

Универзитет у Београду

Факултет за физичку хемију

Nove fizičko-hemijske metode

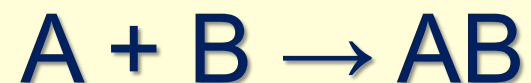
NEKOVALENTNE INTERAKCIJE

Milena Petković

predmet: Nove fizičkohemijske metode
predavanje: Nekovalentne interakcije

?

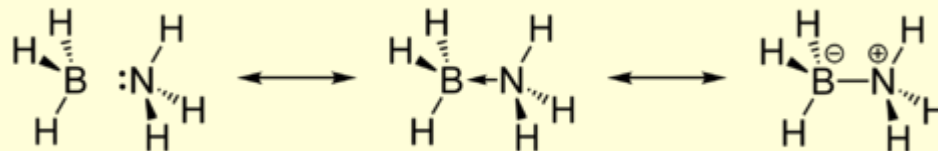
Luisova kiselina i Luisova baza



A – Luisova kiselina (akceptor elektronskog para)

B – Luisova baza (donor elektronskog para)

AB – sistem sa nekovalentnim interakcijama



Nekovalentne interakcije (NI)

Sistemi sa nekovalentnim interakcijama:

jedinjenja koja formira bar jedan par Luisove kiseline i Luisove baze.

poreklo informacija o NI:

- eksperiment (kristalne strukture, spektroskopija)
- teorijski proračuni → kooperativnost

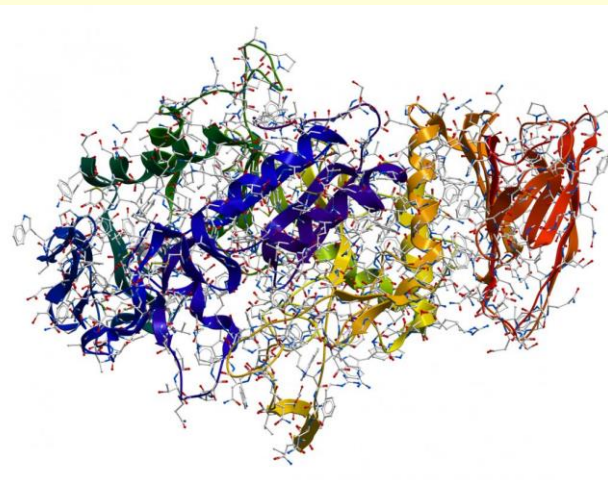
Analizirani sistemi u čvrstom i gasovitom stanju.

Problem: rastvori

Najpoznatiji predstavnici NI:

- vodonične veze
- steking interakcije

Vodonične veze: značaj



Vodonične veze: donori i akseptori

donori vodonika

atomi velike elektronegativnosti: O, N i F

- svi halogeni elementi
- većina halkogenih elemenata
- većina pnikogenih elemenata
- atomi pojedinih metala

akseptori vodonika

atomi sa slobodnim e^- parovima: O, N i F

- sistemi sa πe^-
- pojedine σ veze
- ...



- 1) dokaz da je formirana veza;
- 2) dokaz da se ova veza ostvaruje preko H koji je već vezan za D.

Vodonične veze: uzroci stabilnosti

- elektrostatičke interakcije
- perturbacija elektronske strukture dveju vrsta pri njihovom približavanju
(**unutrašnja** – pomeraj naelektrisanja; **spoljašnja** – prenos naelektrisanja)

kovalentni doprinos
- disperzione interakcije
- sterna odbijanja

Primer: CH...O

povećanje polarnosti C-H veze

- promena hibridizacije C atoma, $sp^3 \rightarrow sp$ ($HC\equiv CH$, $N\equiv CH$)
- supstituenti na C atomu koji privlače elektrone (peptidne grupe u proteinima)

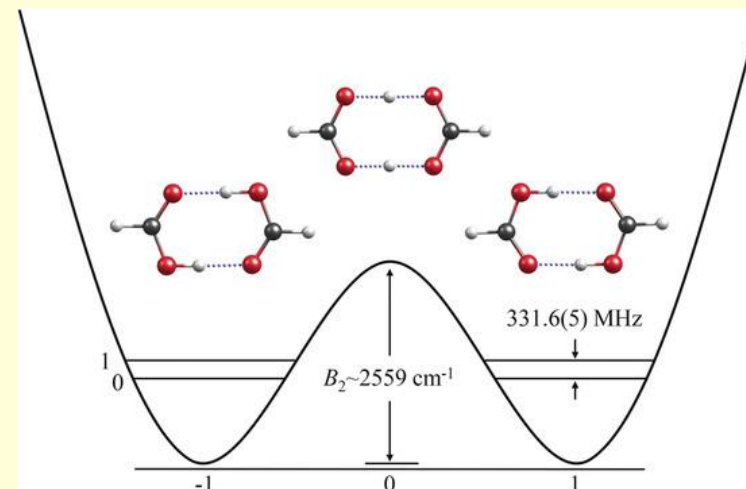
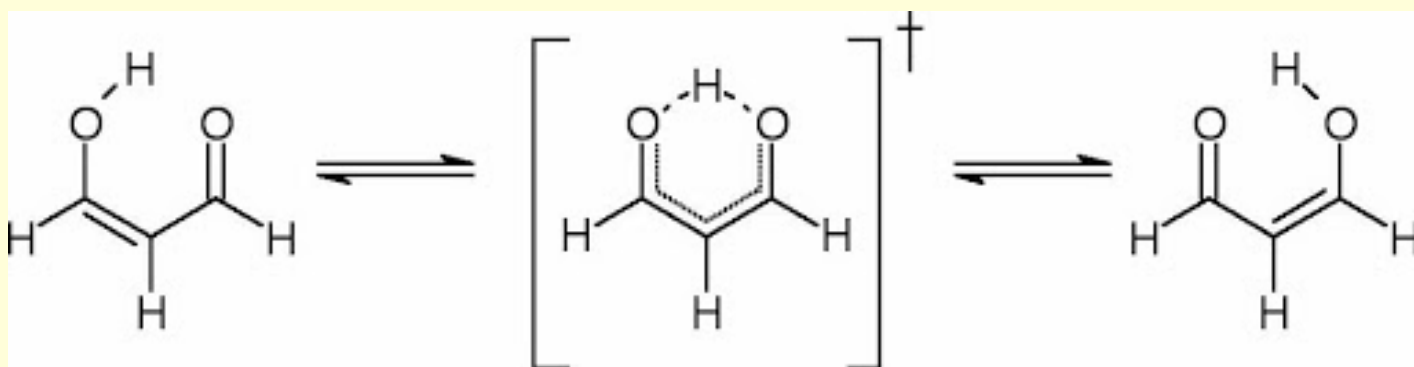
značaj:

- struktura
- mehanizmi enzimskih reakcija
- ...

