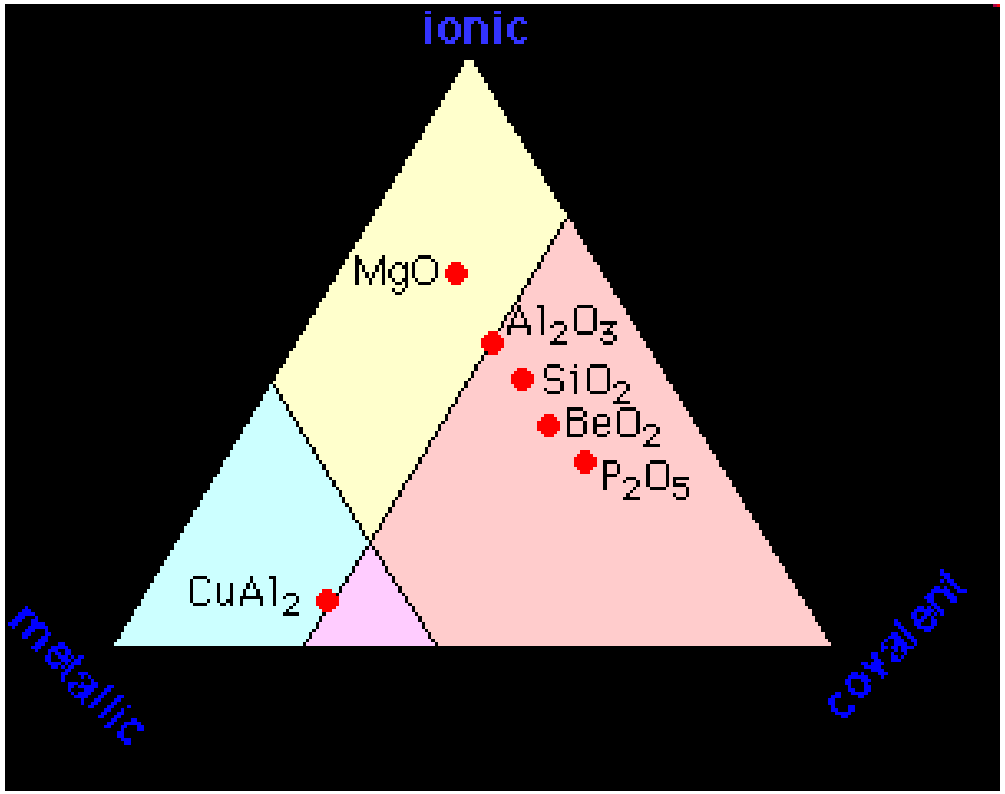
CAPVT II

VEZA

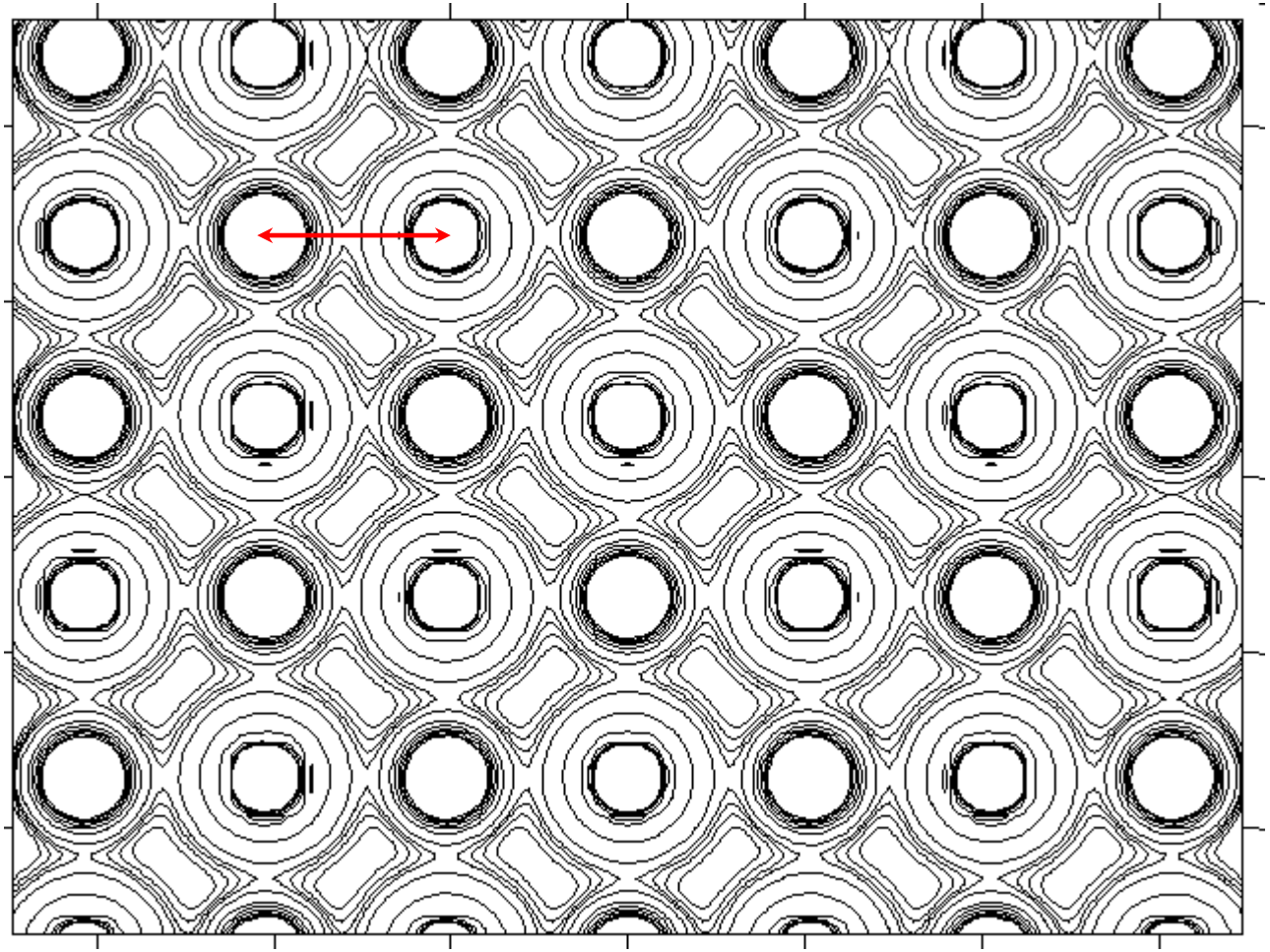
- Kakve kemijske veze mogu biti
  - Kovalentne, ionske, metalne
  - Jednostruke, dvostruke, trostruke...



Svojstva veze

- Duljina
- Energija disocijacije
- Konstanta sile
- Dipolni moment

Duljina veze



1. Udaljenost između jezgara
2. Udaljenost između maksimumâ elektronske gustoće
3. Ravnotežna duljina veze

Duljina veze i kovalentni radijus

$$r_K(\mathrm{S}) = \frac{1}{2} d(\mathrm{S}-\mathrm{S}) = 104\ \mathrm{pm}$$

$$r_K(\mathrm{C}) = \frac{1}{2} d(\mathrm{C}-\mathrm{C}) = 77\ \mathrm{pm}$$

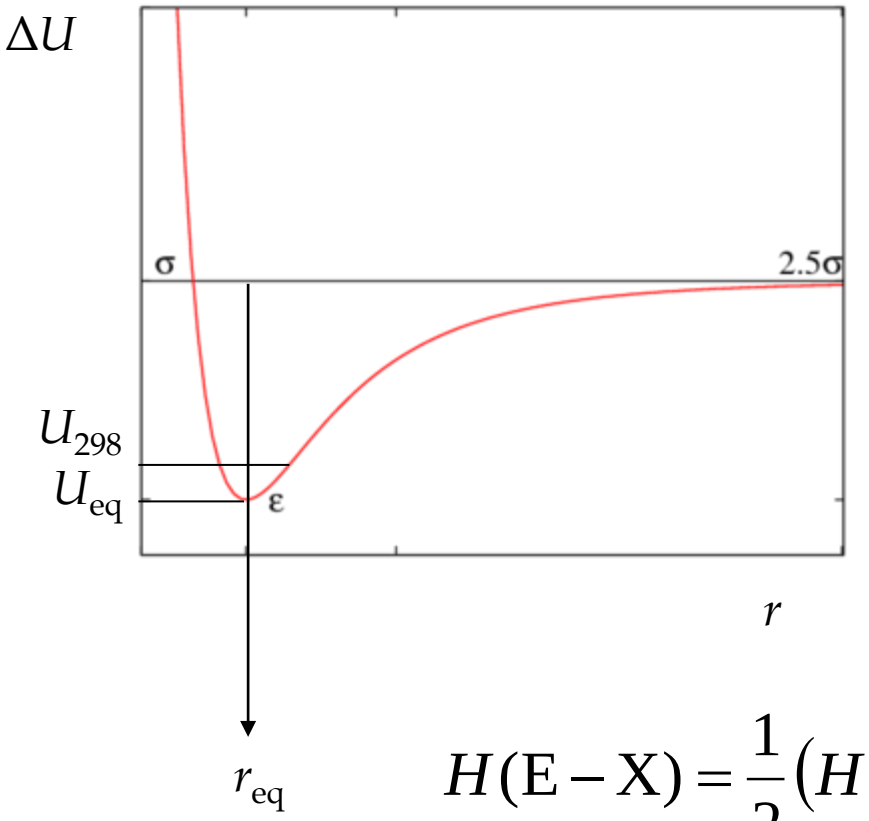
$$d(\mathrm{C}-\mathrm{C}) = r_K(\mathrm{S}) + r_K(\mathrm{C}) = 181\ \mathrm{pm}$$

[181,4 pm u H_3CSH i 180,7 u $(H_3C)_2S$]

$$d(\mathrm{A}-\mathrm{B}) = r_K(\mathrm{A}) + r_K(\mathrm{B}) - k[\chi(\mathrm{A}) - \chi(\mathrm{B})]$$

$(k \approx 9\ \mathrm{pm})$

Energija veze



$$H(\mathrm{E}-\mathrm{X}) = \frac{1}{2}\left(H(\mathrm{E}-\mathrm{E}) + H(\mathrm{X}-\mathrm{X})\right) + k[\chi(\mathrm{X}) - \chi(\mathrm{E})]^2$$

$$k = 96{,}5\ \mathrm{kJ\ mol^{-1}}$$

Konstnta sile

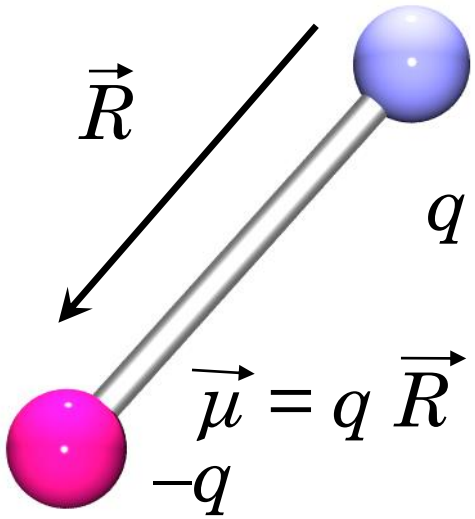
- Mjera za krutost veze (nagib Lennard-Jonesove krivulje)

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

$$k = \frac{(2\pi\nu)^2}{\mu}$$

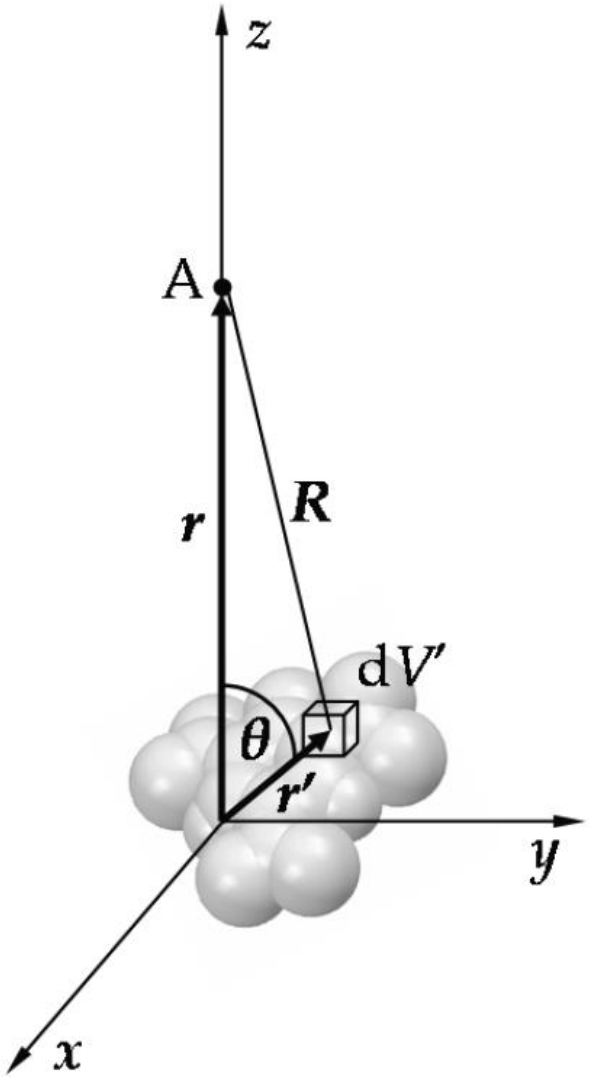
Dipolni moment

- Dipolni moment



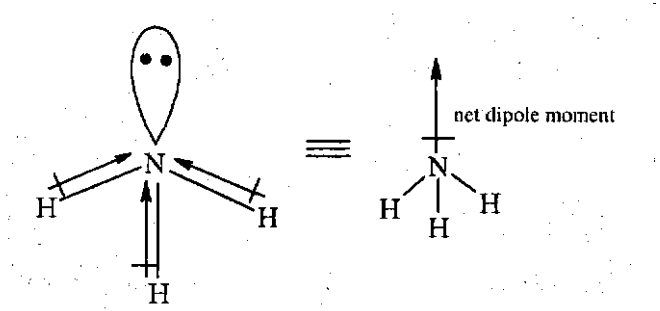
- Molekulski dipolni moment

$$\vec{\mu} = \int_V \vec{r'}\rho(V')dV'$$



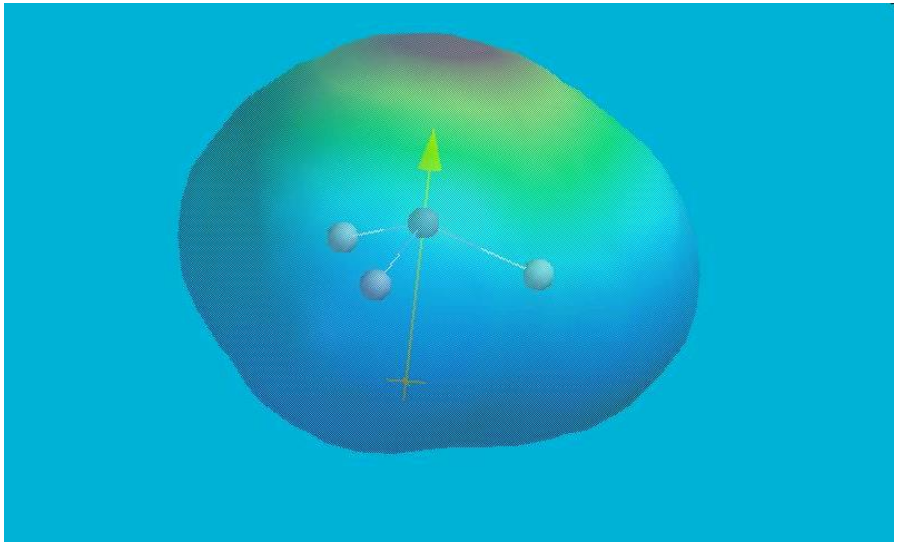
- Ukupni dipolni moment molekule kao suma dipolnih momenata veza.
- Dipolni moment veze sadrži:
  - Atomske dipolne momente
  - Moment prijenosa

A k tomu i dipol neveznog para



NH_3 – dipolni moment od $4{,}76 \cdot 10^{-3}$ C m

(1,846 D)



CO – dipolni moment od 0,122 D

Geometrija molekule

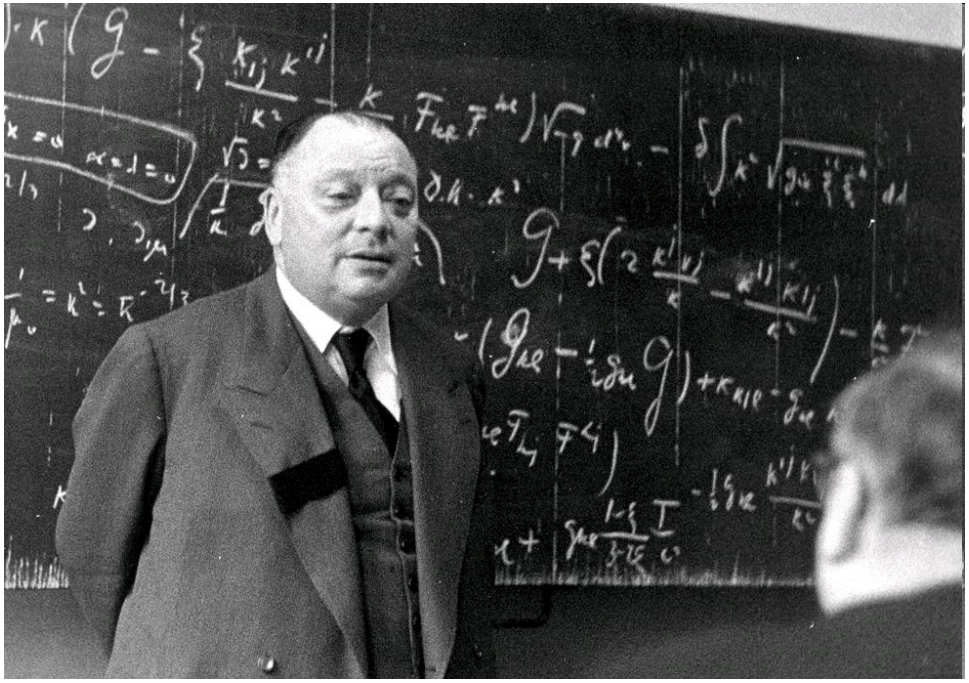
- Određena razmještajem elektrona u molekuli
- Elektroni se odbijaju, a po potrebi i sparuju.

Paulijev princip

Elektronska valna funkcija mora biti antisimetrična s obzirom na izmjenu elektrona

Iliti dva elektrona ne mogu biti u istom stanju (na istom mjestu u isto vrijeme)

Ponašaju se kao da se odbijaju uslijed *"Paulijeve sile"*

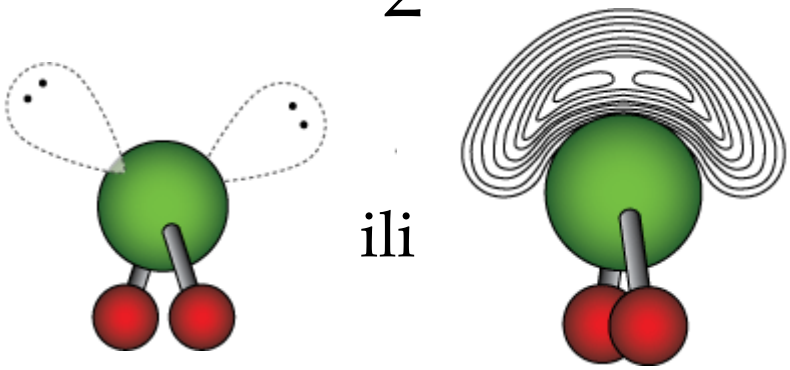


O sparivanju elektrona

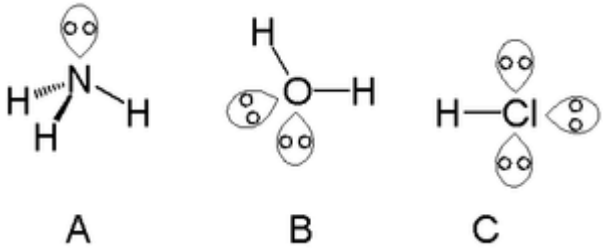
Kažu da zbog Paulija elektroni se sparuju.

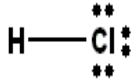
Zašto i koliko to elektroni čine?

H_2O



Monovalentni halogeni



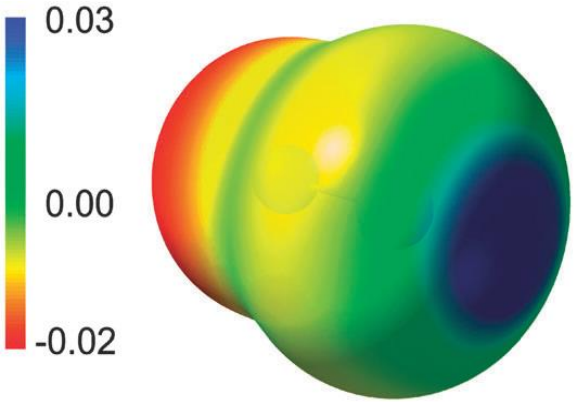


Central atom:	Cl
Cl contributes:	7 e^-
H contibutes:	1 e^-
Total VSE:	8
Total VSEP:	4
Geometry:	Linear (based on tetrahedral)

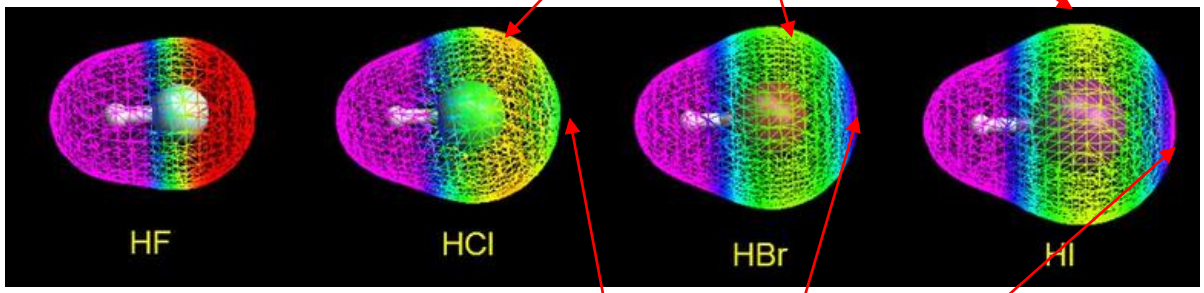
Što ne valja na ovoj slici?

