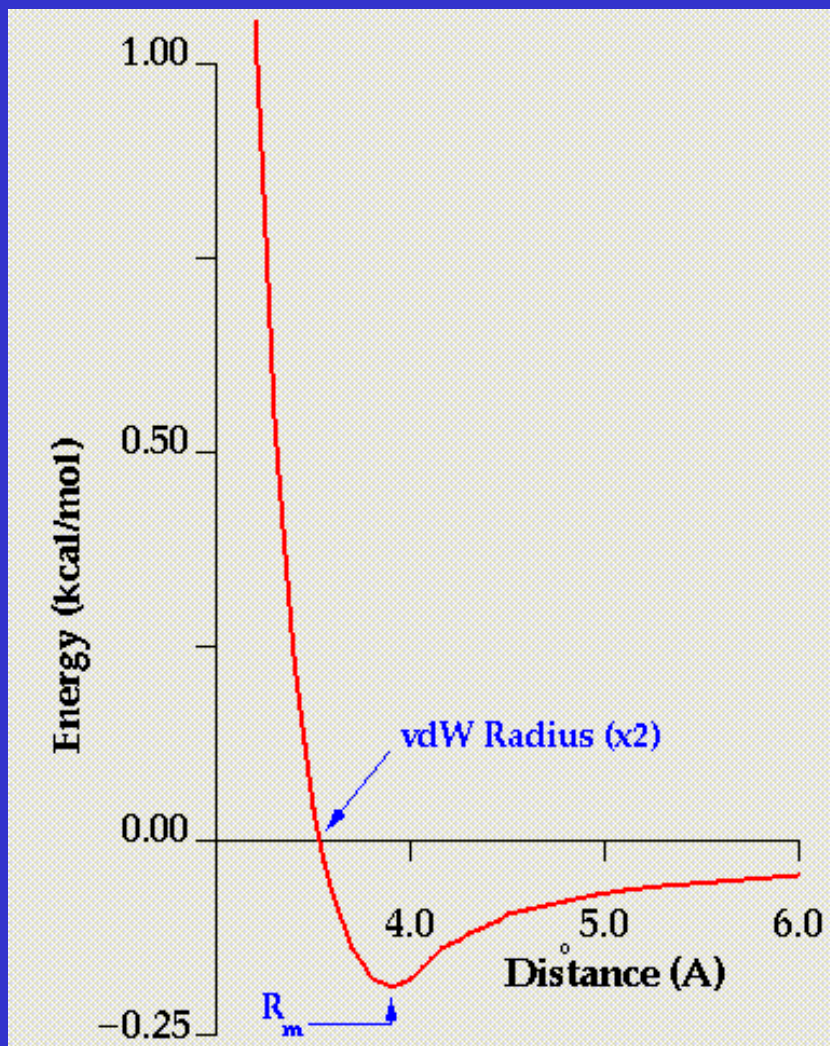
Přitažlivé síly
 $E = 1/r^6$

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 _m
C atom		
- alifat	1.7 Å	2.0 Å
- aromati	1.7 Å	
O atom		
- karbonyl	1.4 Å	1.9 Å
- alkohol	1.5 Å	
N atom		
- amid	1.52 Å	1.80 Å
- amin	1.65 Å	
- ammonium	1.50 Å	
F atom	1.35 Å	
Cl atom	1.80 Å	
Br atom	1.95 Å	
I atom	2.15 Å	
S atom	1.85 Å	

Van der Waalsovy poloměry, Å

Atomový poloměr O 0.73 Å

Iontový poloměr O²⁻ 1.40 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		