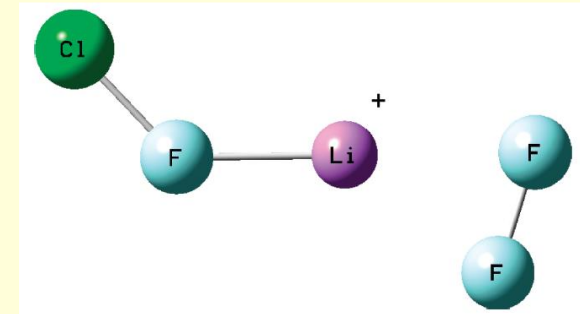
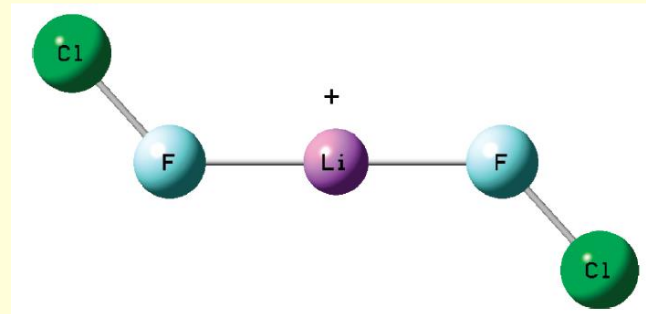
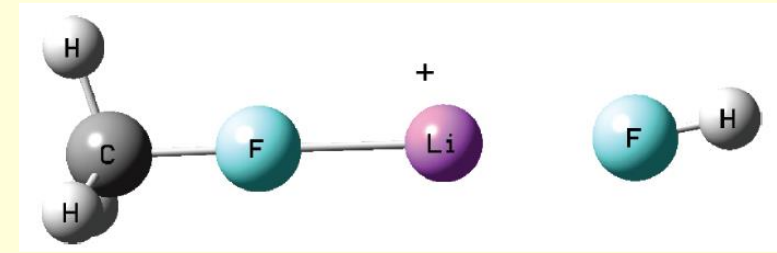
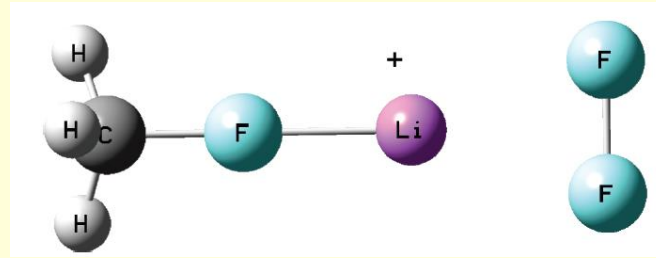
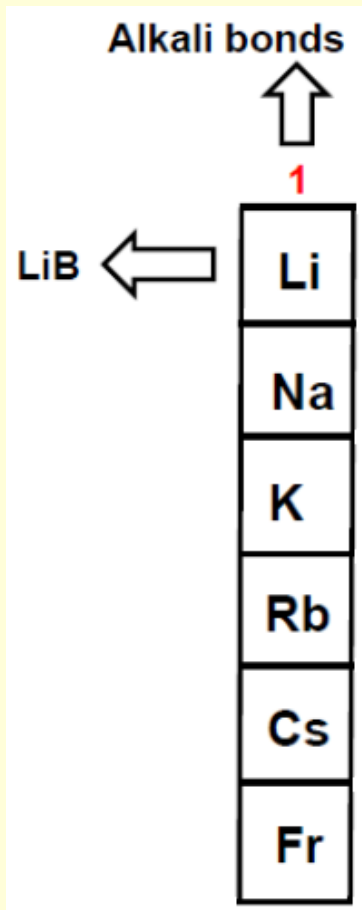
Vodonične veze: prenos H

prenos:

- vodonika ili protona
- intramolekulski i intermolekulski
- u osnovnom i u pobuđenim elektronskim stanjima
- jednostruki ili dvostruki
- simetričan i asimetričan
- ...



Alkalne veze



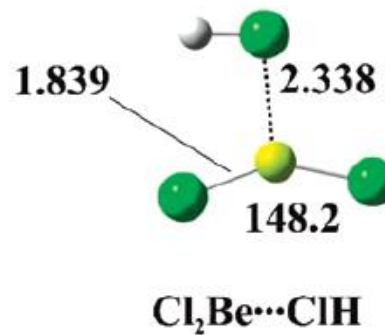
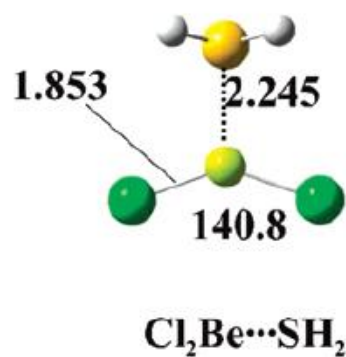
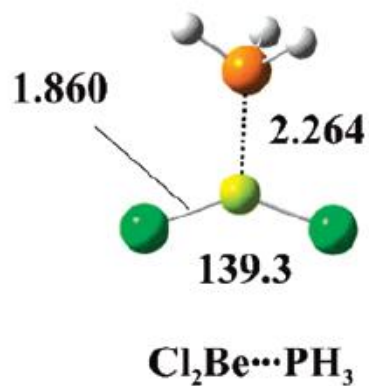
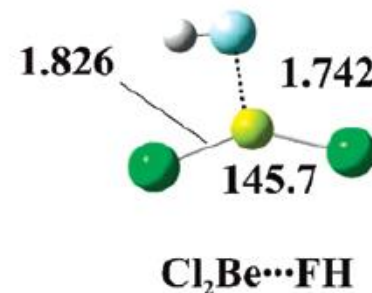
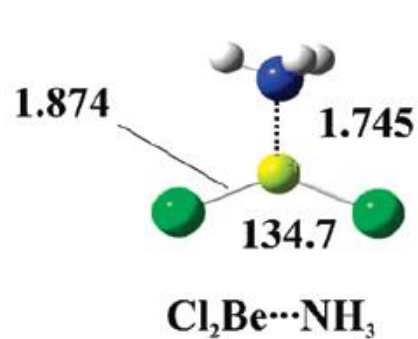
Zemnoalkalne veze

Alkaline earth bonds



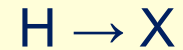
2

Be
Mg
Ca
Sr
Ba
Ra



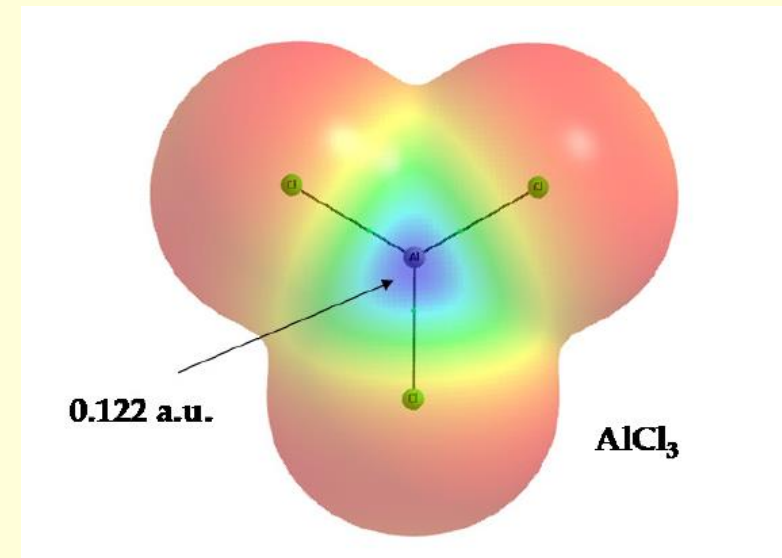
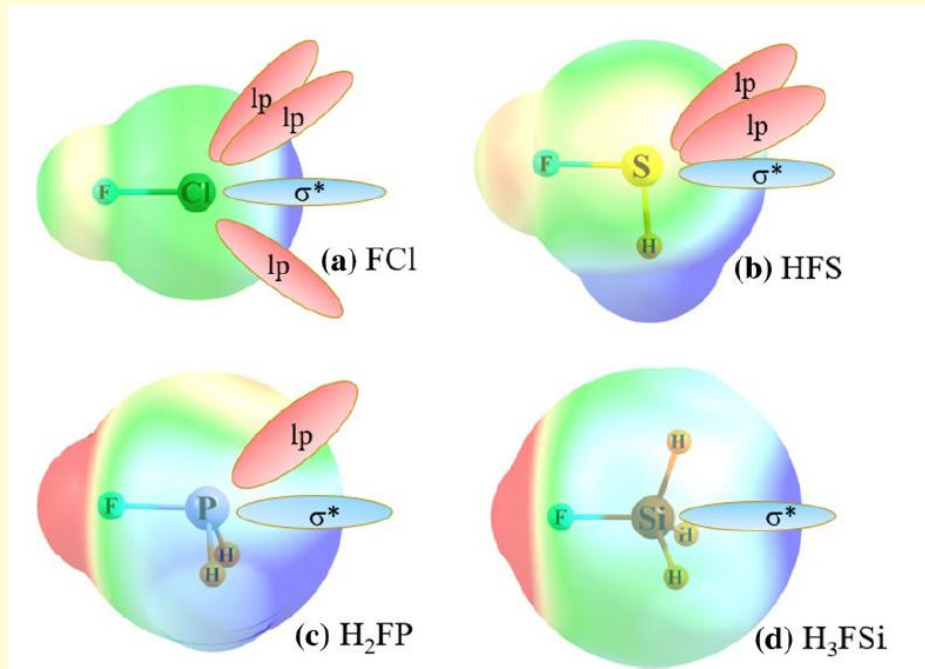
Nova definicija → nove interakcije