Preuzeto od Univerity of Bristol, School of Chemistry, Bristol ChemLabs;
http://www.inchm.bris.ac.uk/schools/vsepr/examples/hcl.htm

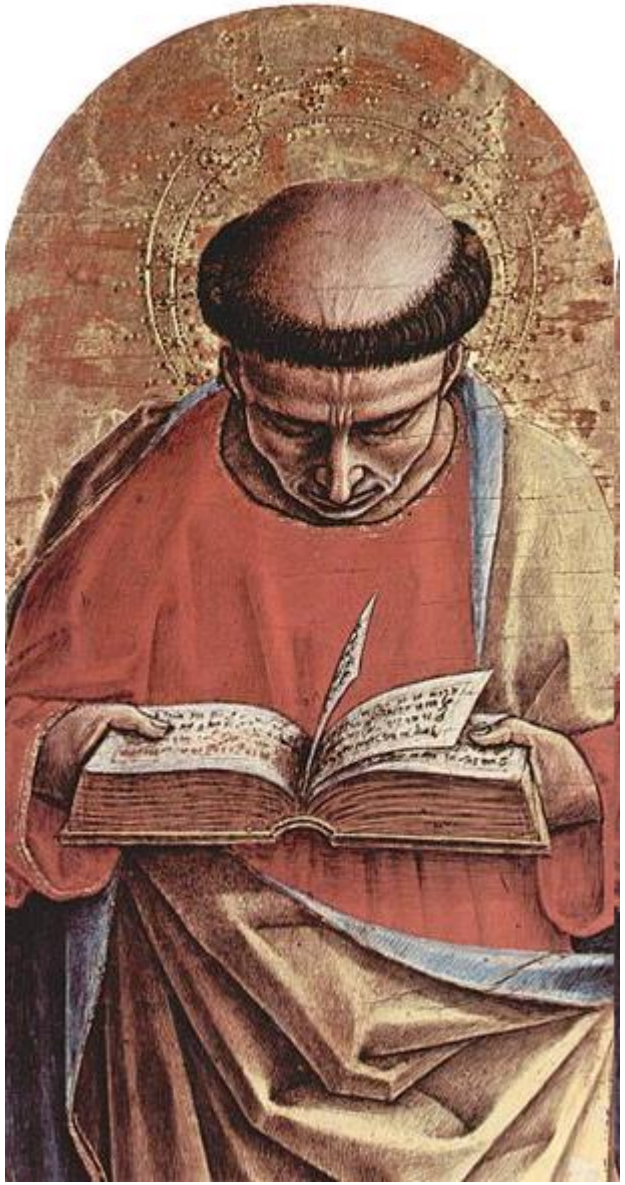
Monovalentni halogeni



povećana elektronska gustoća

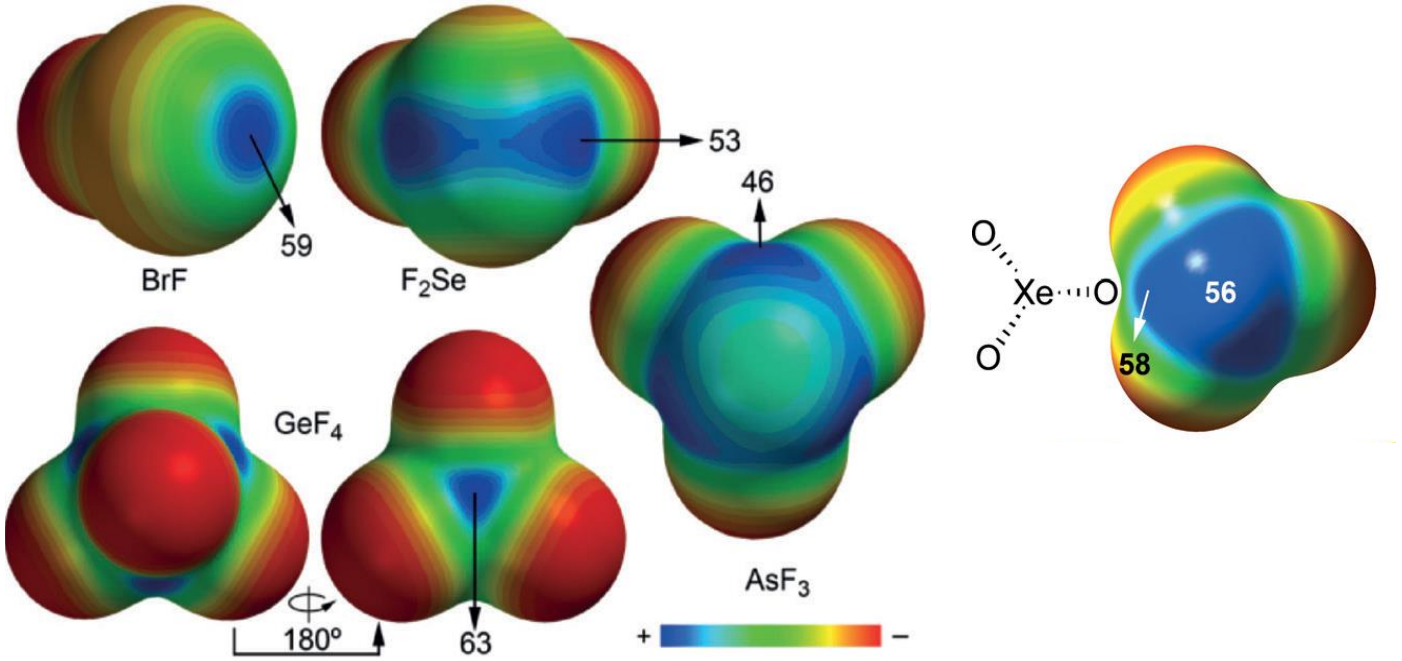


smanjena elektronska gustoća
σ-šupljina (*σ-hole*)

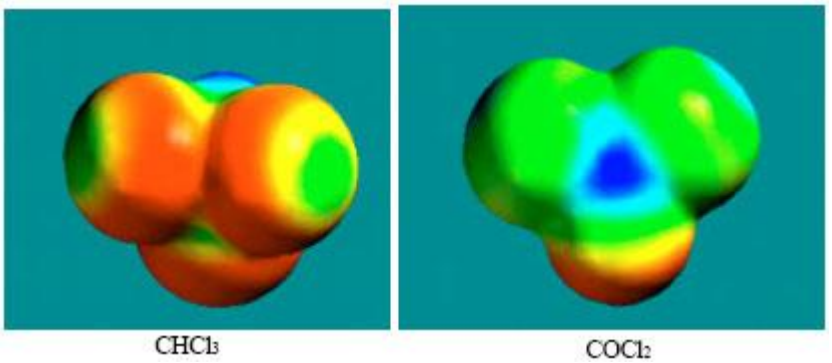


σ-, π- i ostale molekulske rupe

Nedostatak elektronske gustoće javlja se u nastavku **svake** kovalentne veze



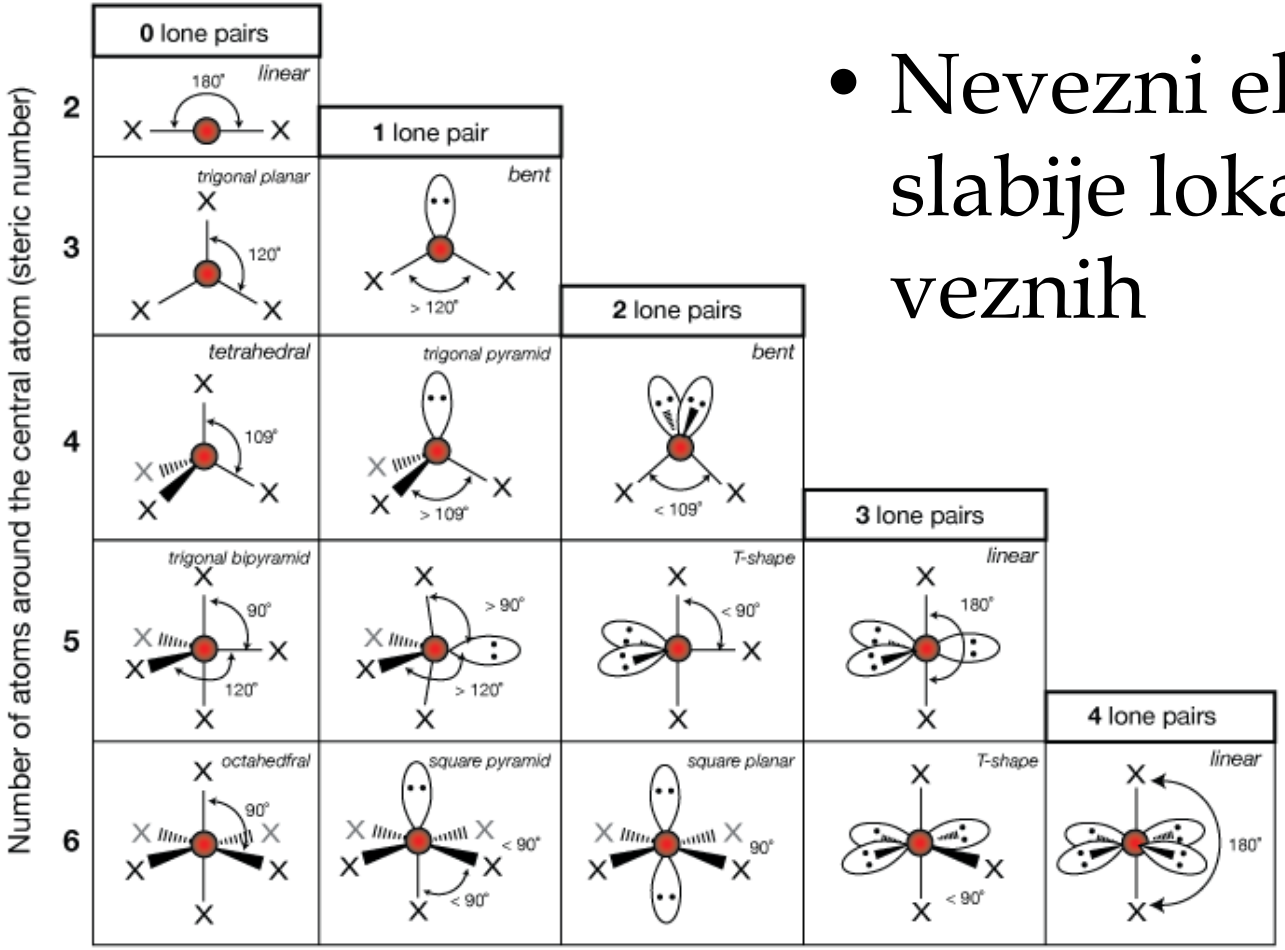
Nedostatak elektronske gustoće kadkad se javlja okomito na (višestruke) kovalentne veze – **π-šupljina**



VSEPR

- **Valence shell electron pair repulsion**
- Vezni i nevezni elektronski parovi razmještaju se tako da budu što dalje jedni od drugih
- Jače lokalizirani parovi se manje odbijaju
- Ne funkcionira za Na_2O i njemu slične
- Ne fukcionira baš ni za preteške atome

VSEPR - binarni spojevi

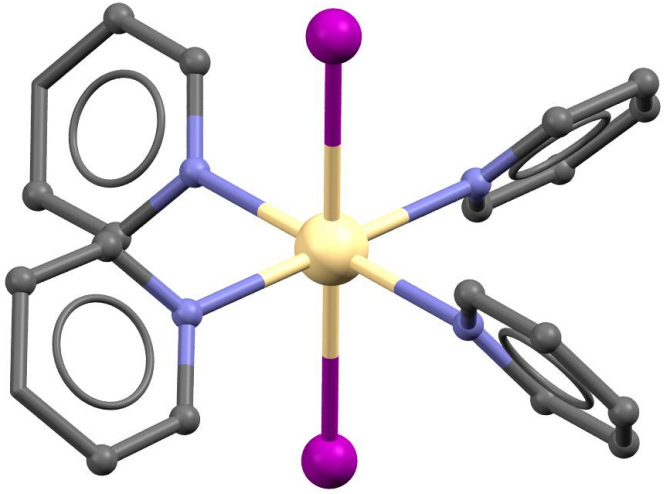


- Nevezni elektroni su slabije lokalizirani od veznih

VSEPR - ternarni spojevi

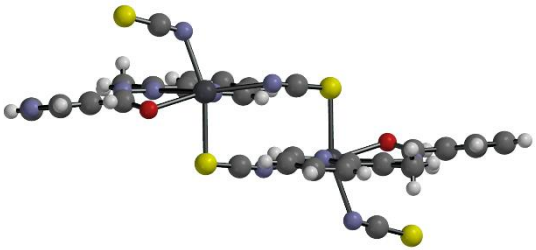
Bentovo pravilo – elektronegativniji supstituenti preferiraju aksijalni položaj (pripadni elektronski parovi su **jače** lokalizirani)

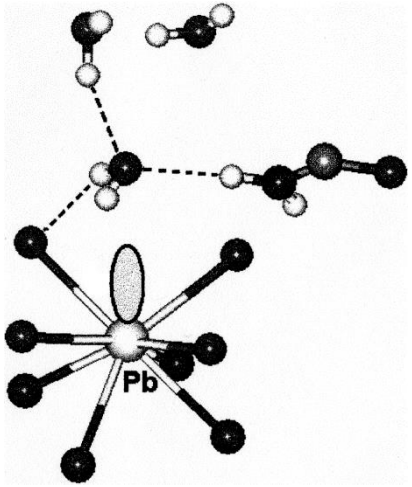
Vrijedi čak i za slučajeve s višeatomnim ligandima (npr. $CdI_2(pyr)_4$)



Olovo(II) i ‘sterički aktivni elektronski par’

- Hemidirekcionalna koordinacija (‘sterički aktivan elektronski par’)





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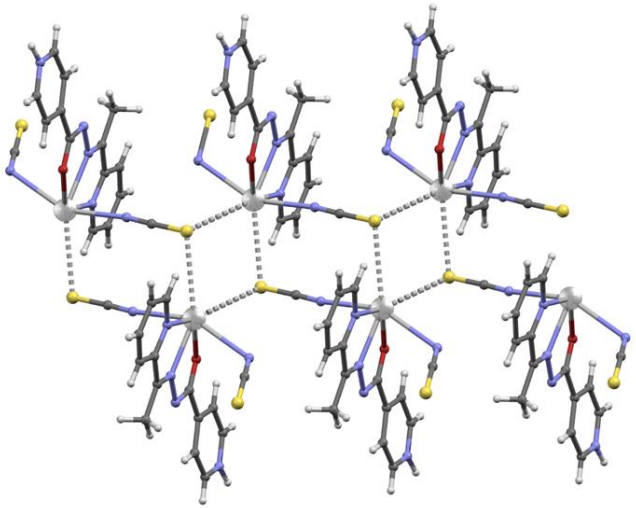
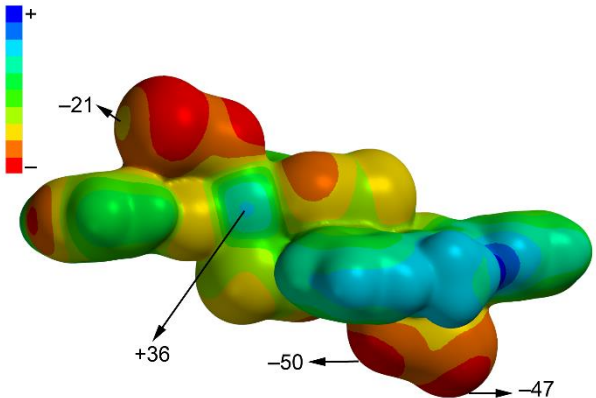
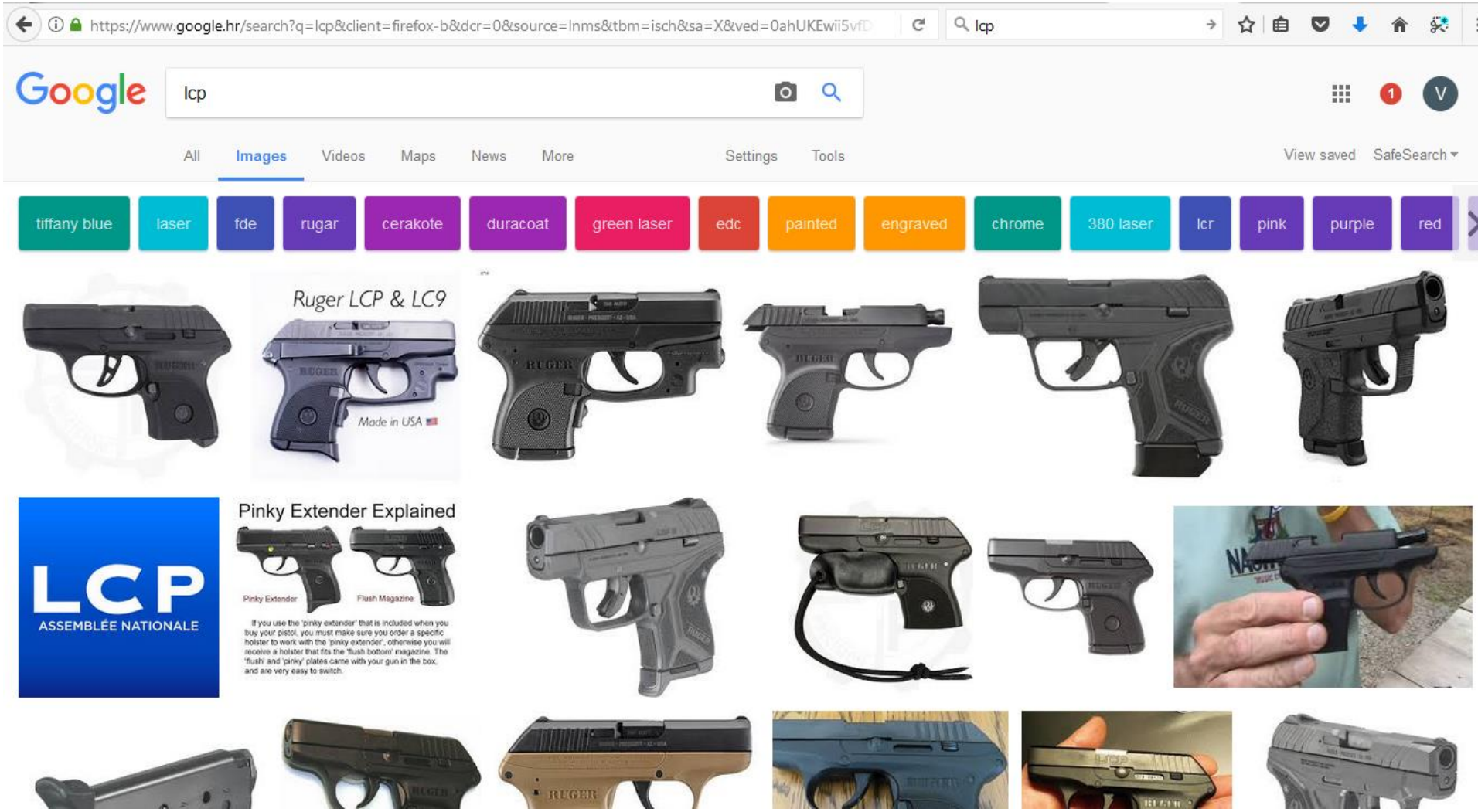




Kad VSEPR ne radi - LCP



LCP

- Gusto pakiranje liganada (Ligand Close Packing) oko centralnog atoma
- Alternativa VSRPR-u (1997./8. Gillespie i Robinson)
- Sterički model

- Nevezna udaljenost se ne mijenja od molekule do molekule
- Intramolekulski nevezni ligandni radius je konstantan za danu kombinaciju središnjeg atoma i liganda
- Ligandi se gusto pakiraju oko centralnog atoma