Vodonična veza: interakcija koja uključuje **premošćujući** atom vodonika.



X atom 14-18. (13) grupe periodnog sistema i ima anizotropnu raspodelu naelektrisanja

↓
 σ (π) šupljina



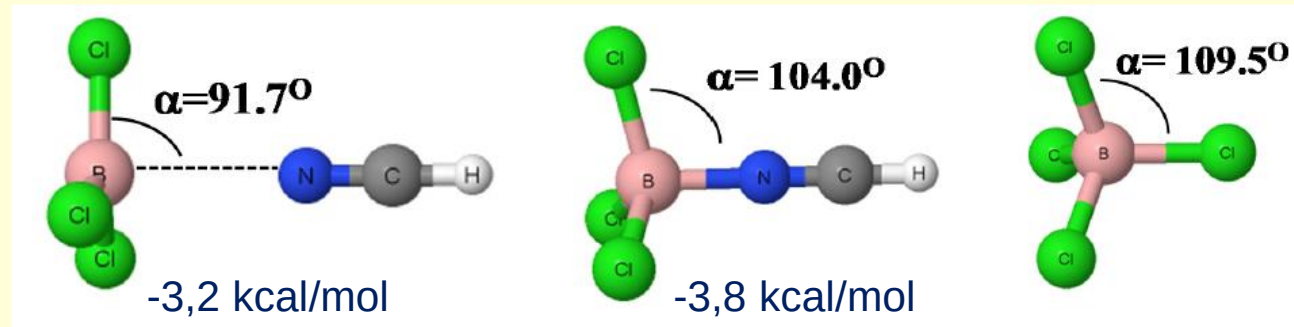
Trielne veze

Triel
bonds



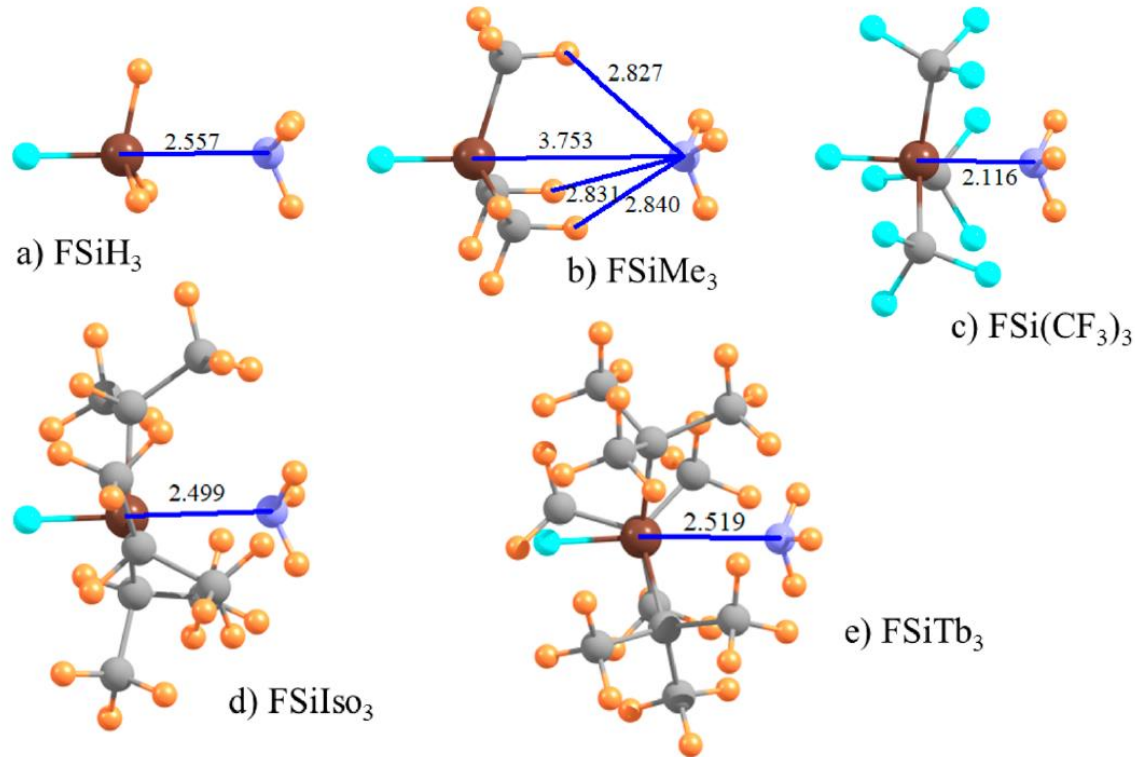
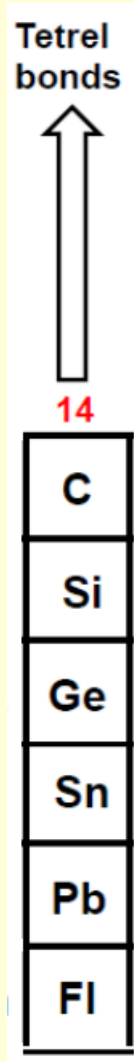
13

B
Al
Ga
In
Tl
Nh



Sistem	Energija veze kcal/mol
$\text{BCl}_3 \cdots \text{N}_2$	-1,5
$\text{AlH}_3 \cdots \text{NCH}$	-17,7
$\text{BH}_3 \cdots \text{NH}_3$	-30,8
$\text{AlCl}_3 \cdots \text{NH}_3$	-38,8
$\text{AlH}_3 \cdots \text{Cl}^-$	-52,2

Tetrelne veze



Sistem	Energija veze sa NH ₃ kcal/mol
FSiH ₃	-5,5
FSiMe ₃	-2,2
FSi(CF ₃) ₃	-18,2
FSiIso ₃	+0,2
FSiTb ₃	+10,8

uticaj:

- veličine T atoma
- veličine supstituenta
- prirode supstituenta

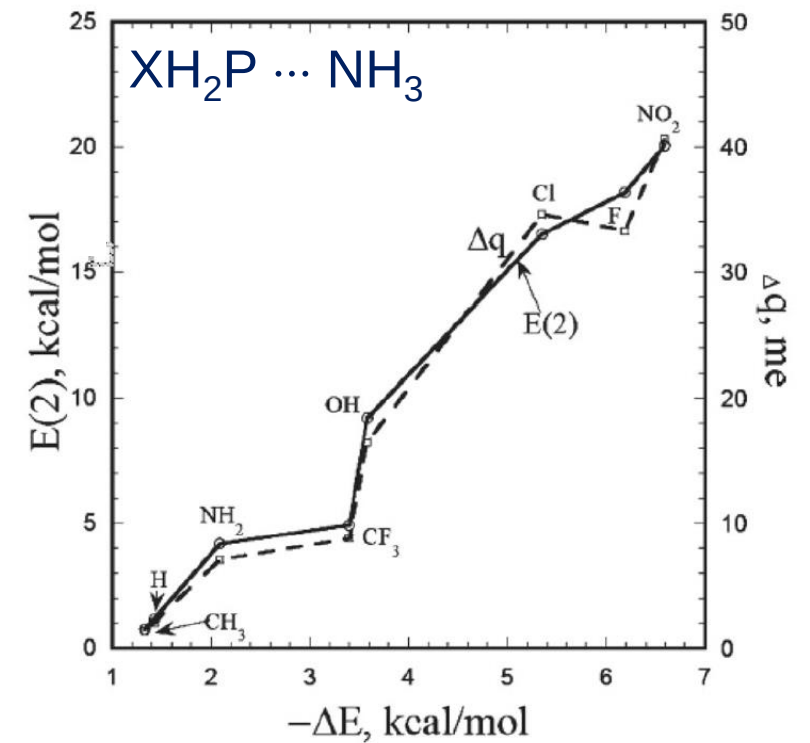
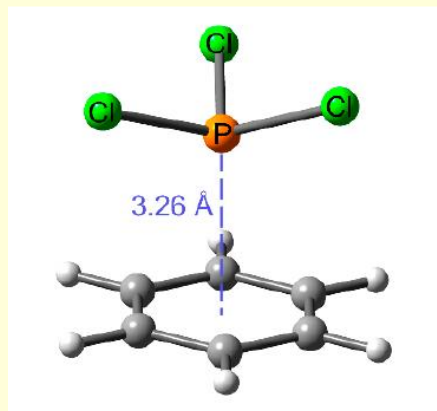
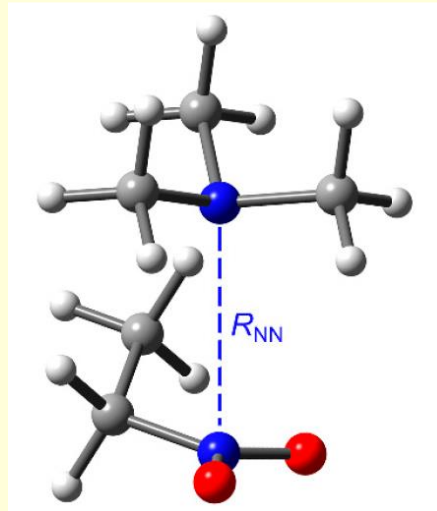
Pnikogene veze

Pnictogen bonds



15

N
P
As
Sb
Bi
Mc



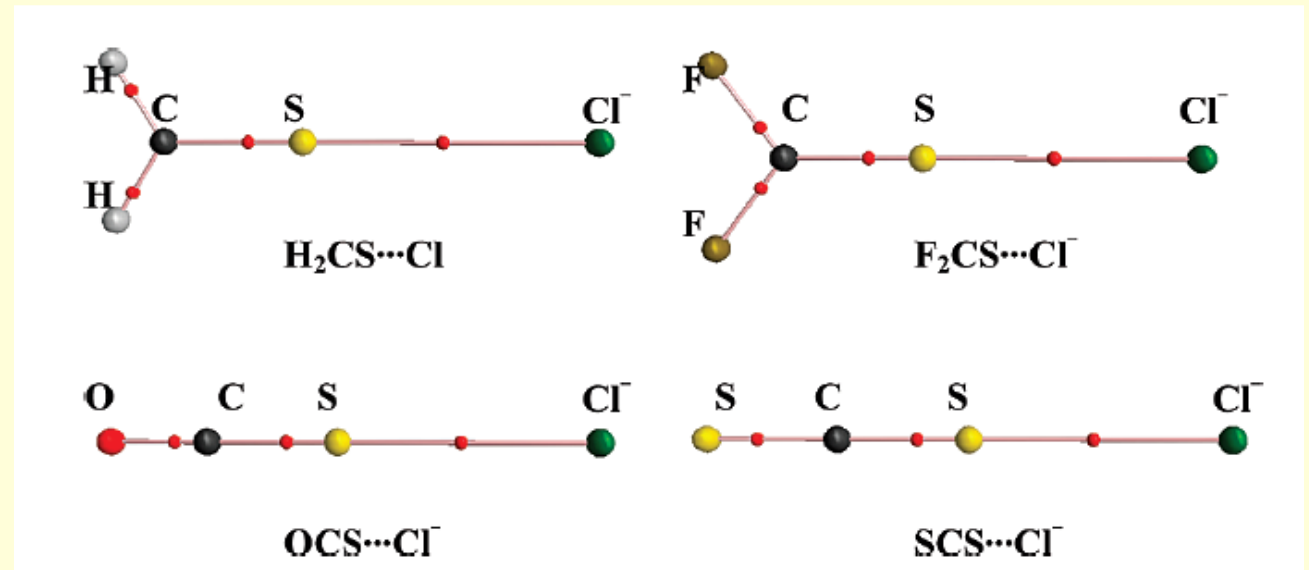
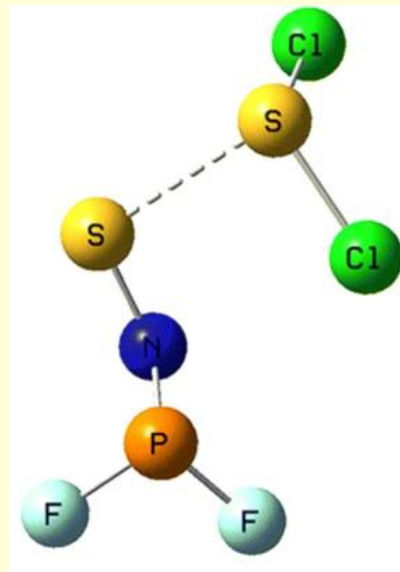
Halkogene veze

Chalcogen bonds



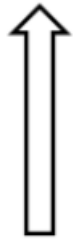
16

O
S
Se
Te
Po
Lv



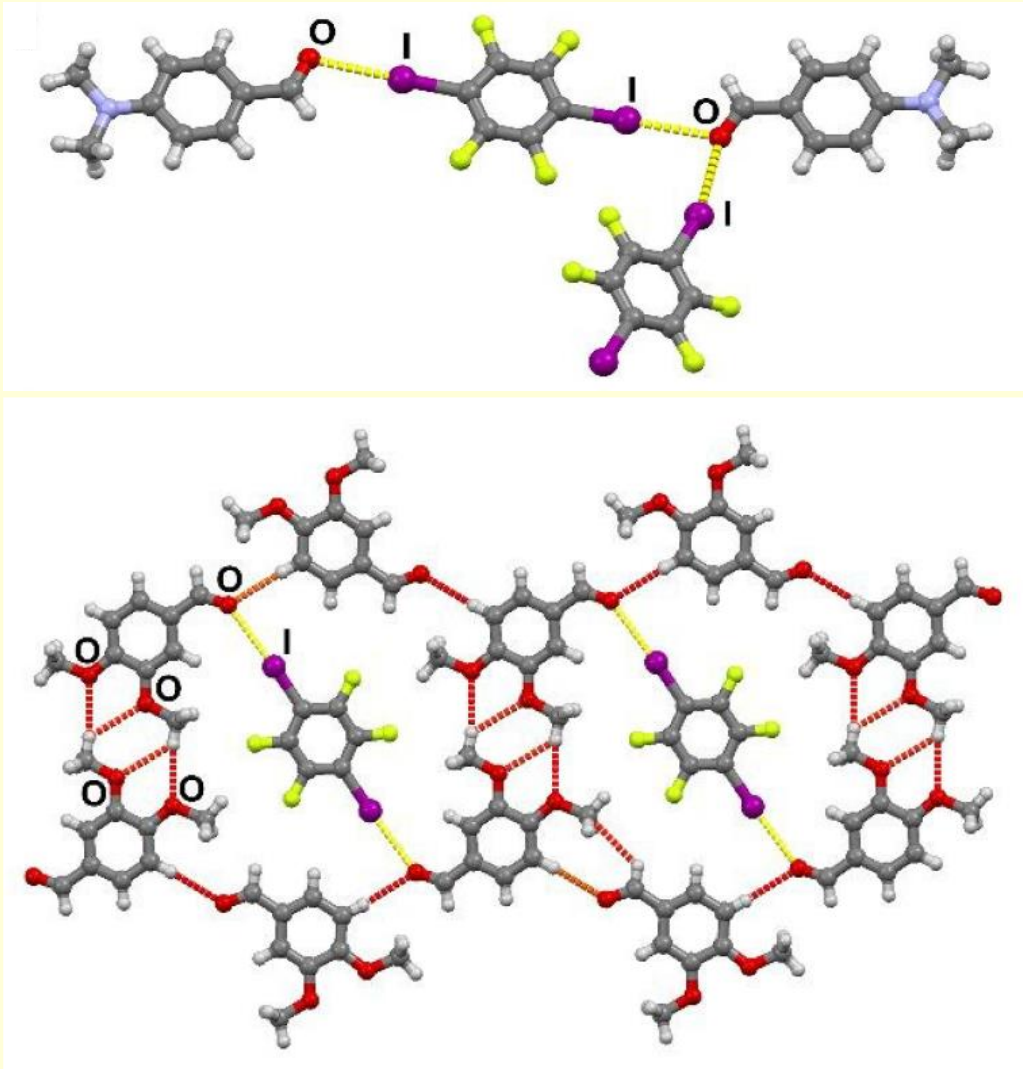
Halogene veze

Halogen bonds



17

F
Cl
Br
I
At
Ts



Aerogene veze

Aerogen bonds



18

He

Ne

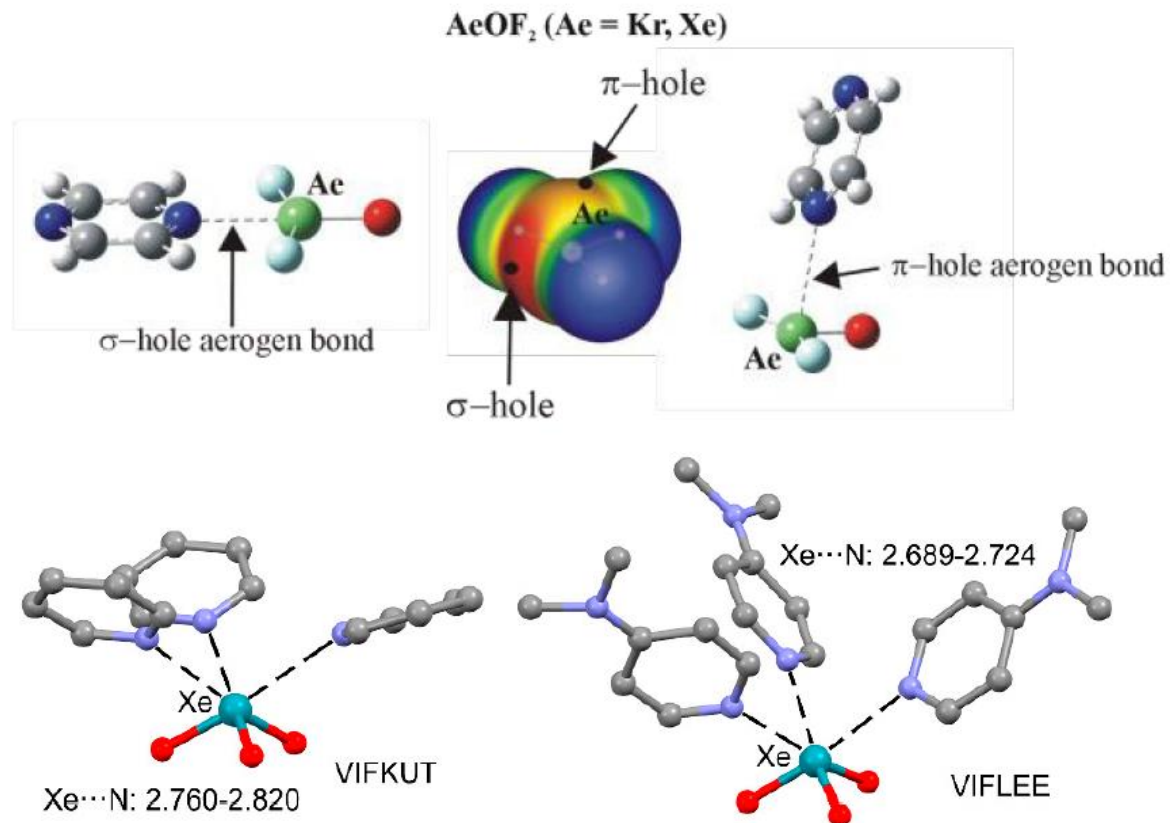
Ar

Kr

Xe

Rn

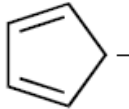
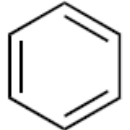
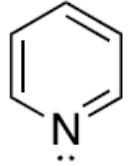
Og



Naziv tipa NI potiče od Luisove kiseline

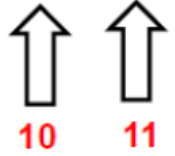
																		Pnictogen bonds					
																		Tetrel bonds					
																		Chalcogen bonds					
																		Halogen bonds					
																		Aerogen bonds					
																		18					
																		He					
																		Regium bonds					
																		13					
																		14					
																		15					
																		16					
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																		12					
																		11					
																		10					
																		9					
																		8					
																		7					
																		6					
																		5					
																		4					
																		3					
																		2					
																		1					
																		HB					
																		H					
																		Alkali bonds					
																		Alkaline earth bonds					
																		BeB					
																		LiB					
																		Li					
																		Be					
																		Na					
																		Mg					
																		K					
																		Ca					
																		Sc					
																		Ti					
																		V					
																		Cr					
																		Mn					
																		Fe					
																		Co					
																		Ni					
																		Cu					
																		Zn					
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																		Rb					
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																		Mo					
																		Tc					
																		Ru					
																		Rh					
																		Pd					
																		Ag					
																		Cd					
																		In					
																		Sn					
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																		Nh					
																		Fl					
																		Mc					
																		Lv					
																		Ts					
																		Og					
																		Spodium bonds					

Luisove baze

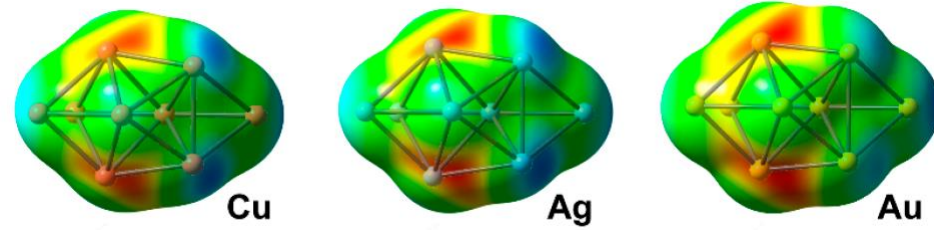
Anions	Neutral molecules			
	Atoms	Bonds	Rings	Groups
H^- F^- CN^- 	He	$\text{H} \equiv \text{H}$ $\text{H} - \text{H}$		 BrCH_3