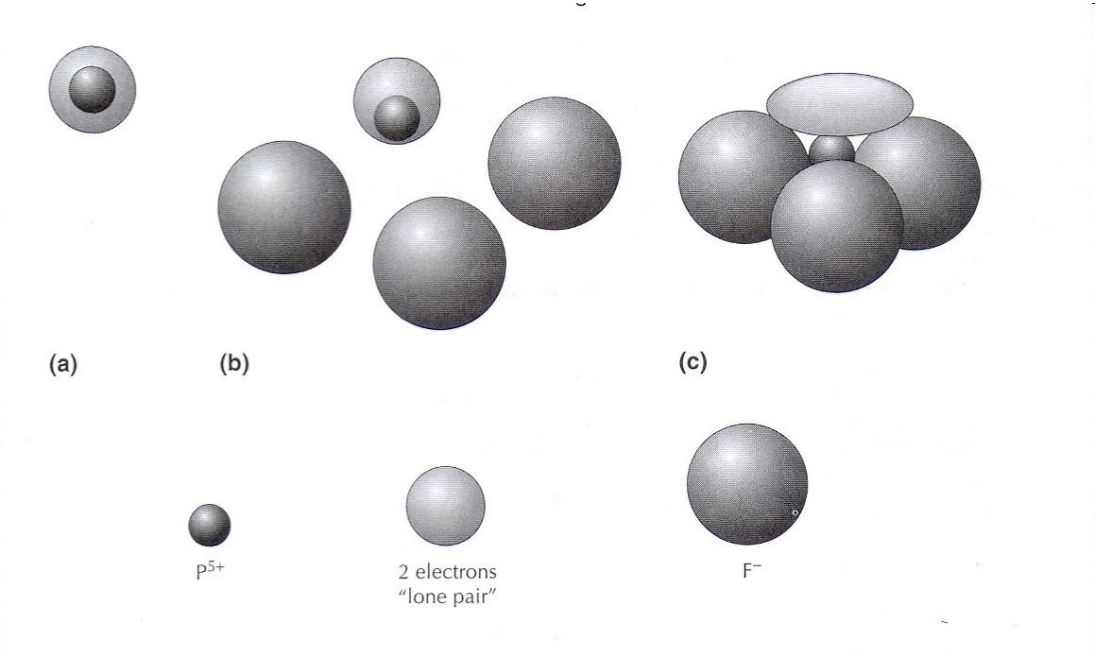
molekula	koordinacijski broj	d(A-F)/pm	$\angle$(F-A-F)/°		d(F...F)/pm
BeF_3^-	3	149	120		258
BeF_4^{2-}	4	155.4	109.5		254
				prosjek	**256**
F_3B	3	130.7	120.0		226
F_2B—OH		132.3	118.0		227
F_2B—NH_2		132.5	117.9		227
F_2B—Cl		131.5	118.1		226
F_2B—H		131.1	118.3		225
F_4B^-	4	138.2	109.5		226
F_3B—CH_3^-		142.4	105 .4		227
F_3B—CF_3^-		139.1	109 .9		228
F_3B—PH_3		137.2	112.1		228
				prosjek	**226**
CF_3^{+a}	3	124.4	120		216
$F_2C{=}CF_2$		131.9	112.4		219
$F_2C{=}CCl_2$		131.5	112.1		218
$F_2C{=}CH_2$		132.4	109.4		216
$F_2C{=}CHF$		133.6	109.2		218
F_4C	4	131.9	109.5		215
F_3C—CF_3		132.6	109.8		217
F_3C—OF		131.9	109.4		215
F_3CO^-		139.2	101.3		215
				prosjek	**216**

Pravilnosti

- U molekuli AX_n duljina veze A-X raste s porastom *n*
- Nevezne udaljenosti između različitih liganada približne su sumi njihovih neveznih radijusa
- Temeljem kovalentnih i ligandnih radijusa, mogu se procijeniti vezni kutevi

Nevezni parovi

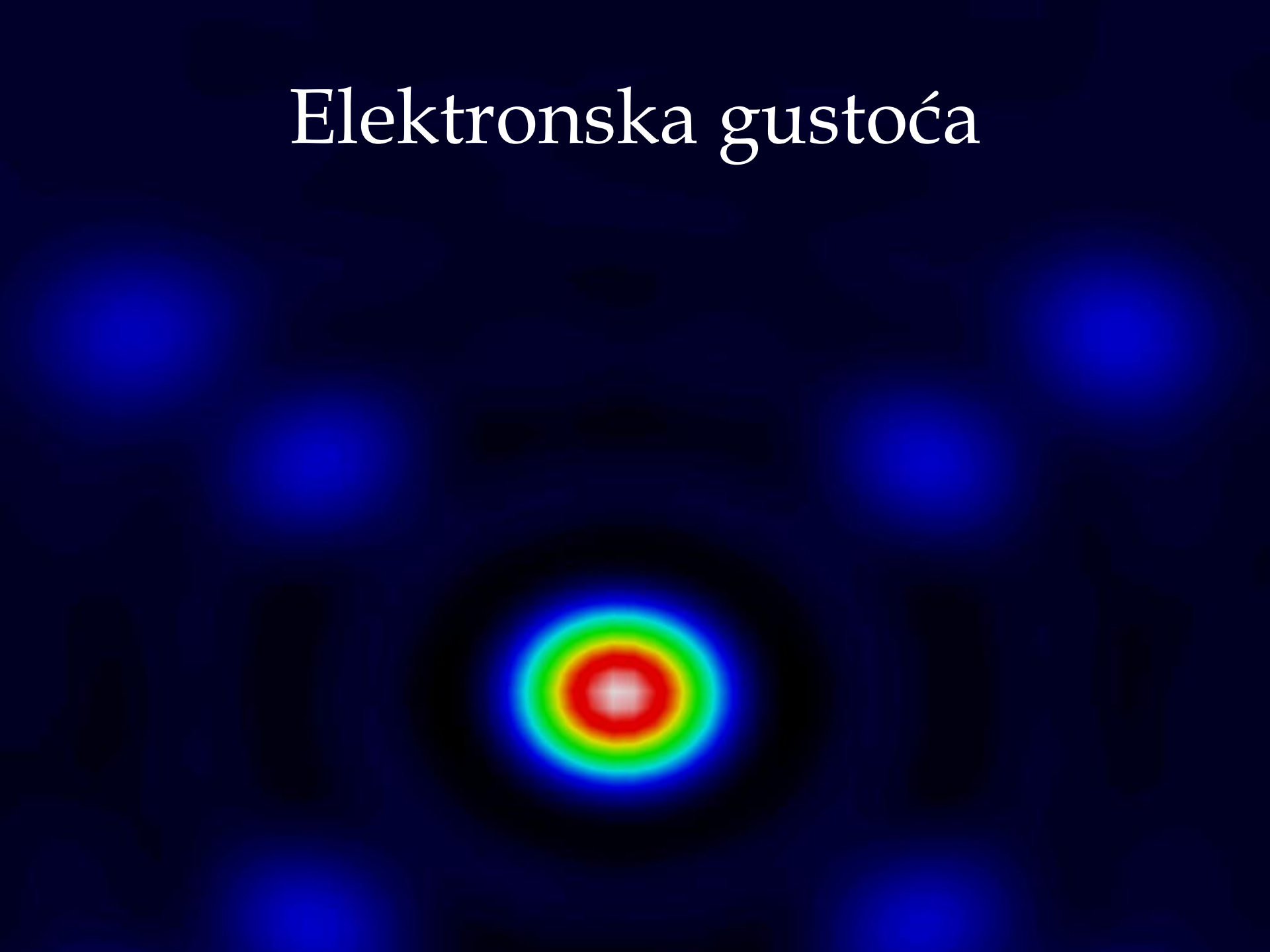
- Središnji se atom ima tretirati kao nesferičan ukoliko ima sparenih neveznih elektrona



Ligandi niske elektronegativnosti

	d(A-O)/pm	$\angle$(O-A-O)/°	$\angle$(A-O-H)/°
LiOH	158.2	—	180.0
$Be(OH)_2$	142.3	180.0	134.5
$B(OH)_3$	136.8	120.0	112.8
$C(OH)_4$	139.3	103.6, 112.5	106.9
$N(OH)_3$	141.3	103.8	102.6
$O(OH)_2$	144.4	100.3	98.7
FOH	143.2	—	98.6

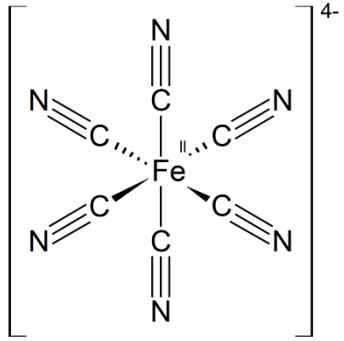
Elektronska gustoća



Kako do gustoće?

Računski: *ab initio,* semiempirijski

Mjerenjem: rentgenska i elektronska difrakcija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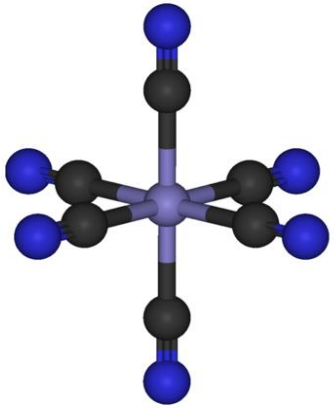

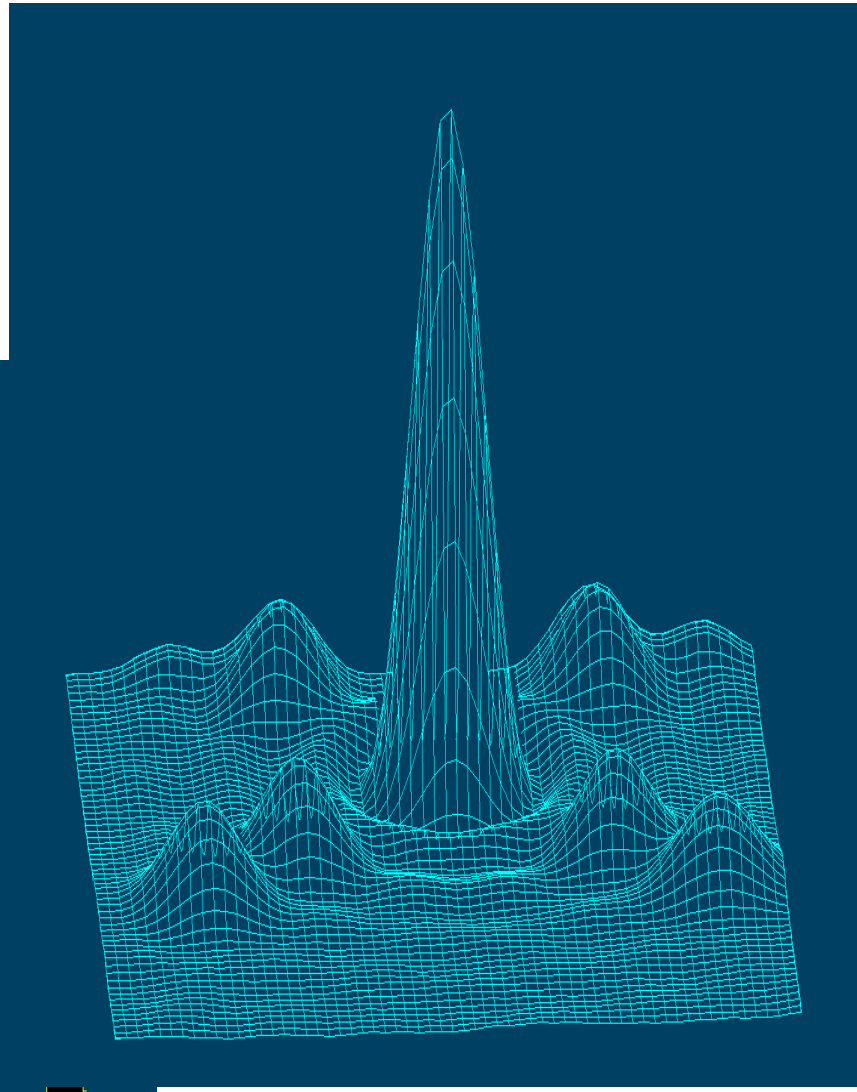

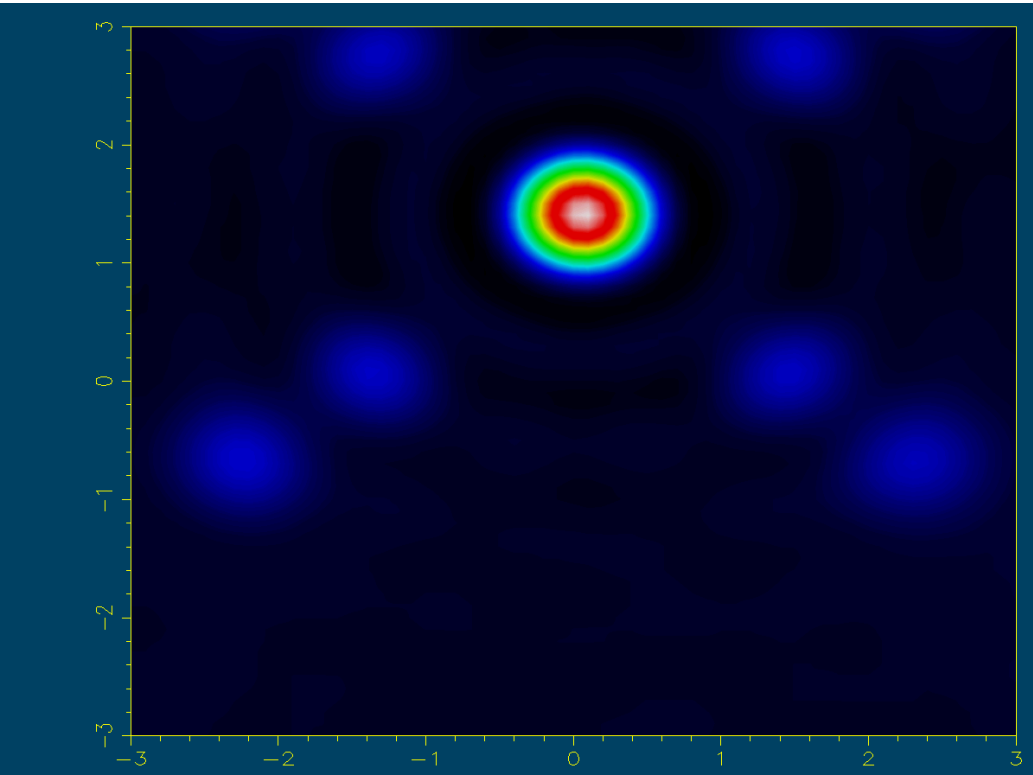
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3

Problemi

Nepotpuni podatci (‘*musavi Fourier*’)

Termičko gibanje (dekonvolucija)

Nesavršenost kristala (artefakti)

Absorpcija i ekstinkcija

Cu – premala rezolucija; Mo,Ag – premali intenzitet

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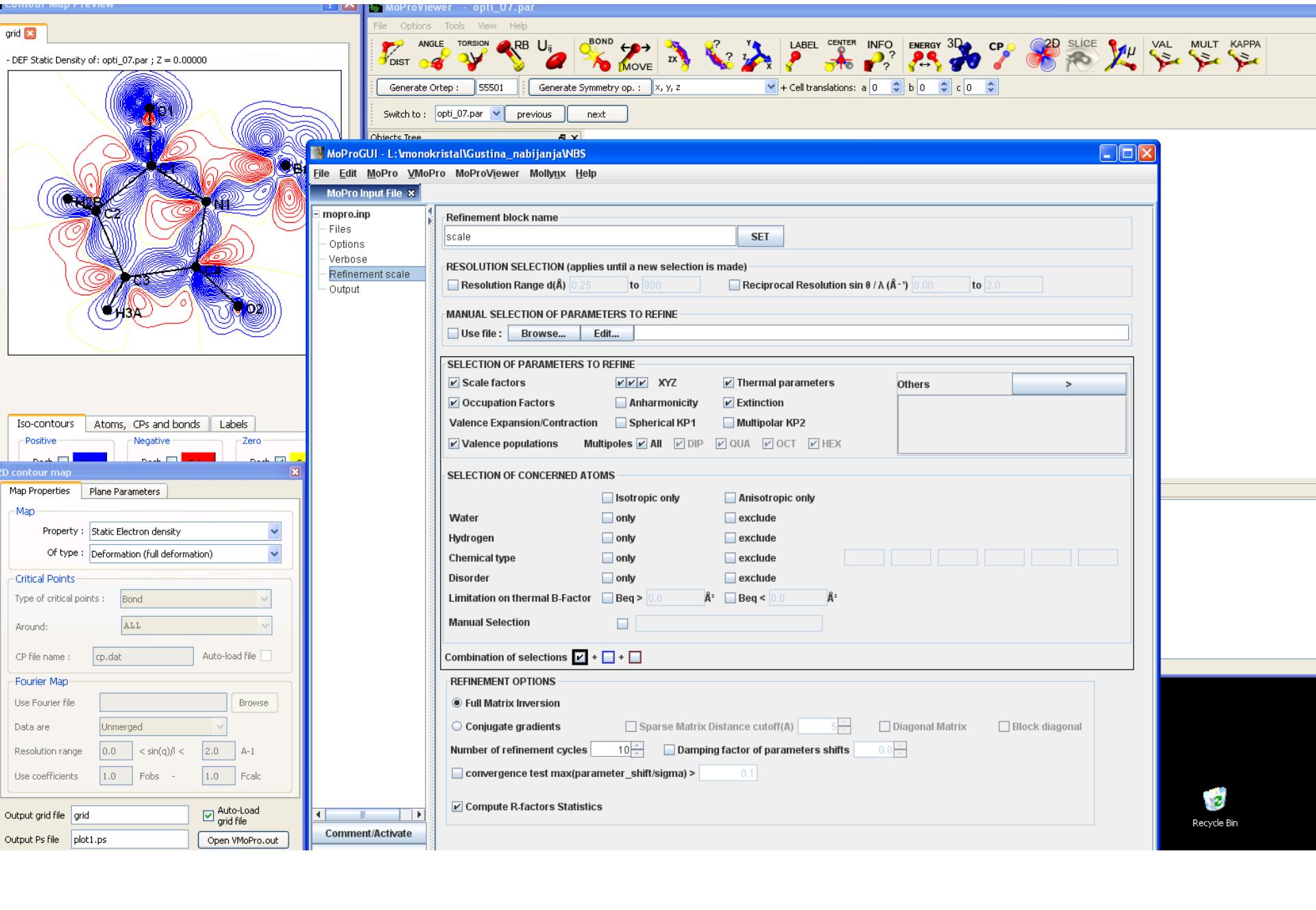
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O1
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C4
H3A
O2
Iso-contours
Atoms, CPs and bonds
Labels
Positive
Negative
Zero
2D contour map
Map Properties
Plane Parameters
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Property : Static Electron density
Of type : Deformation (full deformation)
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Type of critical points : Bond
Around: ALL
CP file name : cp.dat
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Resolution range 0.0 < sin(q)/l < 2.0 A-1
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MoPro Input File
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Files
Options
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Resolution Range d(Å) 0.25 to 900
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MANUAL SELECTION OF PARAMETERS TO REFINE
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SELECTION OF PARAMETERS TO REFINE
Scale factors
XYZ
Thermal parameters
Occupation Factors
Anharmonicity
Extinction
Valence Expansion/Contraction
Spherical KP1
Multipolar KP2
Valence populations
Multipoles All DIP QUA OCT HEX
Others >
SELECTION OF CONCERNED ATOMS
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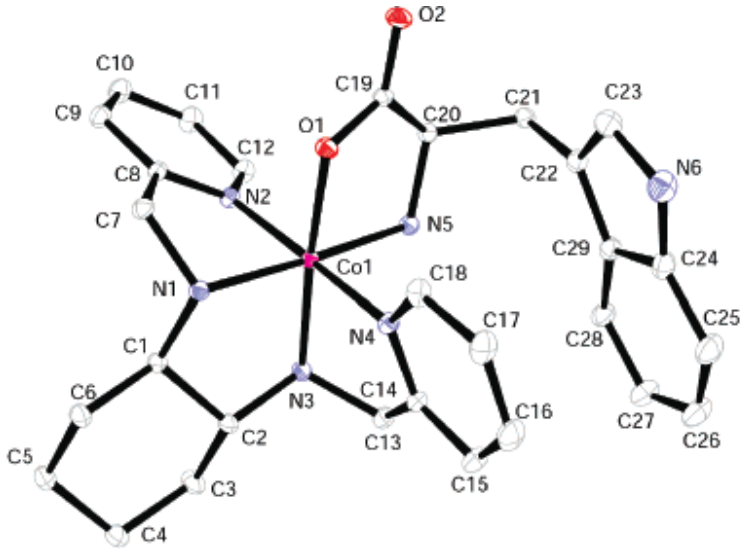
Anisotropic only
Water only exclude
Hydrogen only exclude
Chemical type only exclude
Disorder only exclude
Limitation on thermal B-Factor Beq > 0.0 Å² Beq < 0.0 Å²
Manual Selection
Combination of selections
REFINEMENT OPTIONS
Full Matrix Inversion
Conjugate gradients
Sparse Matrix Distance cutoff(A) 5
Diagonal Matrix
Block diagonal
Number of refinement cycles 10
Damping factor of parameters shifts 0.8
convergence test max(parameter_shift/sigma) > 0.1
Compute R-factors Statistics
Recycle Bin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C29
C24
Co1
C18
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N4
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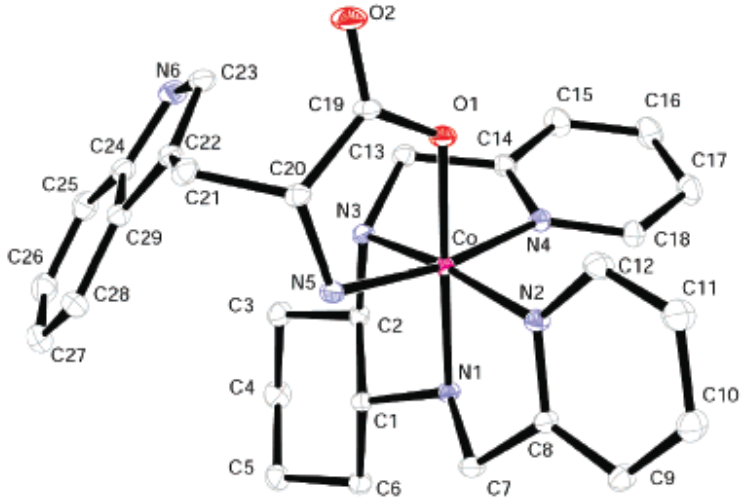
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Co
N4
C18
C29
C26
N5
C12
C28
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C11
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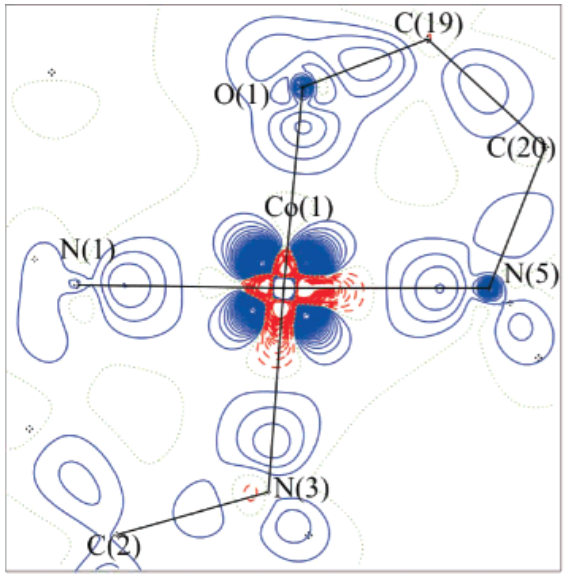
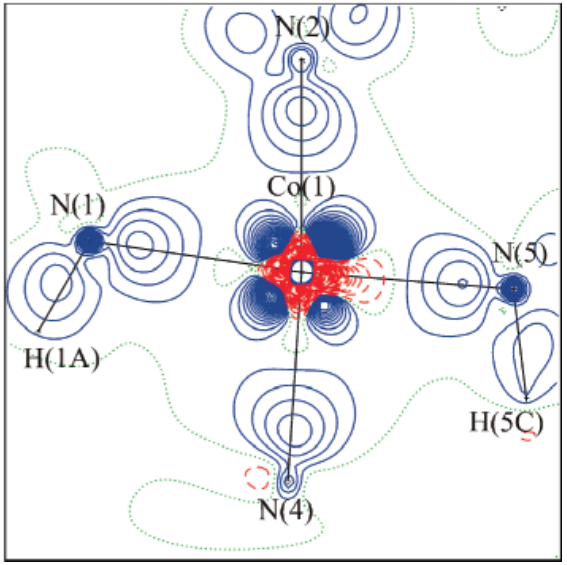
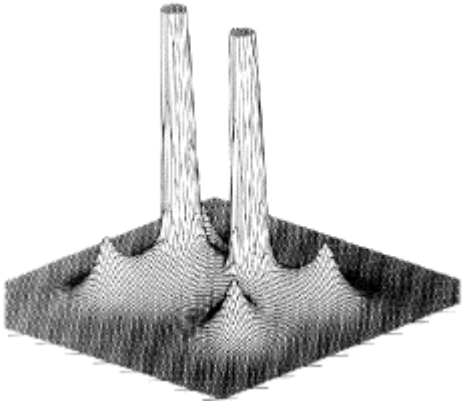
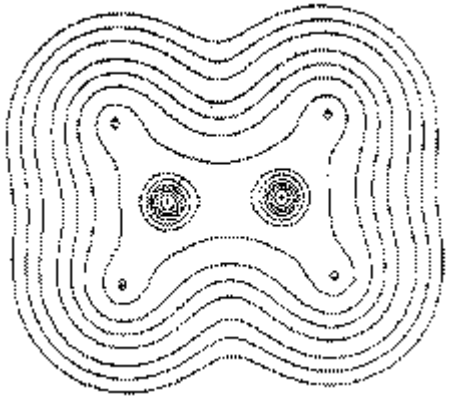
C10
C1
C8
C5
C6
C7
C9