Regijumske veze

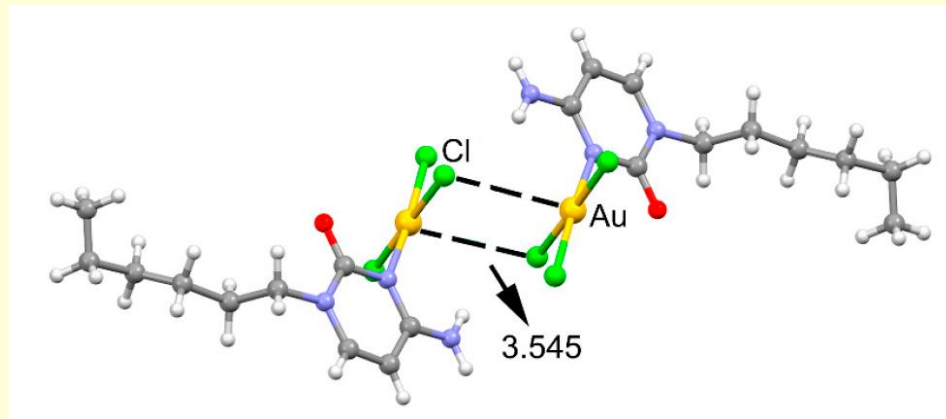
Regium bonds



Ni	Cu
Pd	Ag
Pt	Au
Ds	Rg

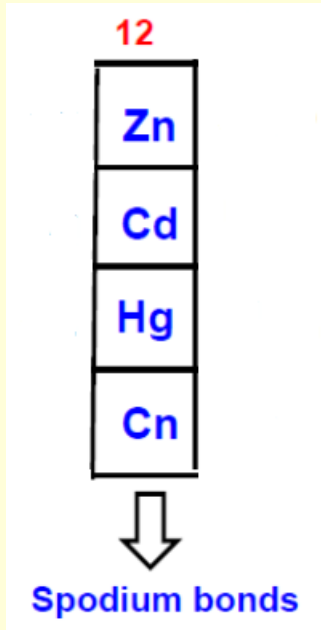


klasteri (nema NI)

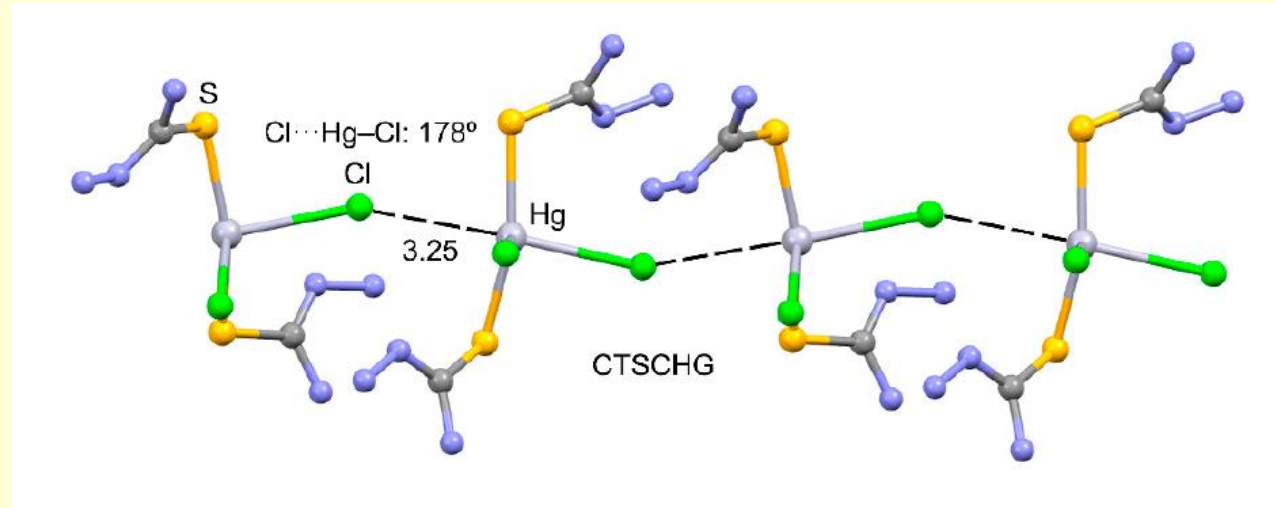


trihloro-(1-heksilcitozin)srebro(III) kompleks

Spodijumske veze



ZnO – spodium (lat)



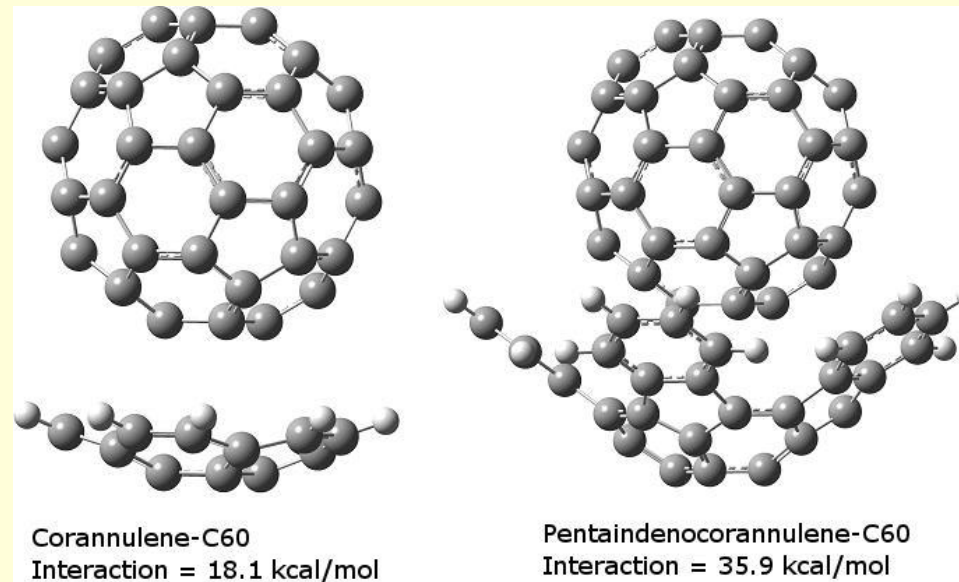
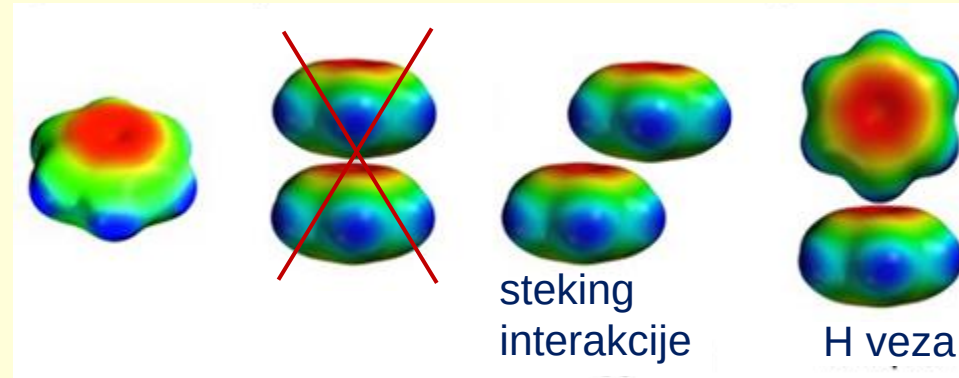
Hg-Cl veza:

- zbir van der Valsovih radijusa: 3,30 Å
- dužina Hg...Cl veze: 3,25 Å
- zbir kovalentnih radijusa: 2,39 Å

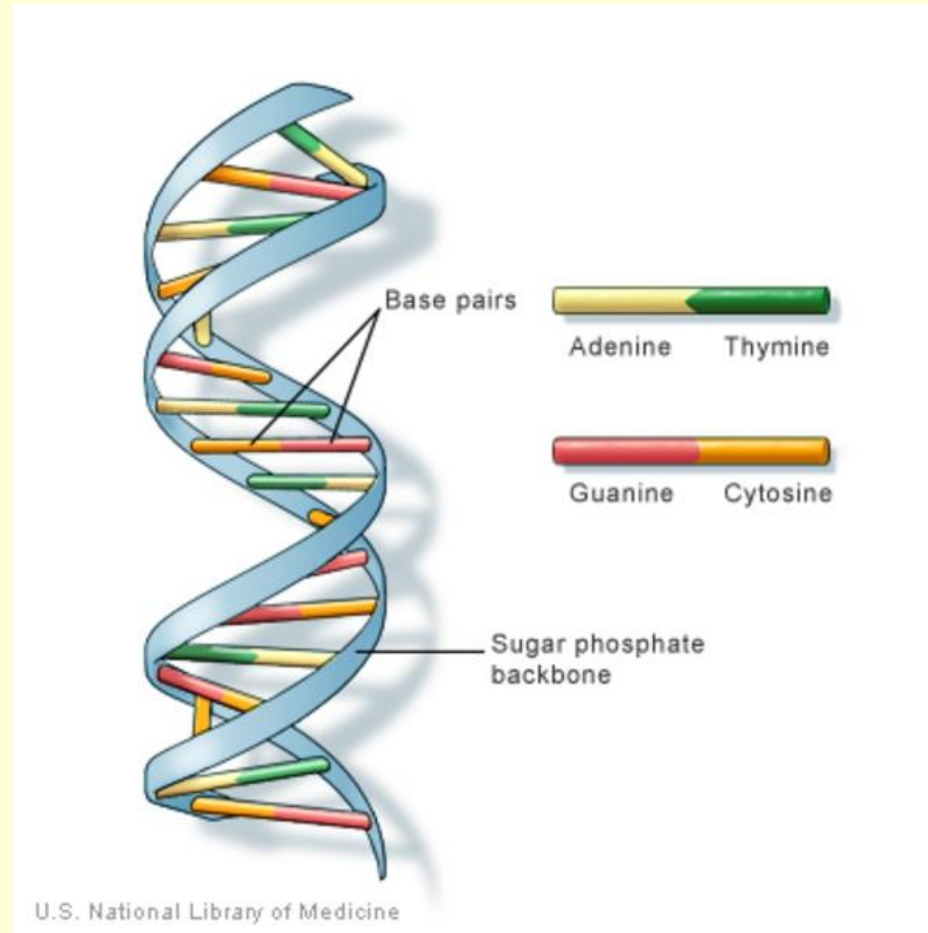
3-9. grupe periodnog sistema

3	4	5	6	7	8	9
Sc	Ti	V	Cr	Mn	Fe	Co
Y	Zr	Nb	Mo	Tc	Ru	Rh
Lan	Hf	Ta	W	Re	Os	Ir
Act	Rf	Db	Sg	Bh	Hs	Mt