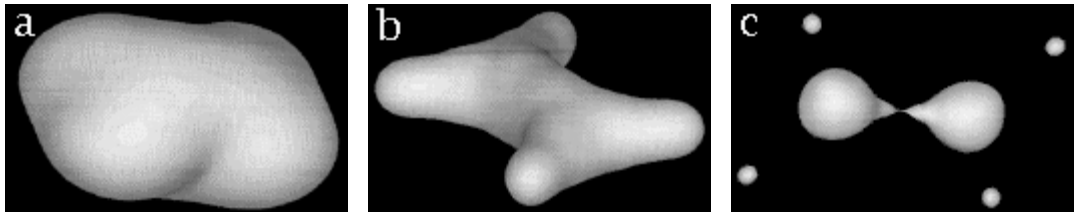

C(19)
O(1)
C(20)
Co(1)
N(1)
N(5)
N(3)
C(2)


N(2)
Co(1)
N(1)
N(5)
H(1A)
H(5C)
N(4)

Prikazi elektronske gustoće





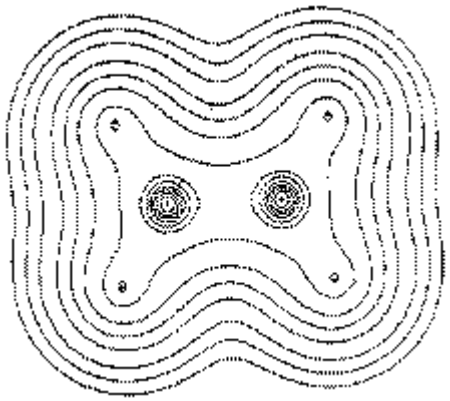


AIM

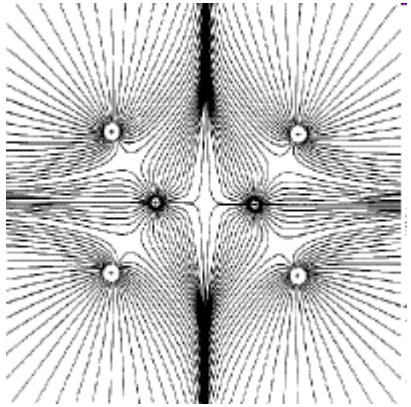
- Atoms In Molecules
- Raspodjela elektronske gustoće u prostoru definira strukturu molekule
- Kako definirati atome, veze itd. u oblaku molekulske elektronske gustoće?

Topologija funkcije gustoće

- Gradijenti, polja, kritične točke i atraktori



envelopa



gradijent

Gradijent – $\nabla\rho$

Vektorsko polje gradijenta – skup svih gradijenatnih putanja

Kritična točka

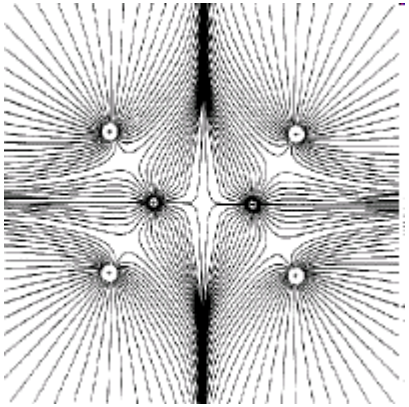
Atraktor – točka u kojoj se spajaju putanje gradijenata – razdjeljuju molekulu na područja pod utjecajem pojedinih atraktora

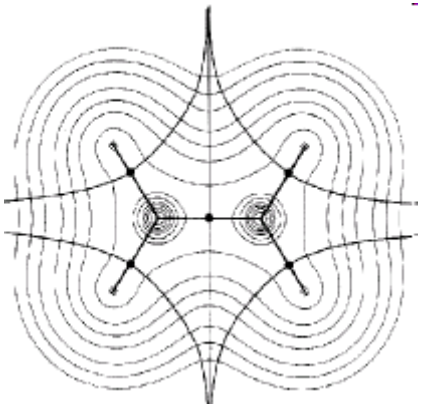
Kritične točke

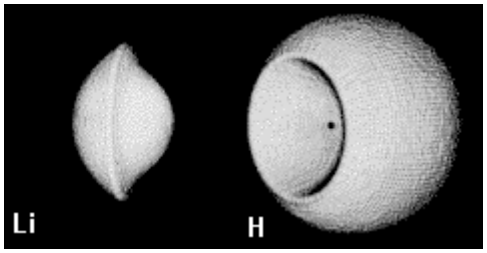
- Atraktori – maksimumi
- Kritične točke veze – sedlaste točke (u 2 smjera maksimum)
- Kritične točke prstena – sedlaste točke (u 2 smjera minimum)
- Kritične točke kaveza - minimumi

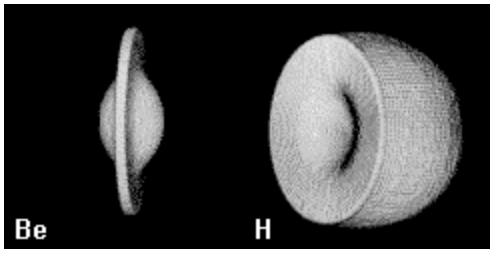
Atom

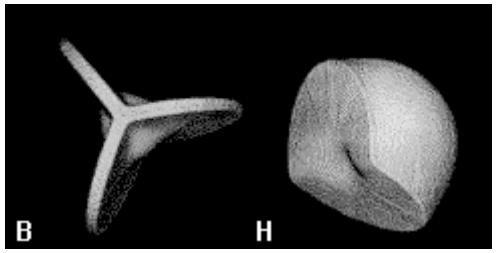
- Jezgra je atraktor
- Pripadni atom je dio prostora u kojemu sve putanje gradijenata imaju isti atraktor
- Postoji skup putanja gradijenata bez atraktora – granice među atomima

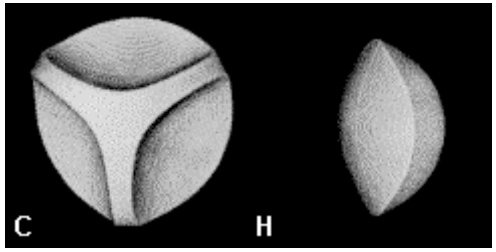


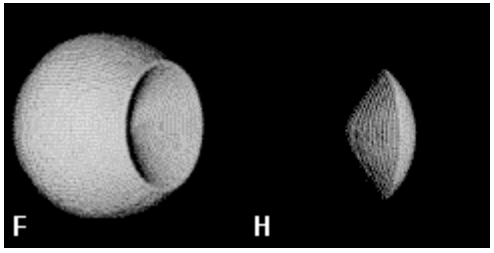


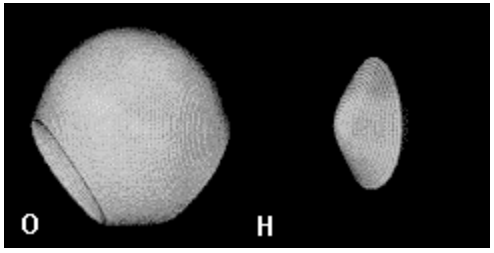

Li
H

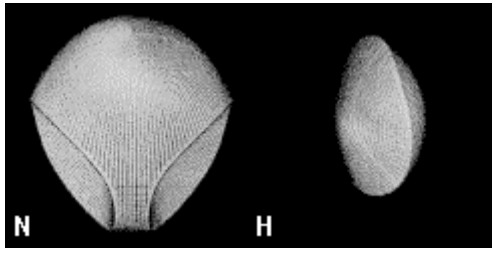

Be
H


B
H


C
H

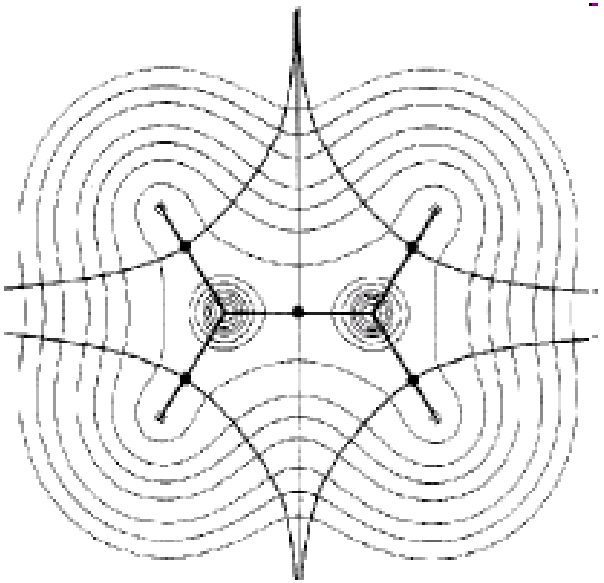

F
H


O
H


N
H

Veza

- Za svaki par atraktora postoji jedna putanja gradijenta koja ih povezuje – veza



Svojstva veze

- Vezna udaljenost
- Gustoća naboja u kritičnoj točki
- Eliptičnost

Kovalentnost i ionskost veze

- Što znači da je veza kovalentna?
- Je li kovalentnija C-O ili C=O?

‘Udio ionske veze’

- Pauling:

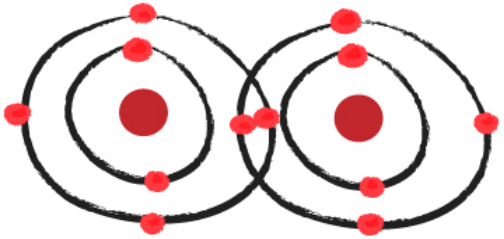
$$\left(1 - e^{-\left(\frac{\Delta\chi}{2}\right)^2}\right) * 100\%$$

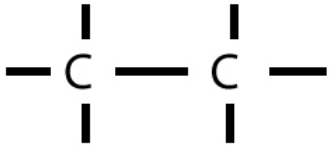
- Preko dipolâ:

$$\left(\frac{\mu_{\text{obs}}}{\mu_{\text{calc}}}\right) * 100\%$$

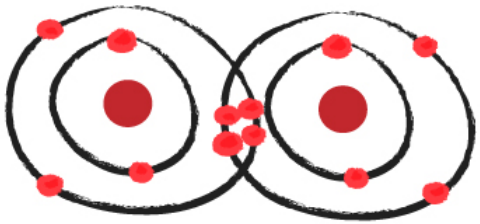
$(\mu_{\text{calc}}) =$ molekulski dipol za slučaj da je veza potpuno ionska ($q = Z$)