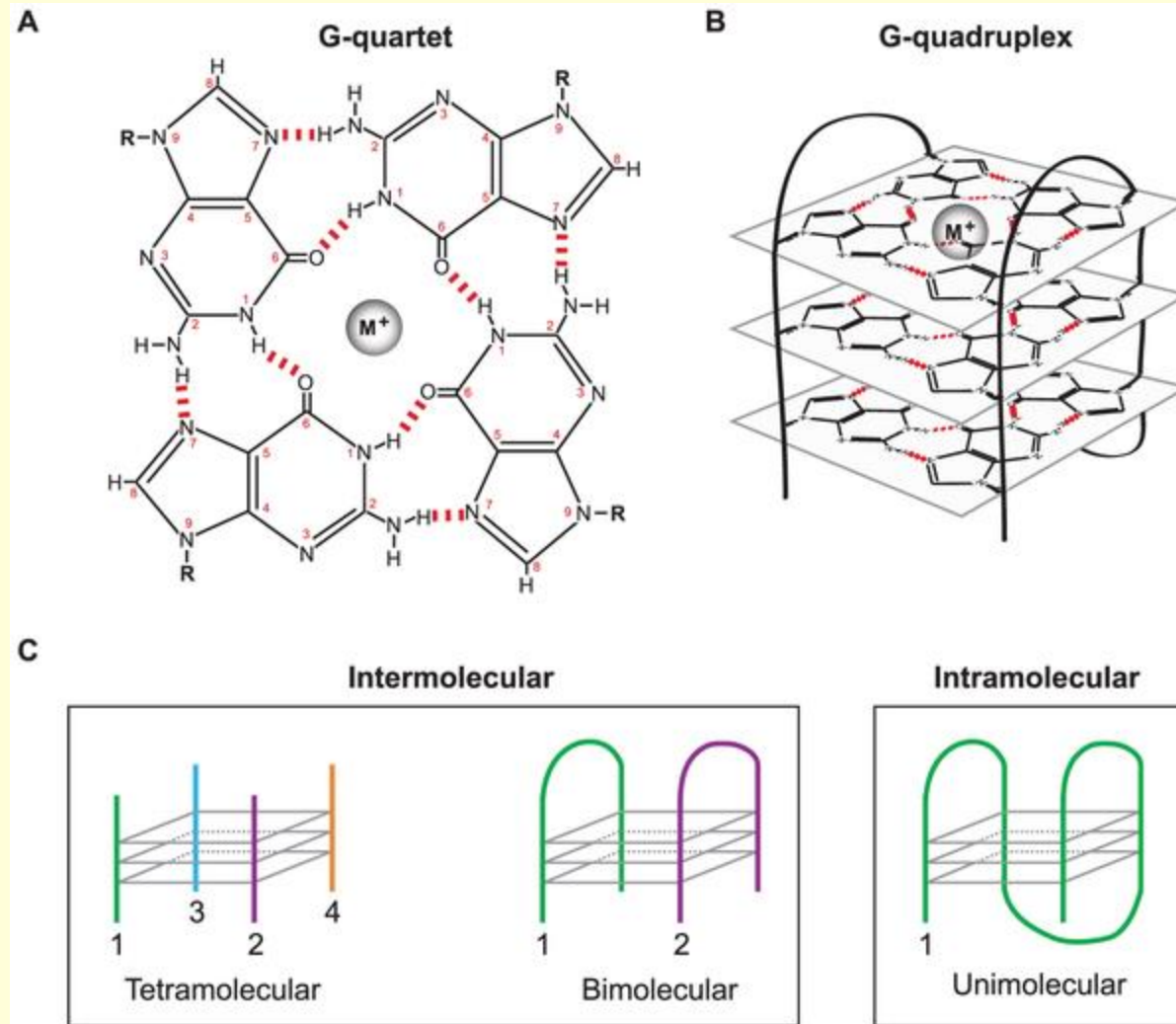
Steking interakcije



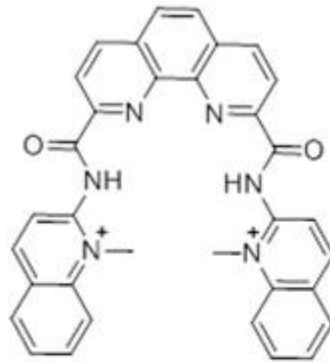
Primer: DNK



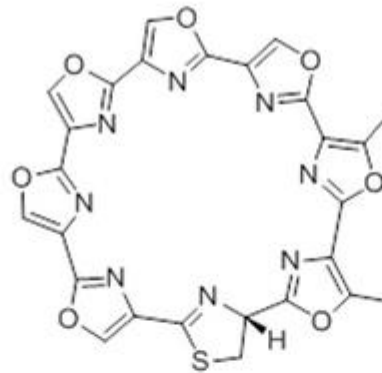
Primer: kvadrupleks guanina



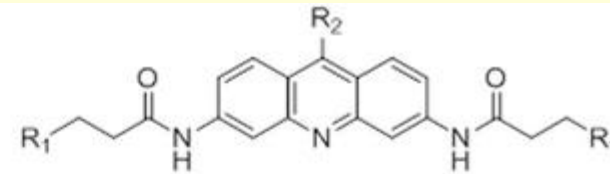
Primer: kvadrupleks guanina – ligandi



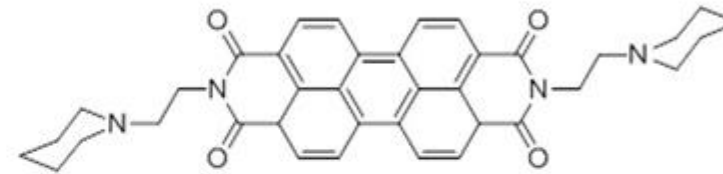
Phen DC₃



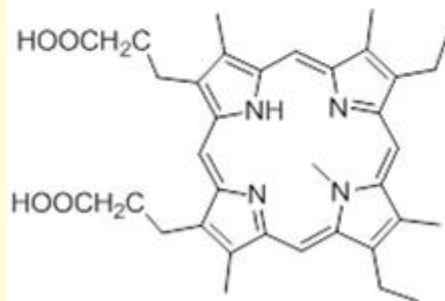
Telomestatin



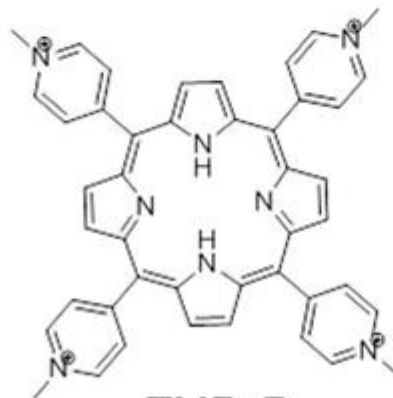
Acridine



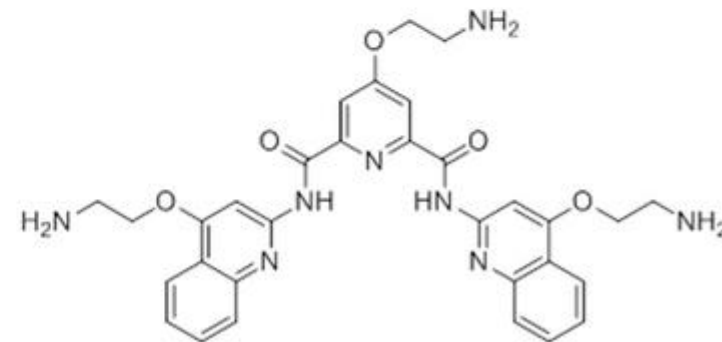
PIPER



NMM

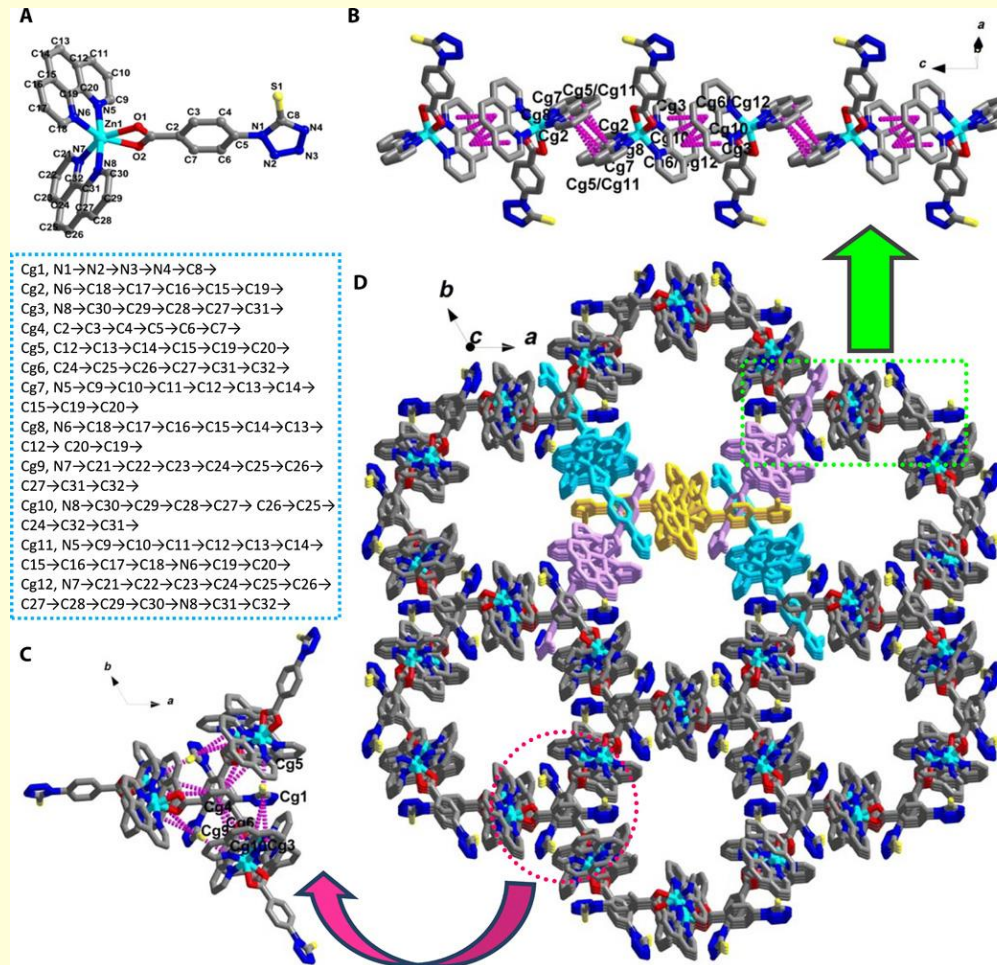


TMPyP₄



Pyridostatin

Primer: porozne supramolekulske strukture



Deng et al. *Sci. Adv.* 6, 2020, eaax9976

Diagram illustrating the periodic table with elements grouped by their valence electron configuration (indicated by red numbers 1 through 18) and labeled with their corresponding chemical bonds:

- Group 1 (Li, Na, K, Rb, Cs, Fr):** Alkali bonds
- Group 2 (Be, Mg, Ca, Sr, Ba, Ra):** Alkaline earth bonds
- Groups 3-10 (Sc, Y, La, Ac; Ti, Zr, Hf, Rf; V, Nb, Ta, Db; Cr, Mo, W, Sg; Mn, Tc, Re, Bh; Fe, Ru, Rh, Pd; Co, Ni, Cu, Zn):** Regium bonds
- Group 11 (Cu, Ag, Au):** Triel bonds
- Group 12 (Zn, Cd, Hg):** Tetrel bonds
- Group 13 (B, Al, Ga, In, Tl):** Pnictogen bonds
- Group 14 (C, Si, Ge, Sn, Pb):** Chalcogen bonds
- Group 15 (N, P, As, Sb, Bi):** Halogen bonds
- Group 16 (O, S, Se, Te, Po):** Aerogen bonds
- Group 17 (F, Cl, Br, I, At):** Aerogen bonds
- Group 18 (He, Ne, Ar, Kr, Xe, Rn, Og):** Aerogen bonds
- Group 12 (Zn, Cd, Hg):** Spodium bonds

➤ **steking interakcije**