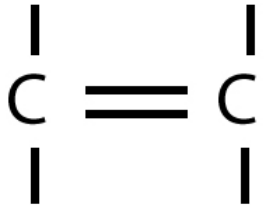
Red veze



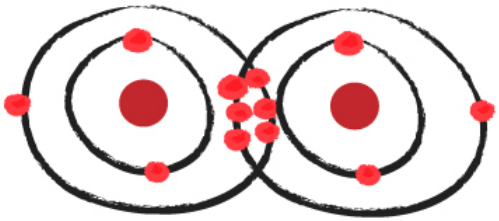


JEDNOSTRUKA



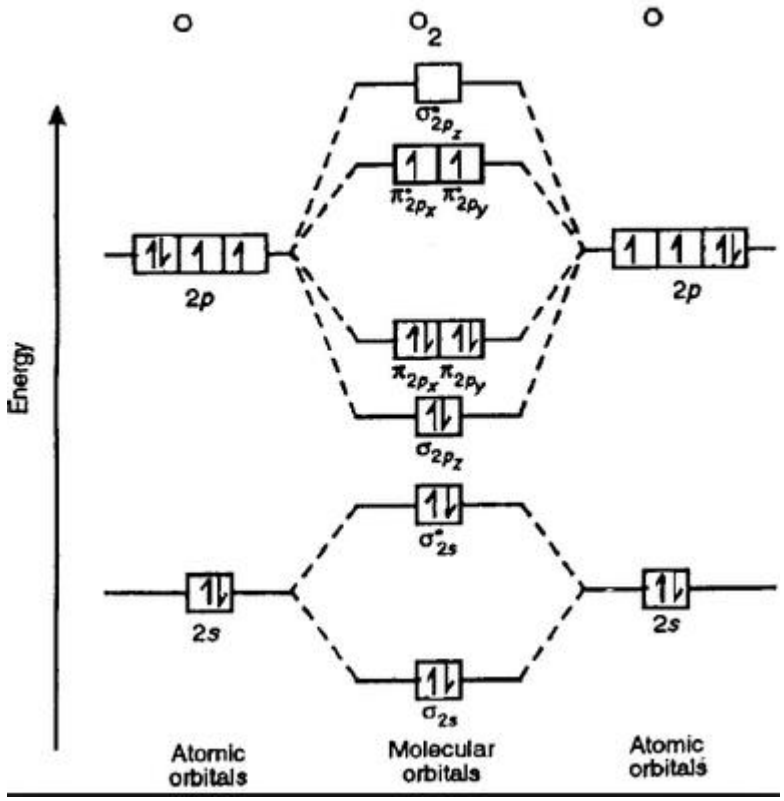


DVOSTRUKA



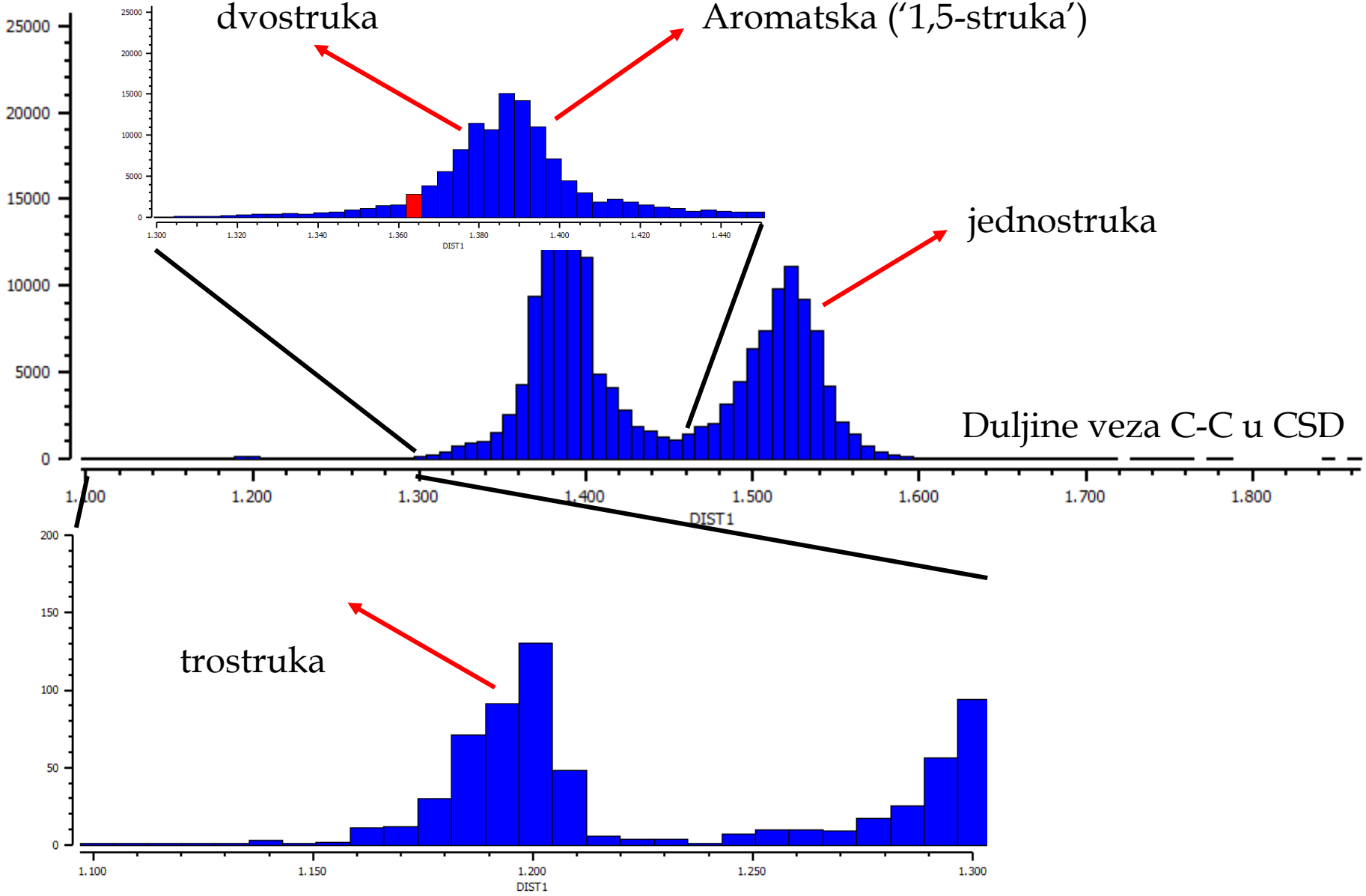
TROSTRUKA

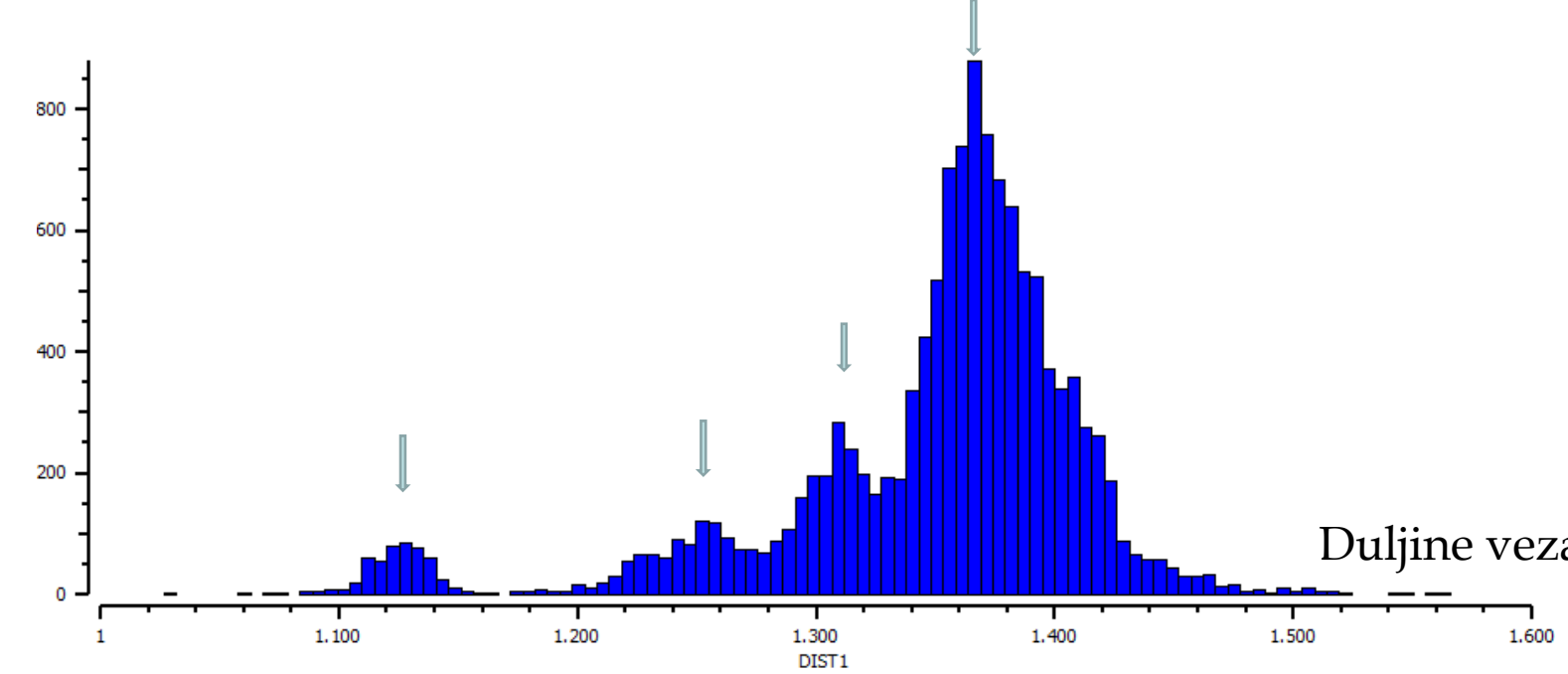
Molekulske orbitale



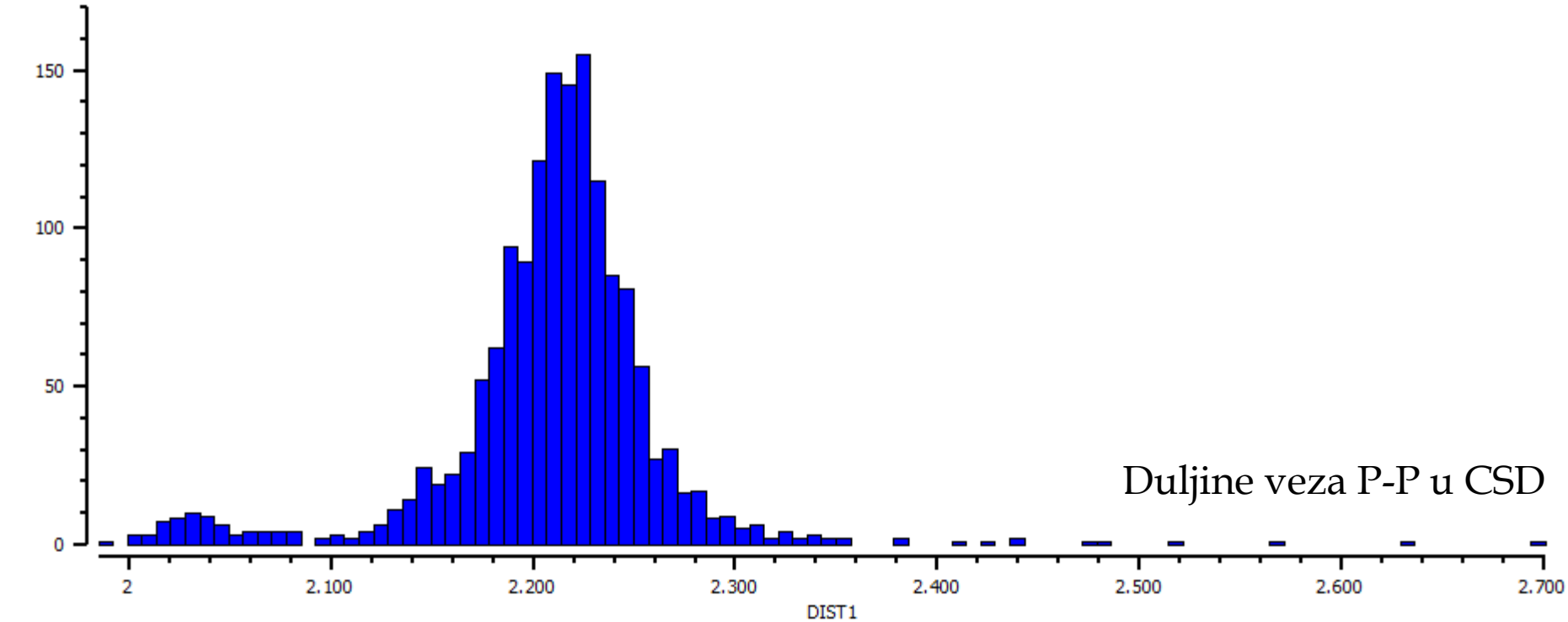
Red veze = $(N(\mathrm{e}_{\mathrm{vezni}}) - N(\mathrm{e}_{\mathrm{protuvezni}}))/2$

Red veze i duljina veze

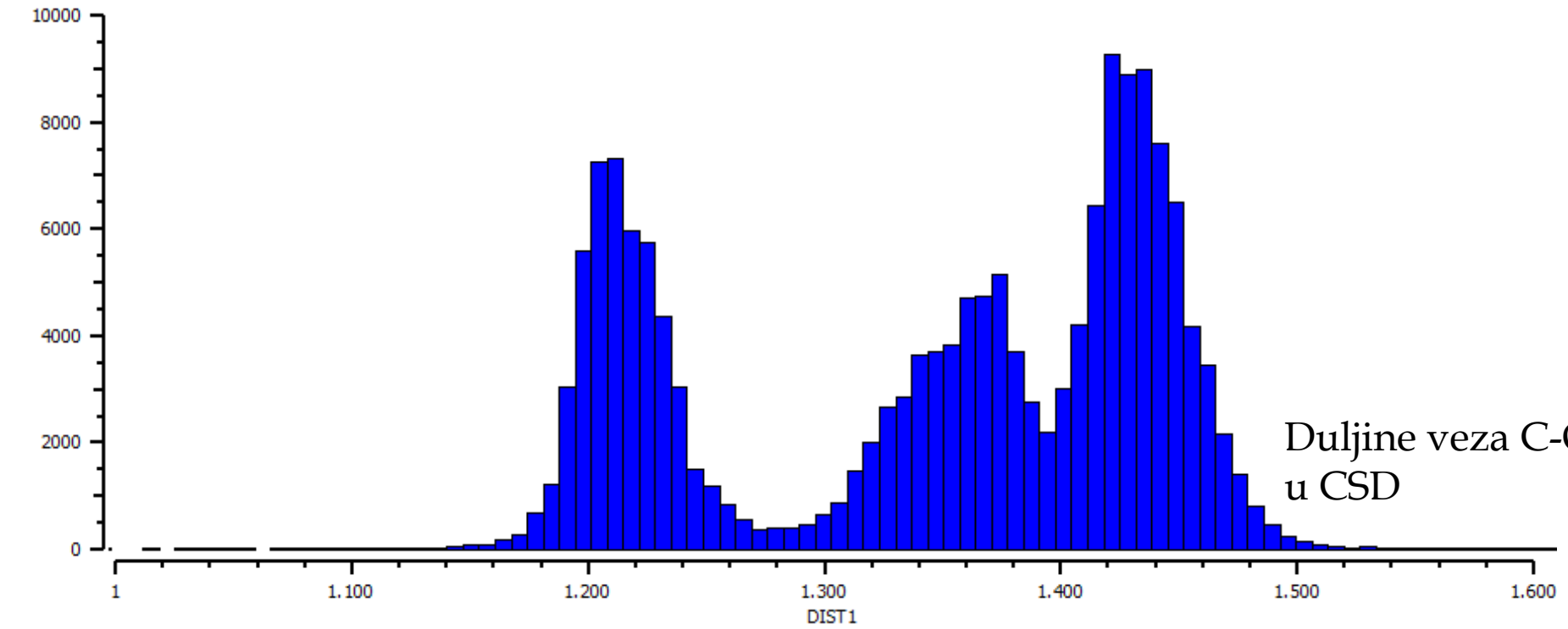




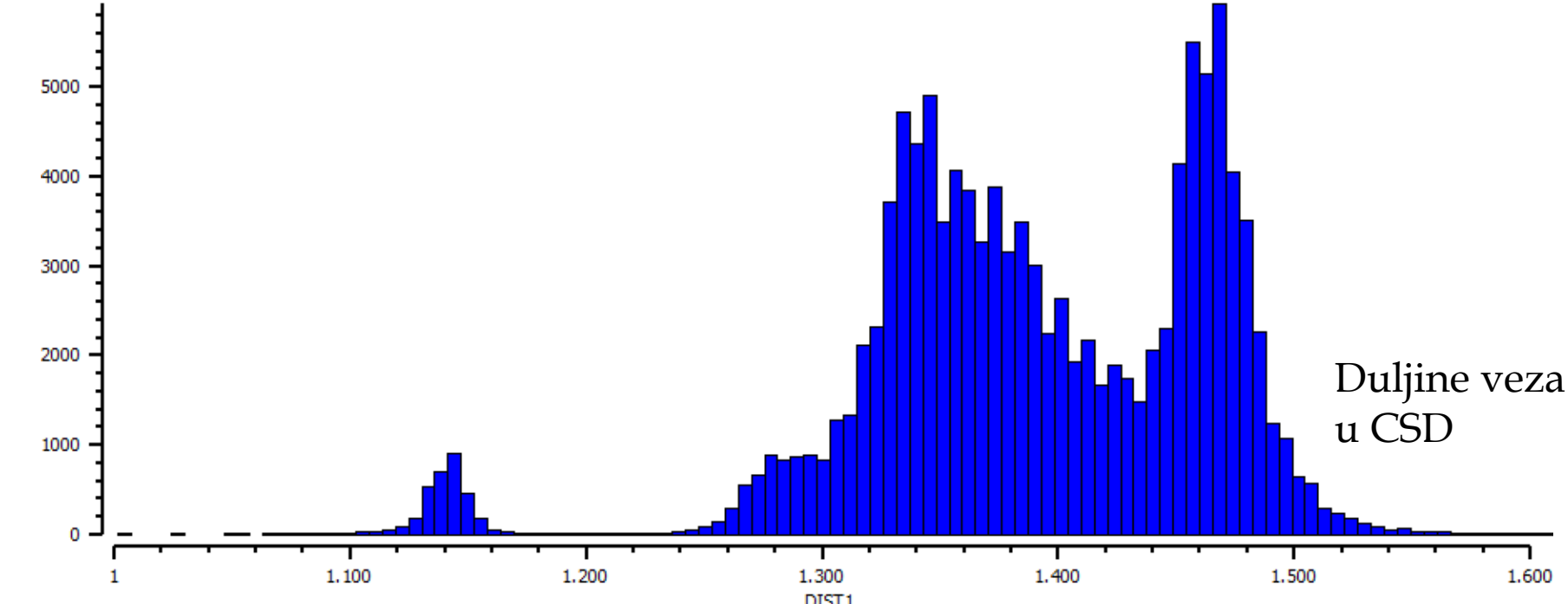
Duljine veza N-N u CSD



Duljine veza P-P u CSD



Duljine veza C-O u CSD



Duljine veza C-N u CSD

Duljina veze i red veze

duljina idealne jednostruke veze

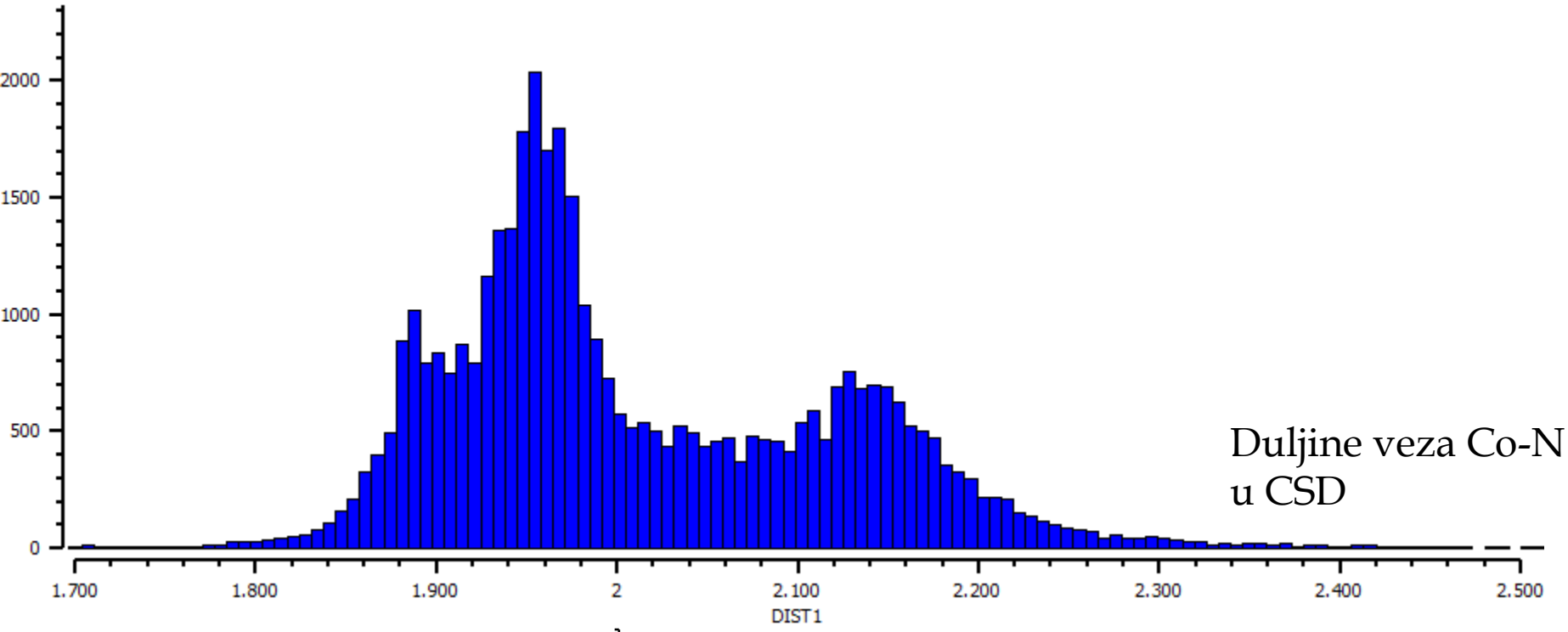
duljina veze

$$S = \exp\left(\frac{d_0 - d}{b}\right)$$

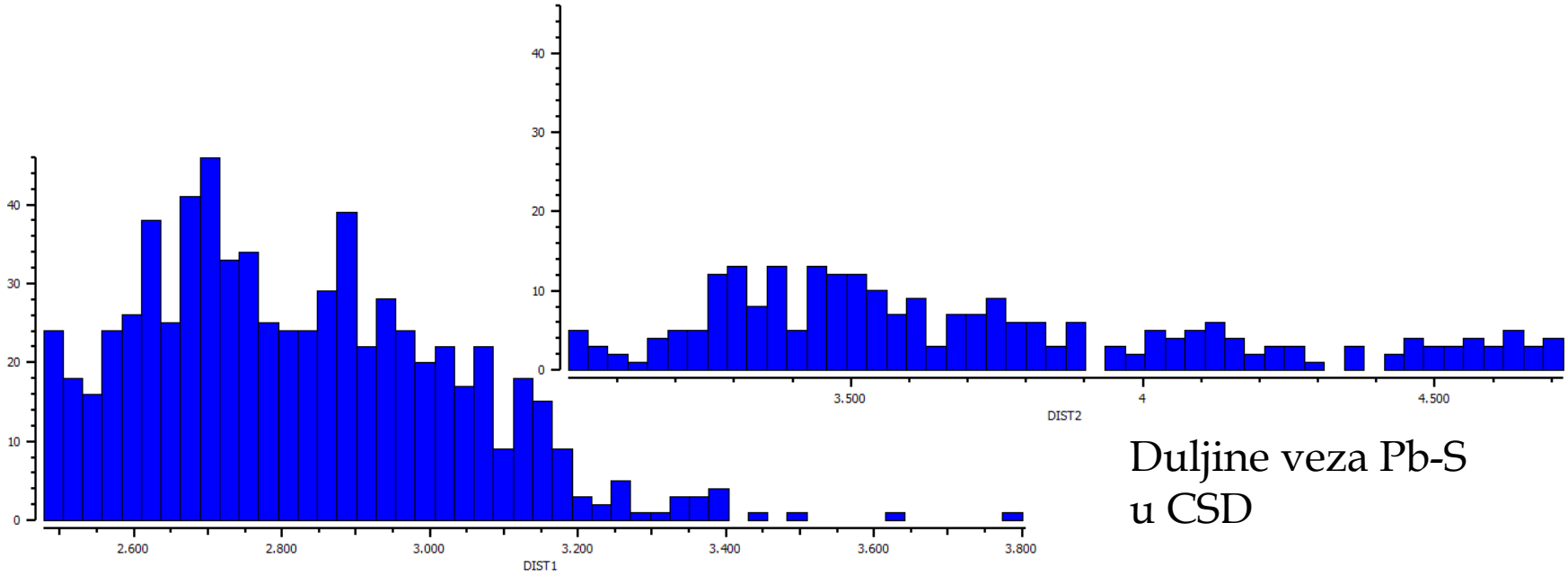
Ugodivi parametar (obično oko 0,37 Å, npr za C 0,352 Å)

Alternativno:

$$S' = \left(\frac{d}{d_0}\right)^{-6}$$



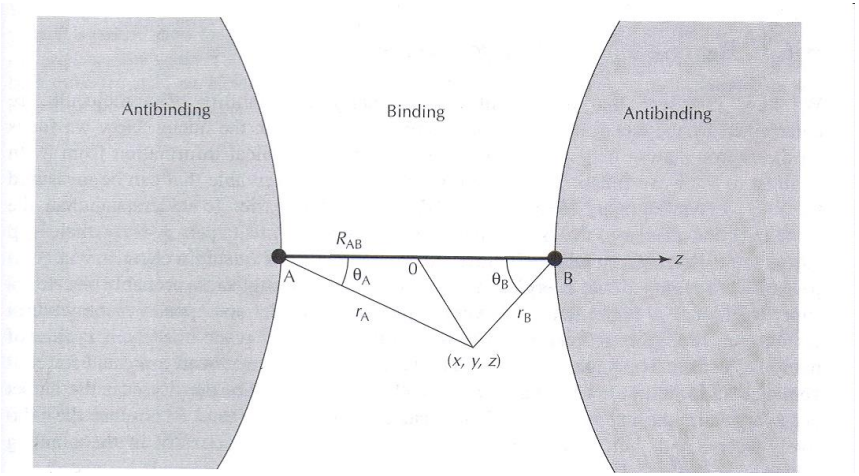
Duljine veza Co-N u CSD



Duljine veza Pb-S u CSD

Ako znamo elektronsku gustoću...

Sila koja djeluje na atomsku jezgru jednaka je zbroju kulonskih sila kojom na nj djeluju ostale jezgre i one kojom na nj djeluje elektronski oblak



$$F_{X_\gamma} = -Z_\gamma \left(\int \mathrm{d}\mathbf{r}\ \rho(\mathbf{r}) \frac{x - X_\gamma}{|\mathbf{r} - \mathbf{R}_\gamma|^3} - \sum_{\alpha \neq \gamma}^{M} Z_\alpha \frac{X_\alpha - X_\gamma}{|\mathbf{R}_\alpha - \mathbf{R}_\gamma|^3} \right).$$

Elektronska gustoća između jezgara je vezna

Elektronska gustoća s vanjske strane jezgara je protuvezna

Razlika integrala vezne i protuvezne = red veze * 2

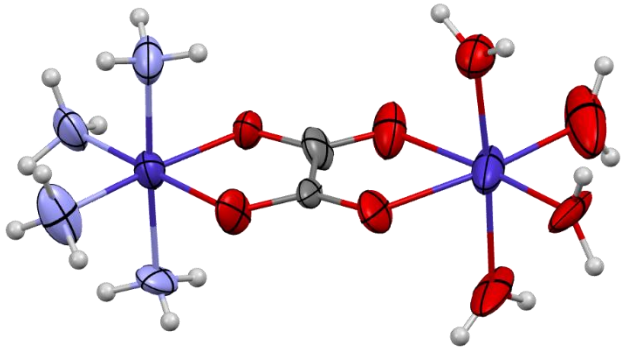
Valencija

Metoda vezne valencije (*bond valency sum*):

Valencija atoma = zbroj redova svih veza koje neki atom čini

- Pogodna metoda za određivanje oksidacijskih stanja temeljem geometrijskih parametara

BVS = 3,49

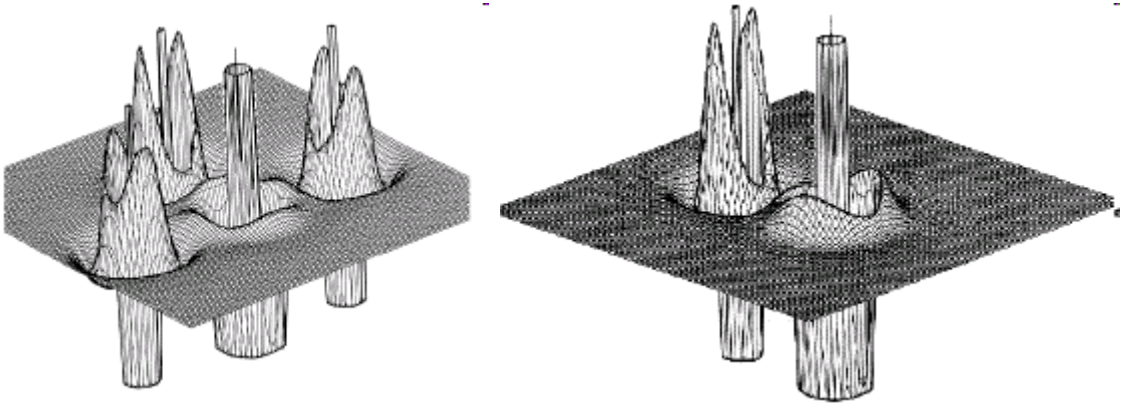


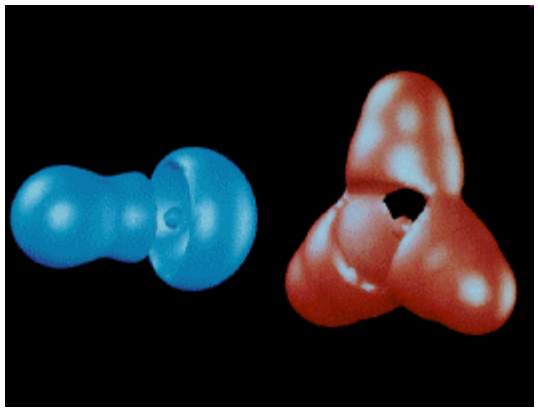
BVS = 2,10

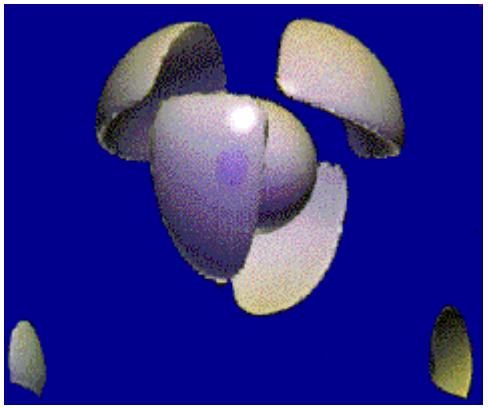
$[(NH_3)_4CoC_2O_4Co(H_2O)_4]^{3+}$.

Nevezni parovi – Laplacian elektronske gustoće

- Suvišak ($\nabla^2\rho < 0$) ili manjak ($\nabla^2\rho > 0$) elektronske gustoće – lociranje neveznih elektrona

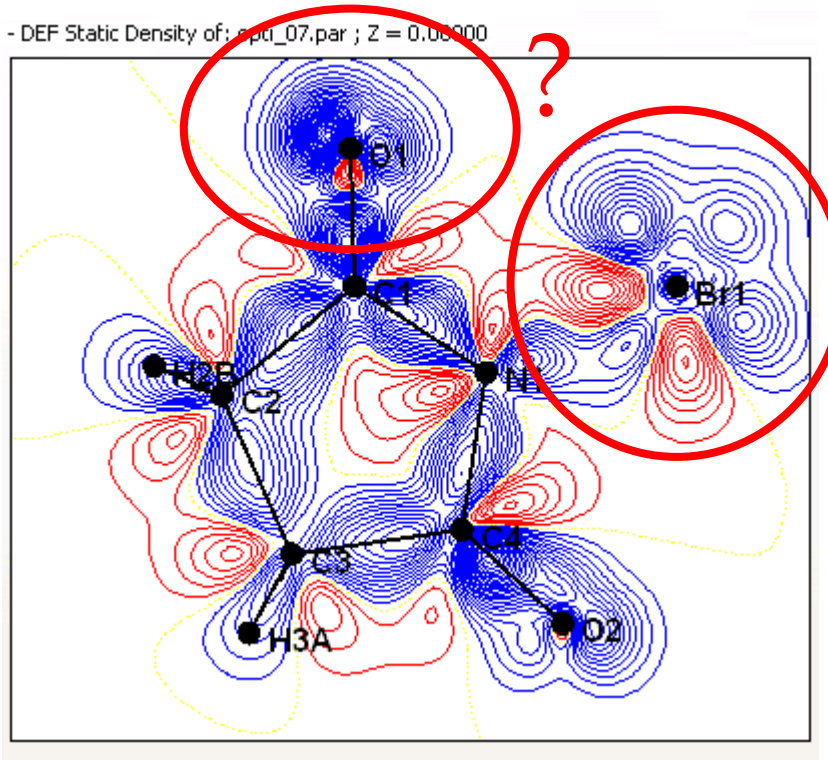


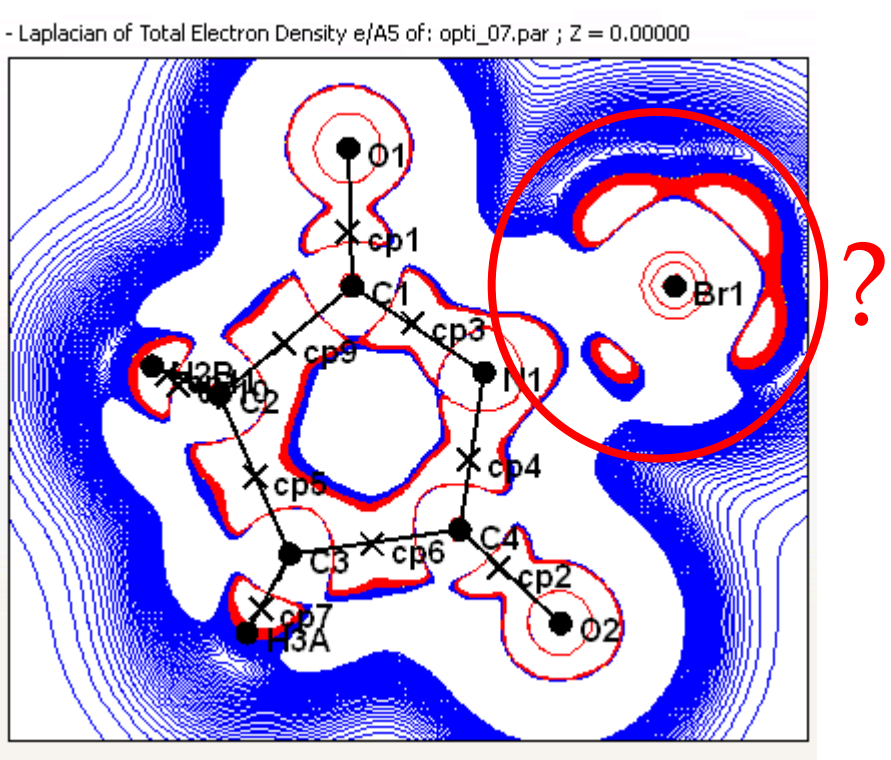




Ali...

- Za gledati fine detalje treba i fina mapa elektronske gustoće...





CAPVT IIa

Vezno, nevezno (ali ne i bezvezno)

Međumolekulske interakcije

- Interakcija permanentnih dipola (Keesomova sila)
- Interakcija permanentnog i induciranog dipola
- Interakcija induciranih dipola (disperzna, Londonova sila)
- Jaka vodikova veza
- Slaba vodikova
- Halogenska veza
- Međuhalogenska veza

- Interakcija π—π
- Interakcija π—kation
- Interakcija π—anion
- Interakcija π—halogen
- Interakcija π—halkogen (O, Te)
- Interakcija π—N
- N–H··· Cl_2–M
- Interakcija halkogen—halkogen
- ...

Najjednostavnije međumolekulske interakcije

- Interakcija permanentnih dipola (Keesomova sila)
- Interakcija permanentnog i induciranog dipola
- Interakcija induciranih dipola (disperzna, Londonova sila)

} van der Waalsove sile (interakcije)

Da bi molekula imala električni dipol

- Mora biti polarne simetrije.
- Mora imati pogodnu raspodjelu naboja – prisuće atomâ velikih razlika u elektronegativnosti.
  - Dipolni momenti obično reda veličine (10^{-30} – 10^{-29}) C m.
  - Pogodna jedinica

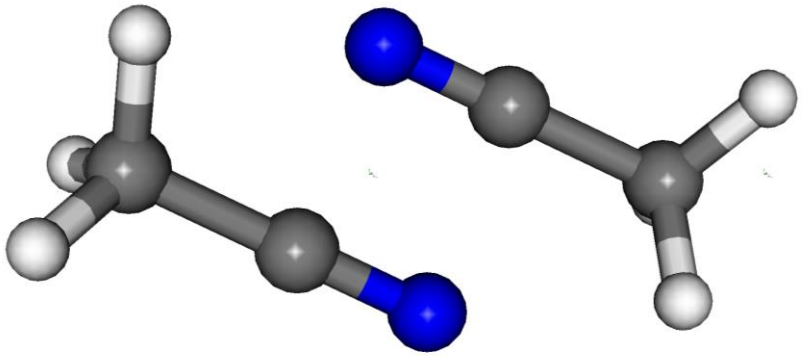
  D ≈ 3.33564×10^{-30} C·m

Molekula	μ/D
H_2O	1,8546(40)
HF	1,82618(6)
HCl	1,1086(3)
NH_3	1,14718
$CHCl_3$	1,04(2)
$(CH_3)_2CO$	2,88(3)
$(CH_3)_2SO$	3,96(4)
C_2H_5OH	1,69(3)
HCN	2,985188

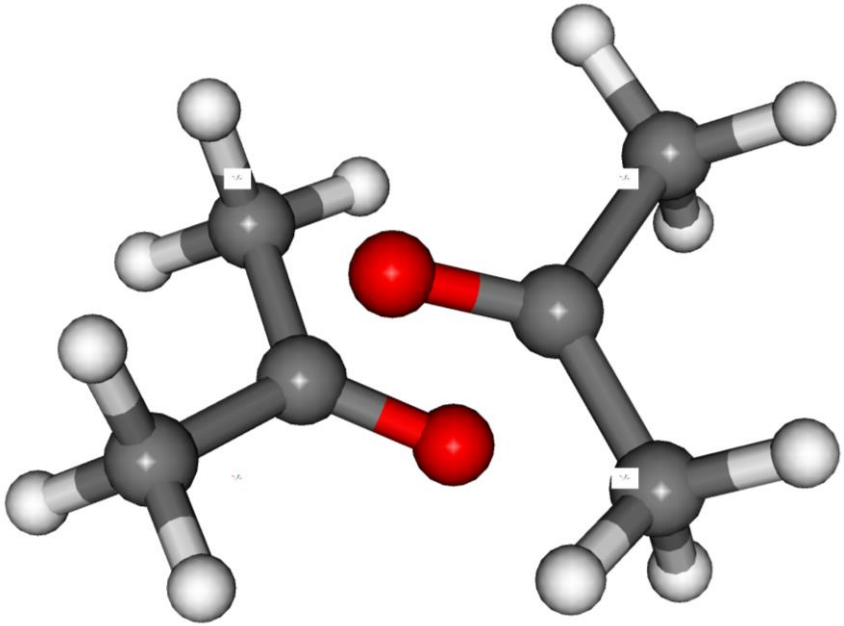
Određivanje dipolnog momenta molekule

- Mjerenjem dielektrične konstante (Clausius-Mosotti-Debyeova jednadžba).
- Iz rotacijskih spektara (Starkov učinak).
- Račun (*ab initio* ili semiempirijski) – nuždno poznavanje razmještaja atomâ u molekuli.

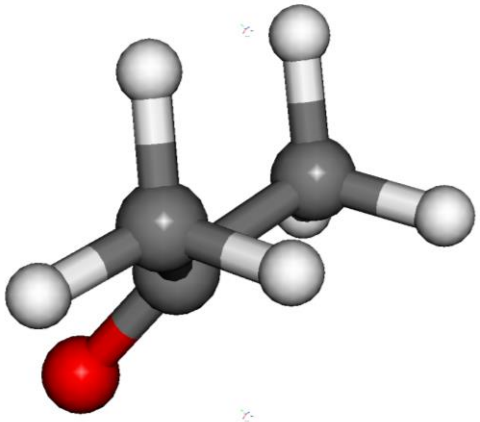
Energije dipolnih interakcija



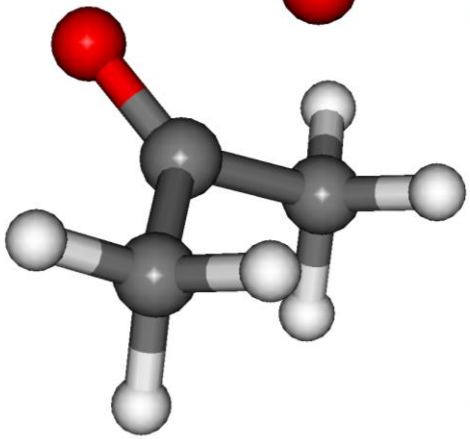
-16,0 kJ mol^{-1}



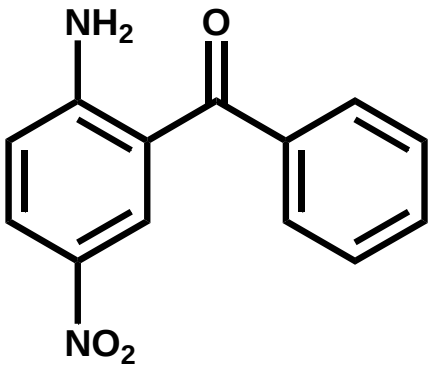
-22,3 kJ mol^{-1}

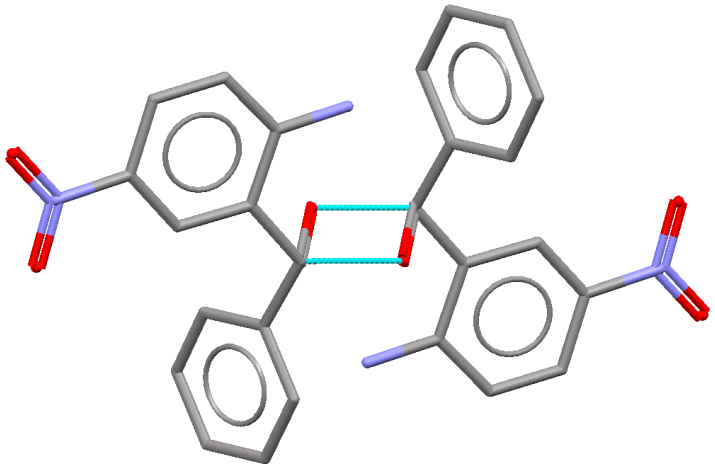


-7,6 kJ mol^{-1}



Približavanje karbonila – dipolna interakcija ili početak nukleofilne adicije?





Vodikova veza

An *A*–H···*B* interaction is called a hydrogen bond if 1) it constitutes a local bond, and 2) *A*–H acts as a proton donor to *B*.

***Interakcija* A–*H*···B *naziva se vodikovom vezom ako je 1) u pitanju lokalna veza, i 2)* A–*H djeluje kao proton-donor prema* B.**

T. Steiner, *Angew. Chem.*, **41** (2002), 41-76.

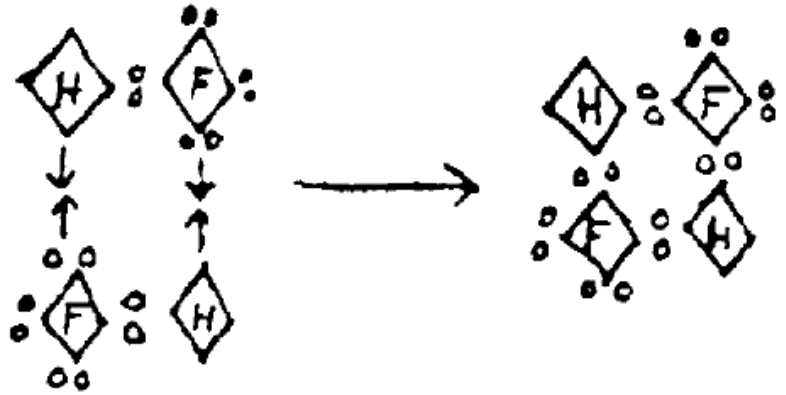
Podjela prema G. A. Jeffreyju (1997.)

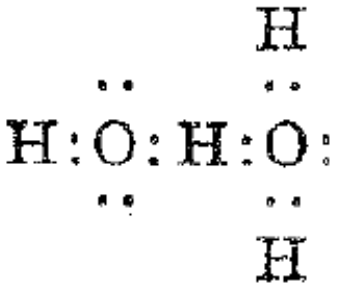
	jaka	srednja	slaba
vrsta interakcije	kovalentna	elektrostatska	elektrostatska / disperzijska
duljina veze H···*A* (Å)	1,2 – 1,5	1,5 – 2,2	> 2,2
produljenje veze *X*–H (Å)	0,08 – 0,25	0,02 – 0,08	< 0,02
omjer *X*–H/H···*A*	*X*–H ≈ H···*A*	*X*–H < H···*A*	*X*–H << H···*A*
X···*A* (Å)	2,2 – 2,5	2,5 – 3,2	> 3,2
usmjerenost	jaka	srednja	slaba
kut (°)	170 – 180	> 130	> 90
energija veze (kcal mol^{-1})	15 – 40	4 – 15	< 4
rel. pomak u IR spektru (cm^{-1})	25 %	10 – 25 %	< 10 %

Kovalentna?

G. N. Lewis, 1916.

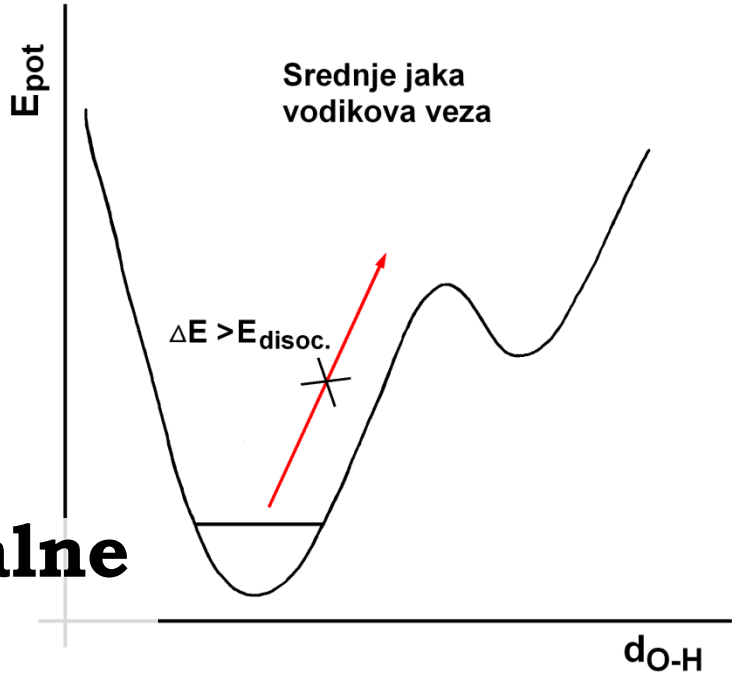
M. L. Huggins, 1919.





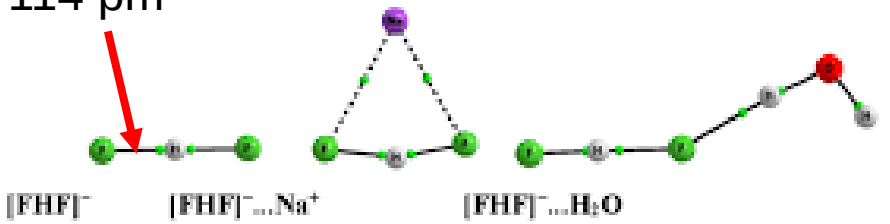
Latimer & Rodebush, 1920.

Potencijalne jame

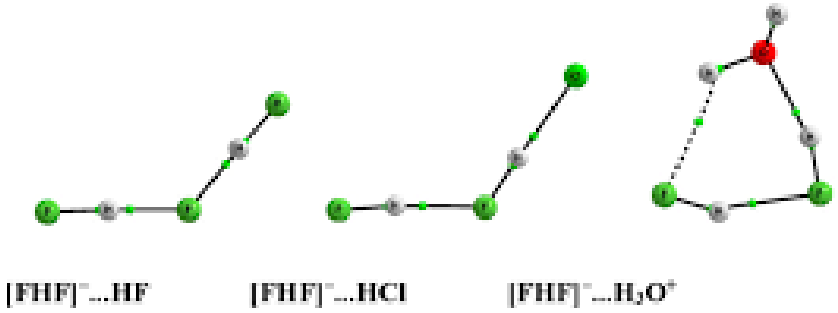


Jaka vodikova veza: hidrogendifluoridni anion (HF_2^-)

114 pm

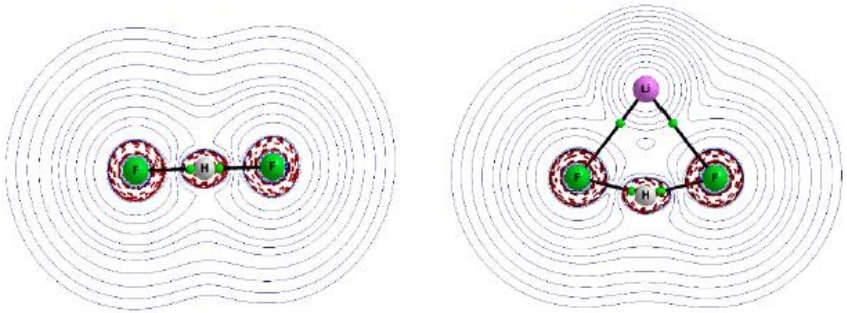


[FHF]⁻ [FHF]⁻...Na⁺ [FHF]⁻...H₂O



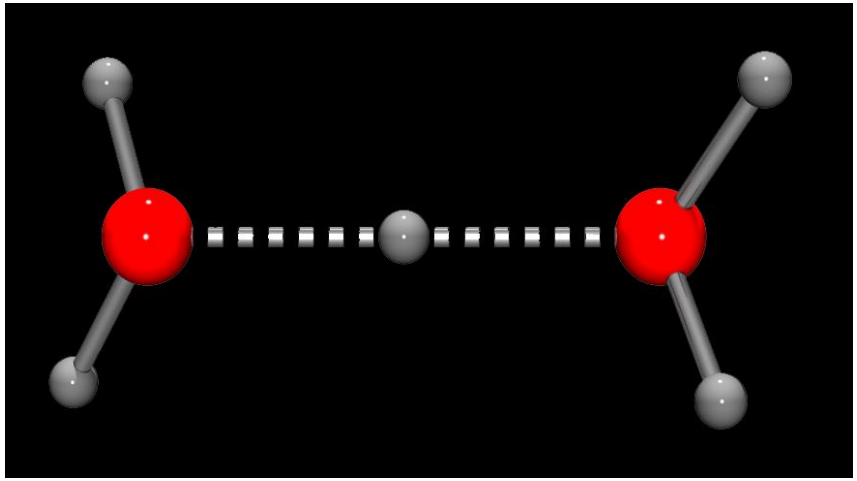
[FHF]⁻...HF [FHF]⁻...HCl [FHF]⁻...H₃O⁺

Energija veze > 155 kJ/mol. (energija veze u molekuli HF 565 kJ/mol, a u molekuli F_2 = 155 kJ/mol).

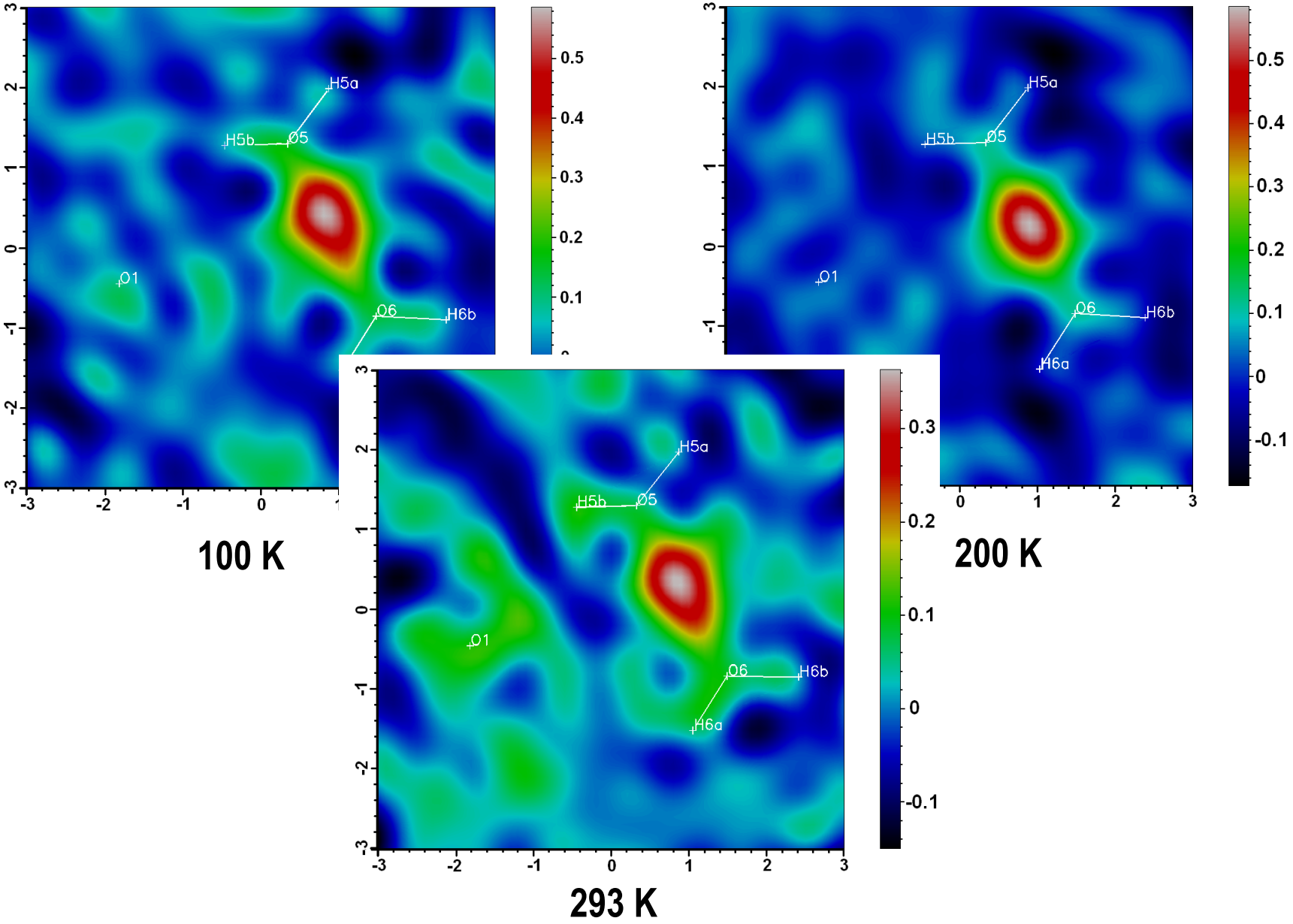


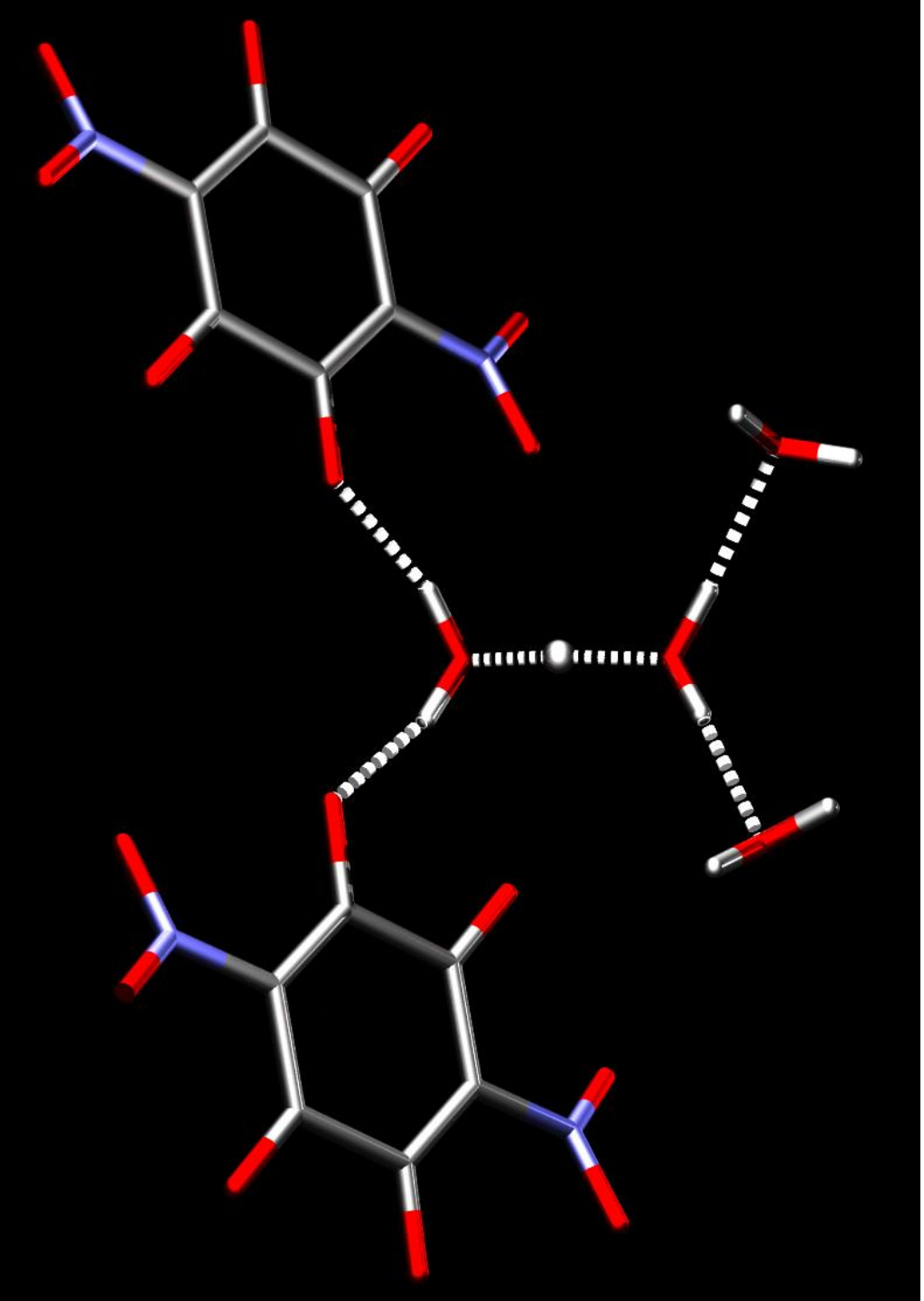
[FHF]⁻ [FHF]⁻...Li⁺

Jaka vodikova veza: Zundelov ion ($H_5O_2^+$)



Gdje je proton?

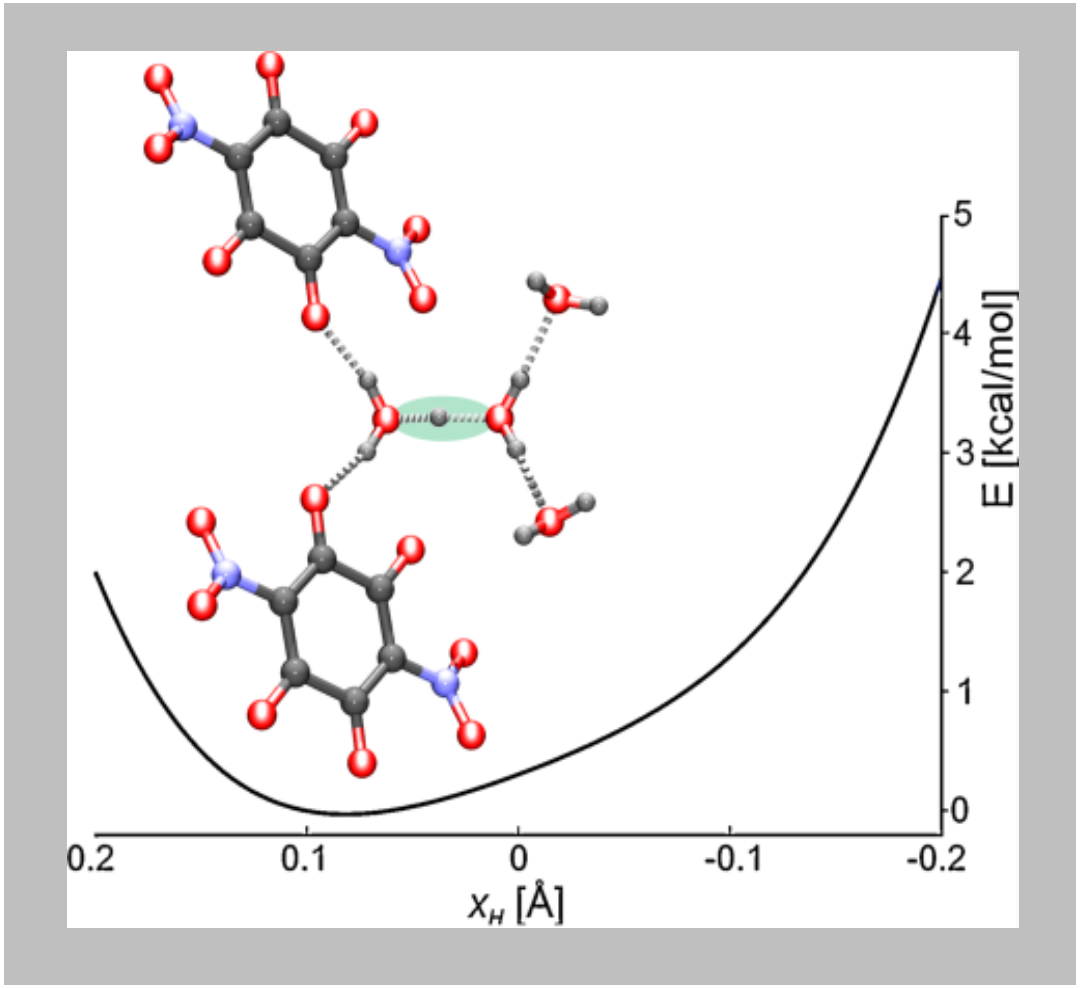




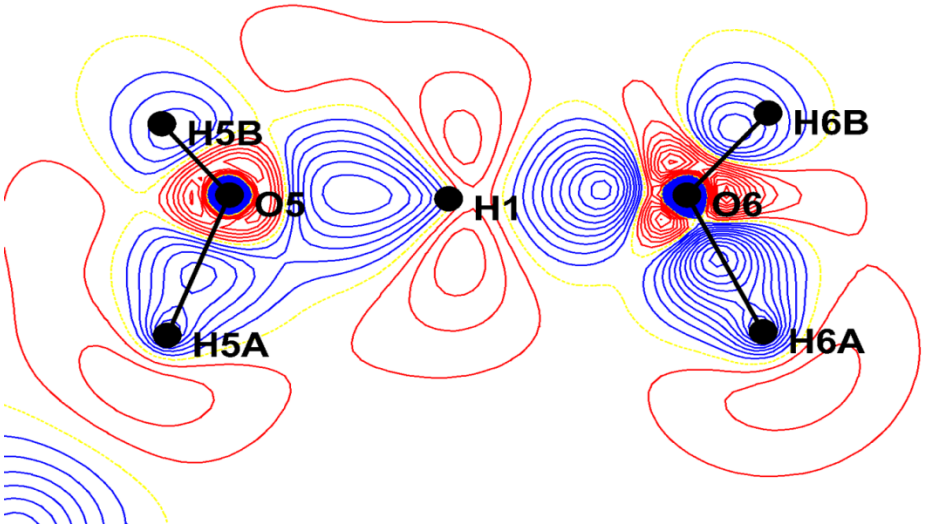
Duljina veze
O···H···O:

100 K	**2.433(2)**
150 K	**2.433(2)**
200 K	**2.433(2)**
250 K	**2.436(2)**
293 K	**2.438(2)**

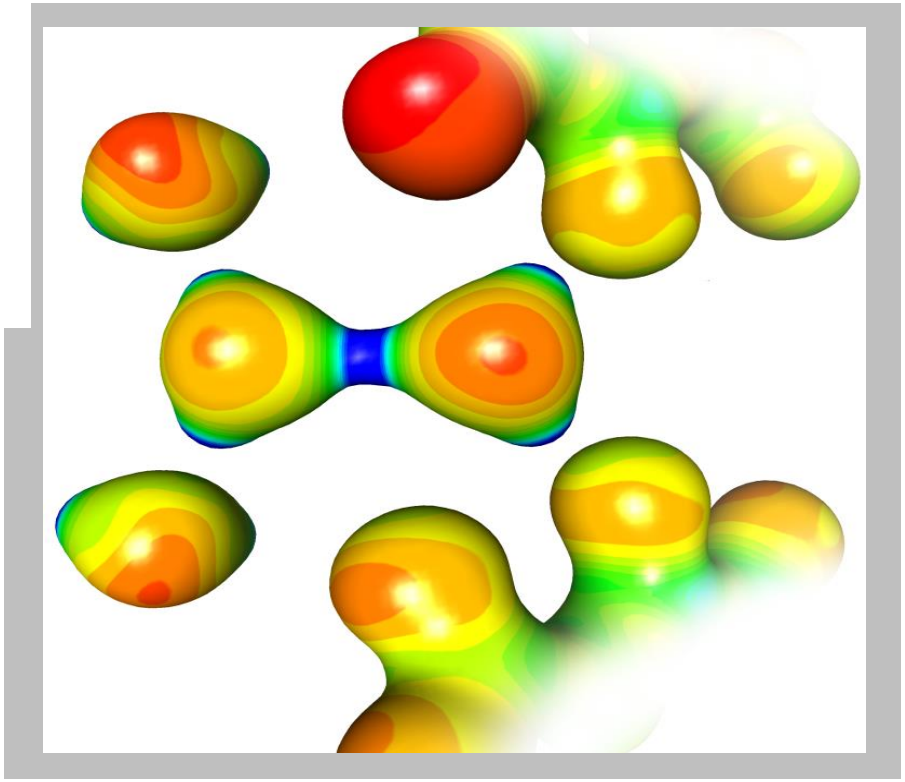
Iz kvantno-kemijskih računa:



Gustća naboja na Zundelovom ionu



Površina: 0,5 e Å-3

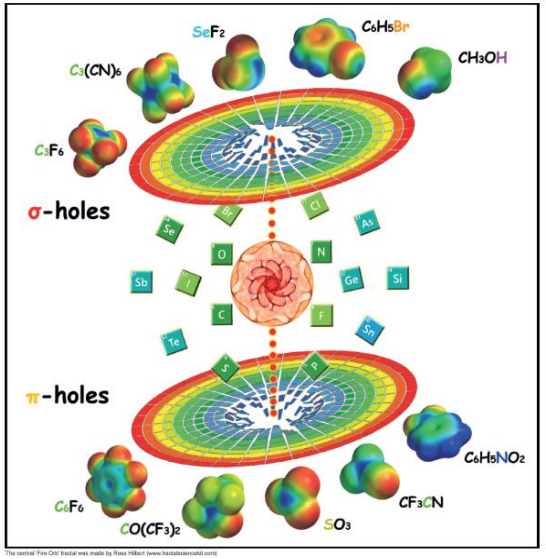


Molčanov, K., Jelsch, C., Wenger, E., Stare, J., Madsen, A.Ø., Kojić-Prodić, B. CrystEngComm, 2017, 19(28), 3898-3901

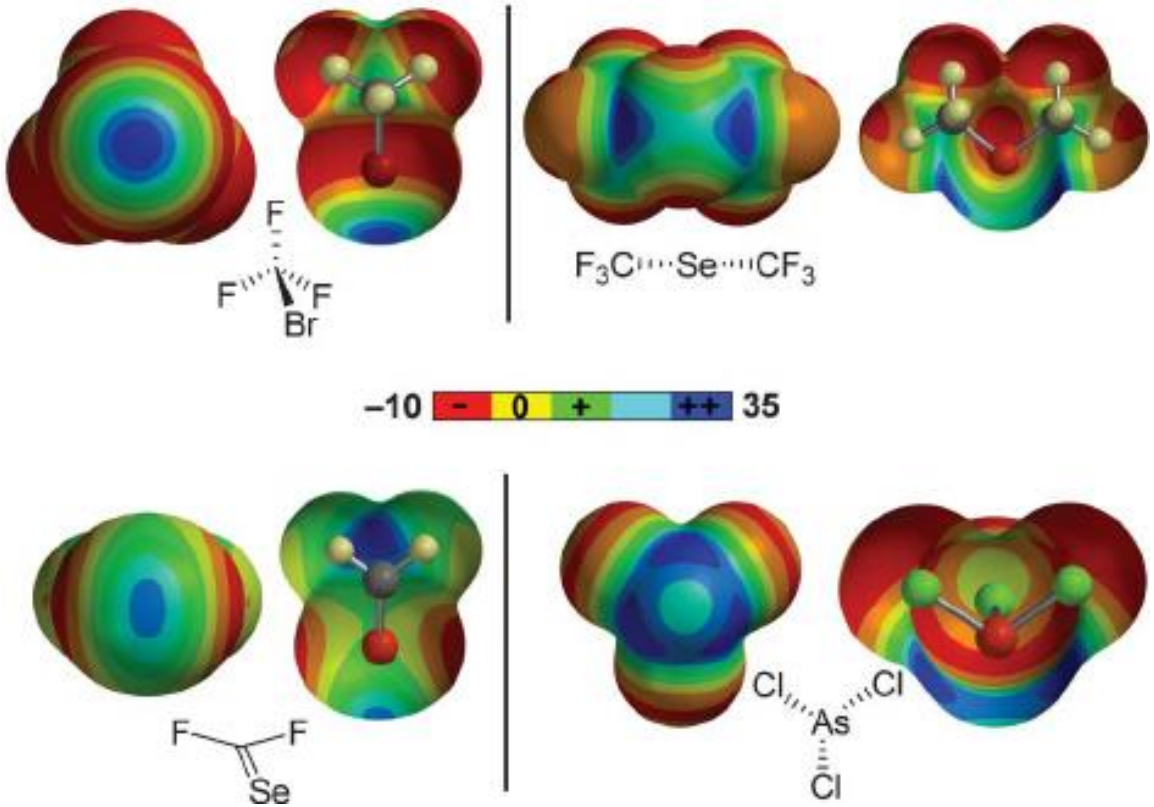
Interakcije σ-šupljine

Svi teški atomi su polarizabilni – nasuprot kovalentne veze imaju manjak elektrionske gustoće – Lewisove kiseline (elektrofili)

Halogenska veza
Halkogenska veza
Pnikogenska veza
Tetrelna veza
Trielna veza
Aerogenska veza



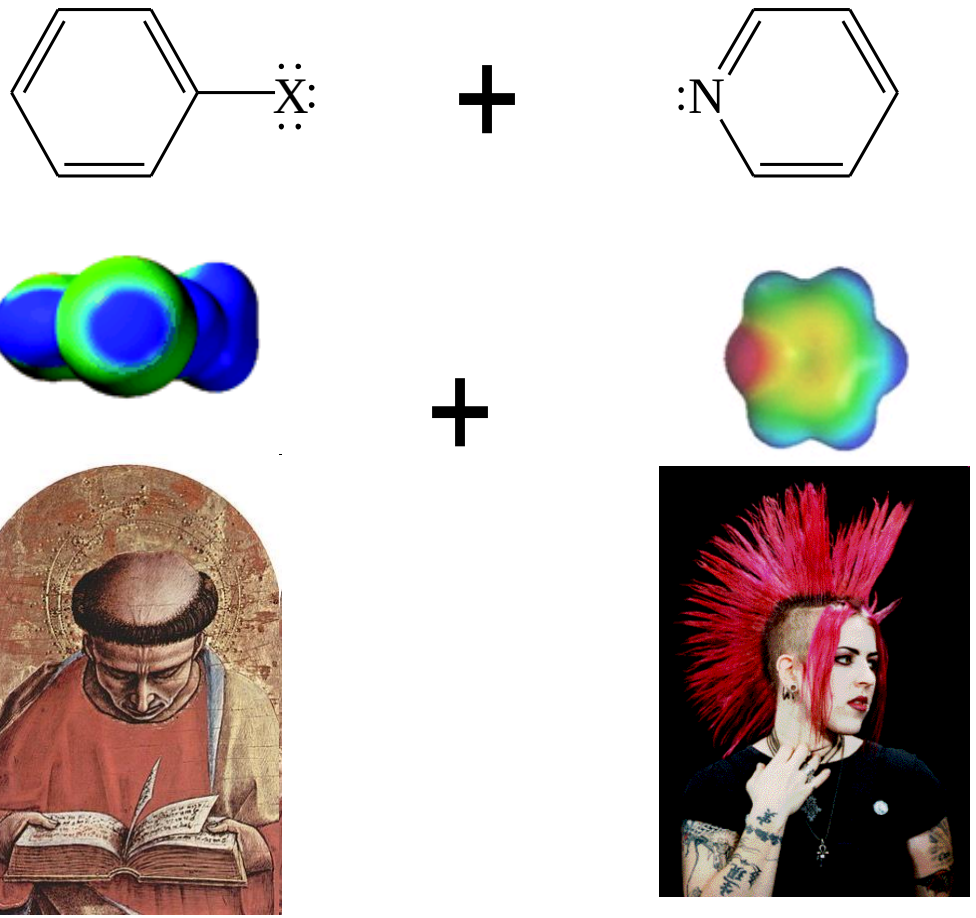
A. Bauza, T.J. Mooibroek, A. Frontera, The Bright Future of Unconventional σ/π-Hole Interactions, *ChemPhysChem.*, 2016, 16, 2496.



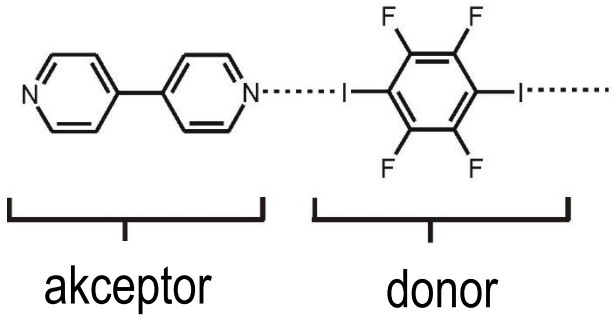
Halogenska veza

•A halogen bond occurs when there is evidence of a net attractive interaction between an electrophilic region associated with a halogen atom in a molecular entity and a nucleophilic region in another, or the same, molecular entity.

Pure Appl. Chem., 2013, 85, 1711.



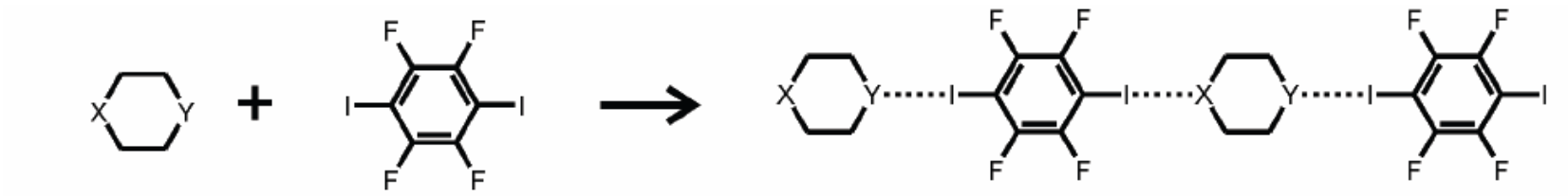
Halogenska veza

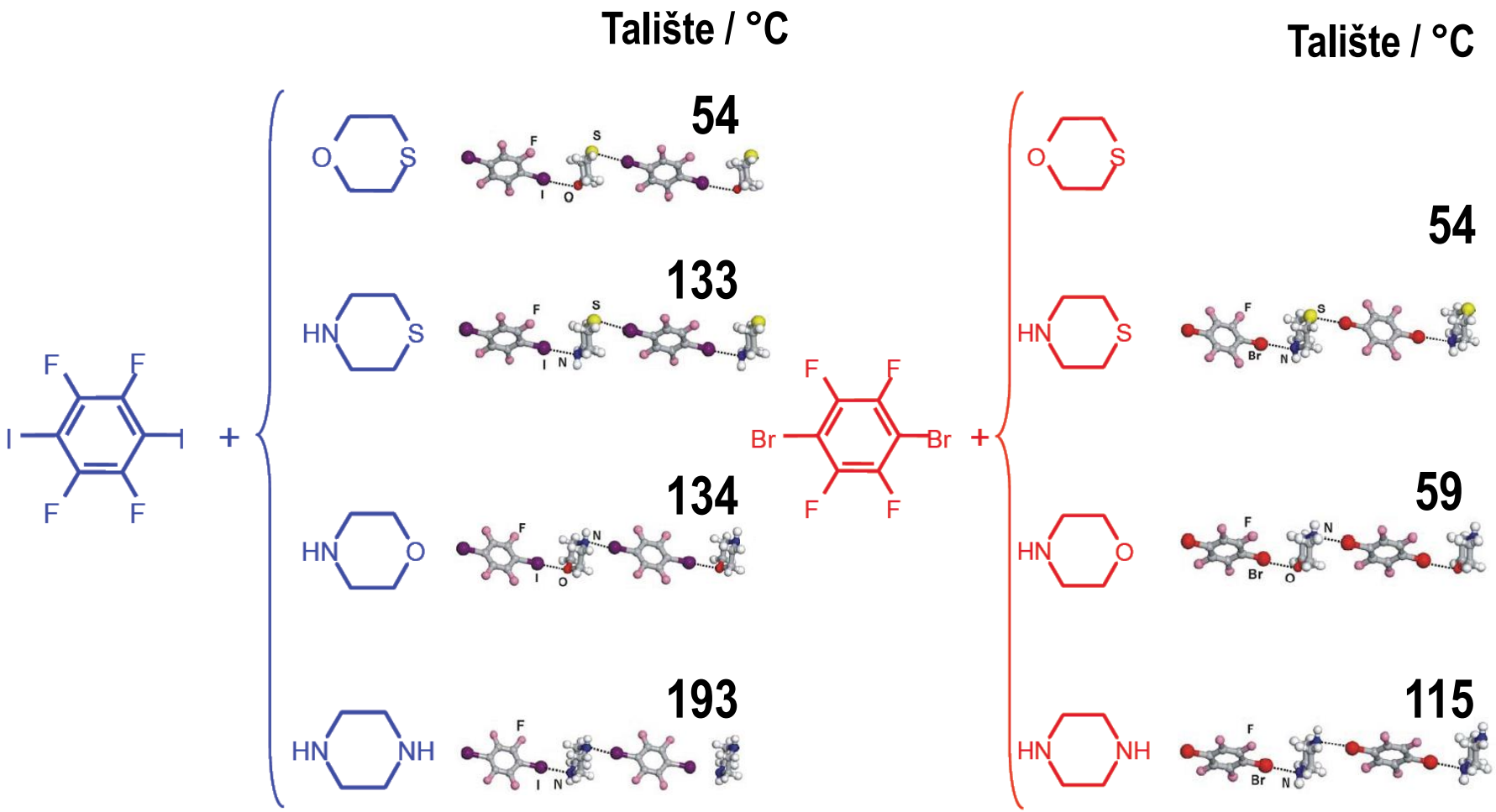


A··· X–Y

- Donor – polarizabilni (& polarizirani) atom halogena (I>Br>Cl>>F)
- Akceptor – Lewisove baze (N>O>S)
- Linearne (kut Y-X···A blizu 180°) i jake (neutralne 10–90 kJ mol^{-1} ionske > 150 kJ mol^{-1})

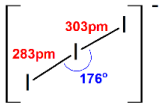
Heteroatomni derivati cikloheksana i *p*-dihalogentetrafluorbenzeni



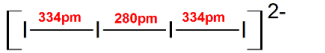


D. Cinčić, T. Friščić, W. Jones, *Chem. Eur. J.* 14 (2008) 747–753.

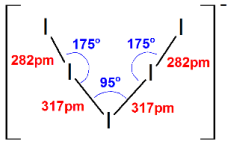
Jaka halogenska veza: polihalogenidni anioni



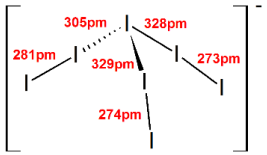
$[I_3]^-$ in $Cs^+[I_3]^-$



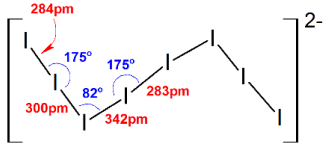
The linear $[I_4]^{2-}$ ion in $[Cu(NH_3)_4]^{2+}[I_4]^{2-}$



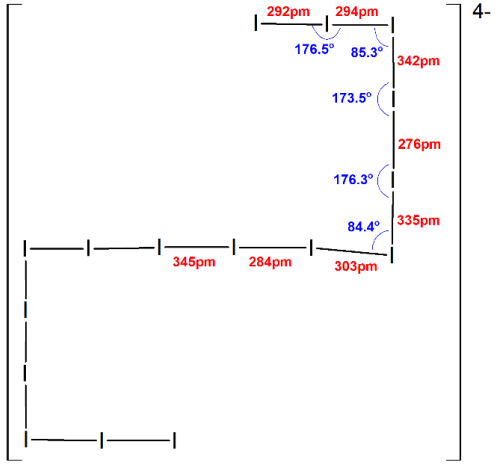
$[I_5]^-$ in $[Me_4N]^+[I_5]^-$



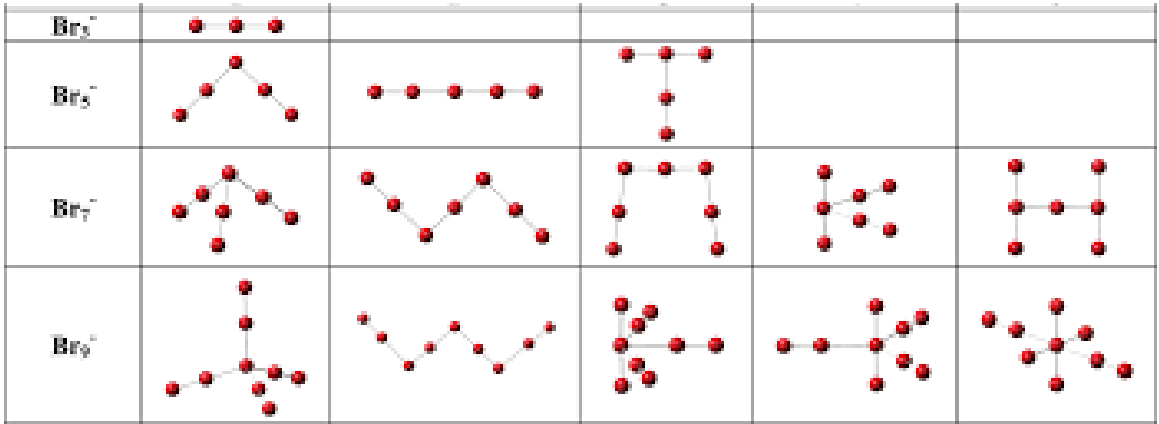
$[I_7]^-$ in $[Ph_4P]^+[I_7]^-$

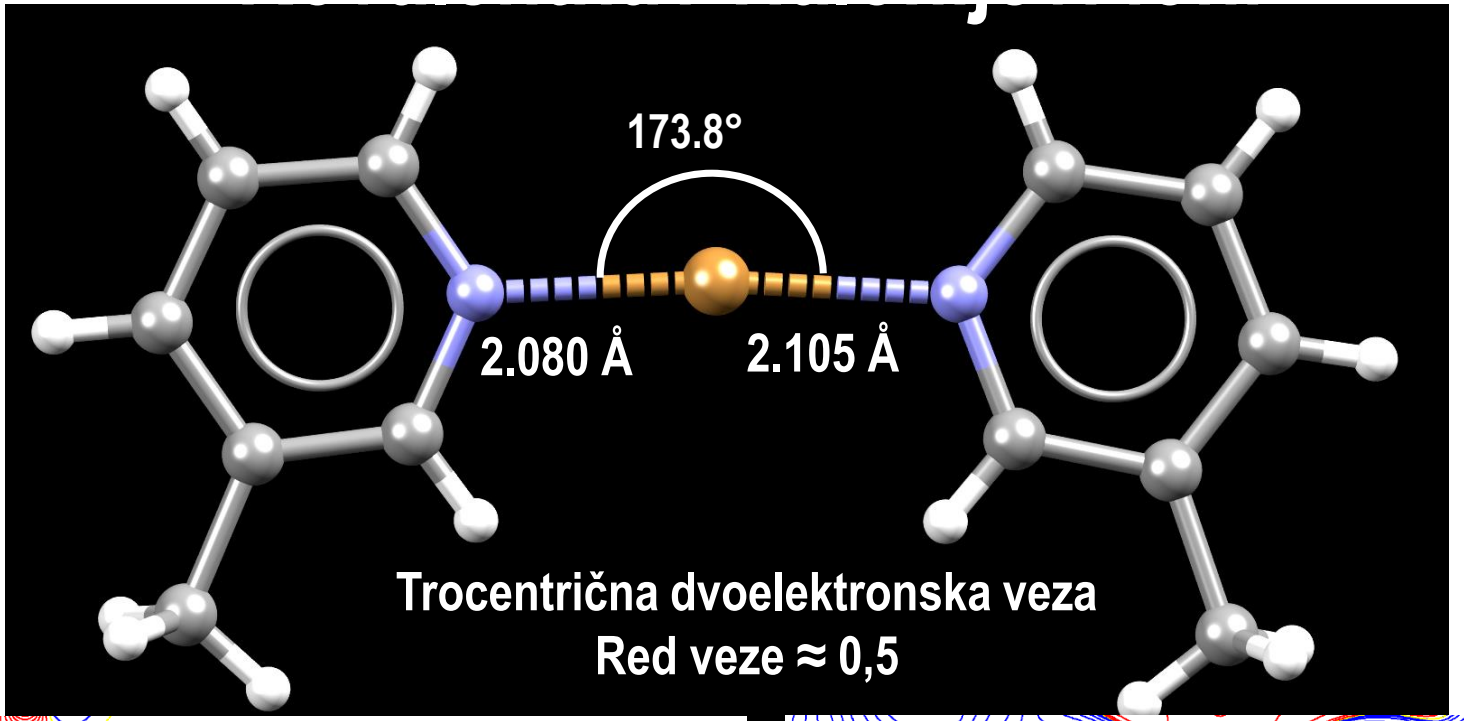


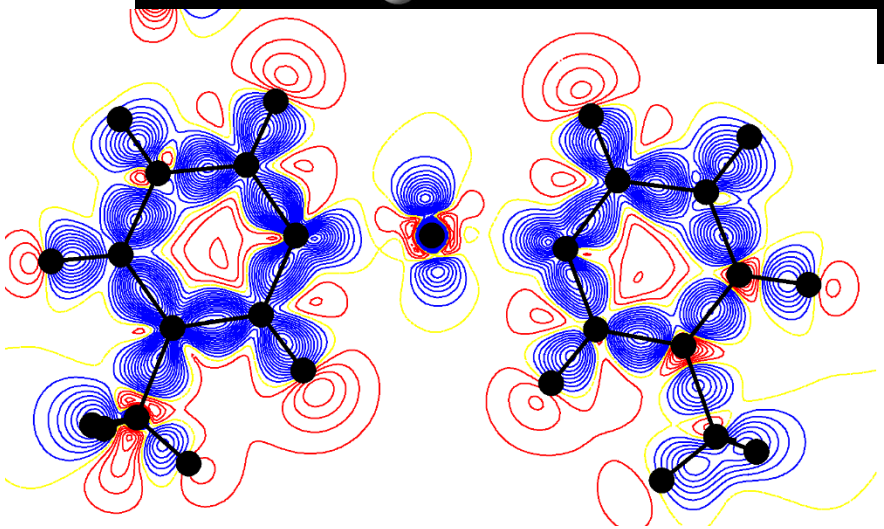
The centrosymmetric $[I_8]^{2-}$ ion in $Cs_2[I_8]$

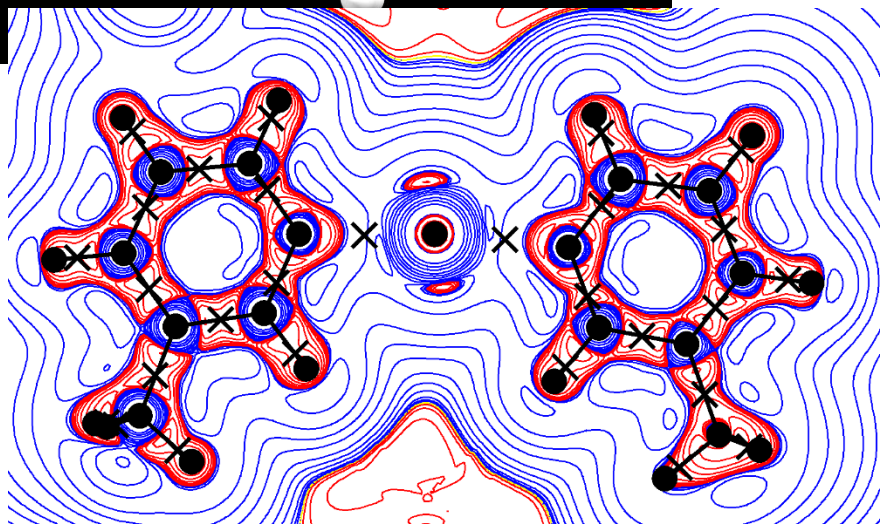


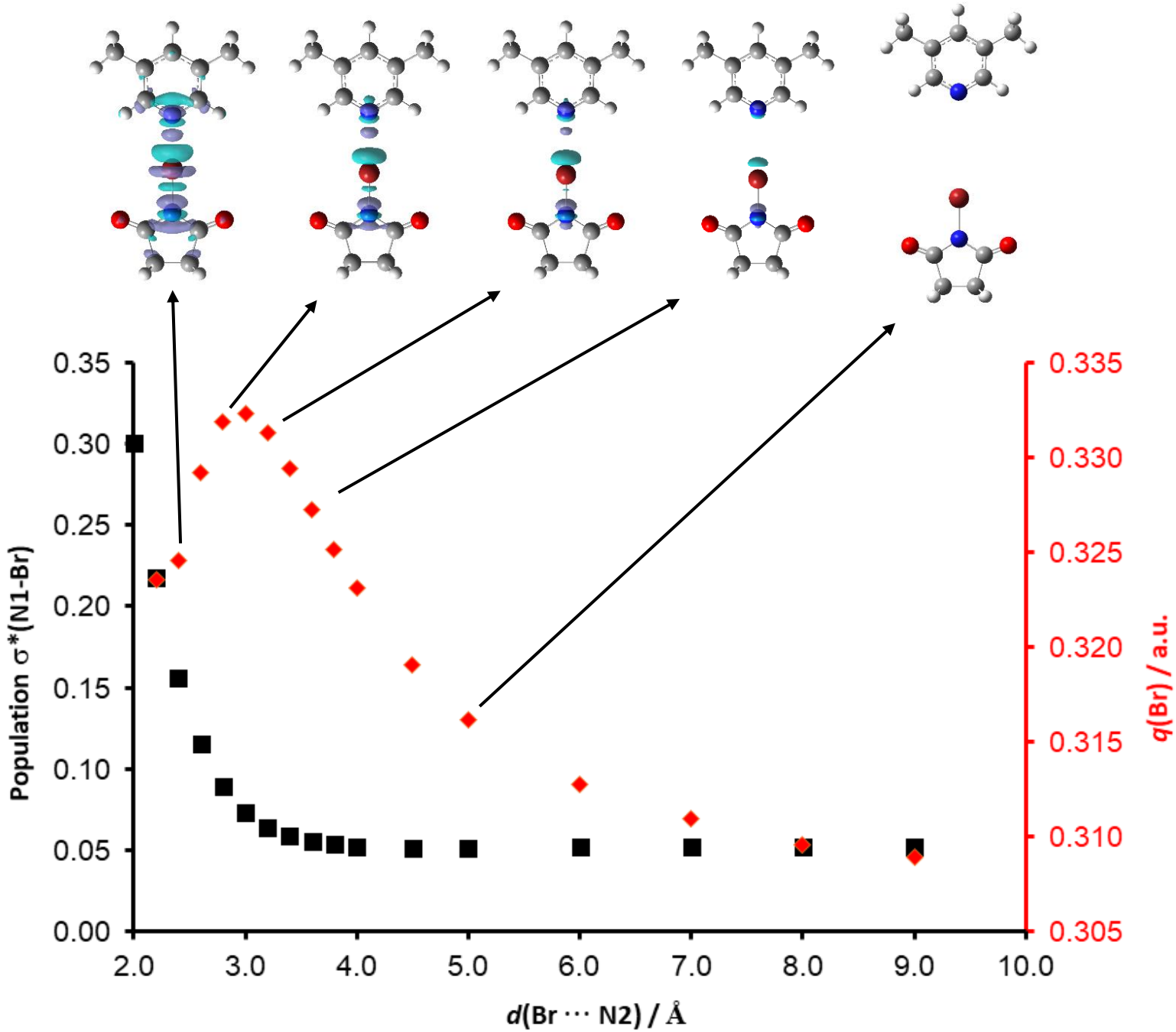
The centrosymmetric $[I_{16}]^{4-}$ ion in $[C_7H_9N_4O_2]_4[I_{16}]$, $[C_7H_9N_4O_2]^+$ is the protonated theobromine ion




173.8°
2.080 Å
2.105 Å
Trocentrična dvoelektronska veza
Red veze ≈ 0,5





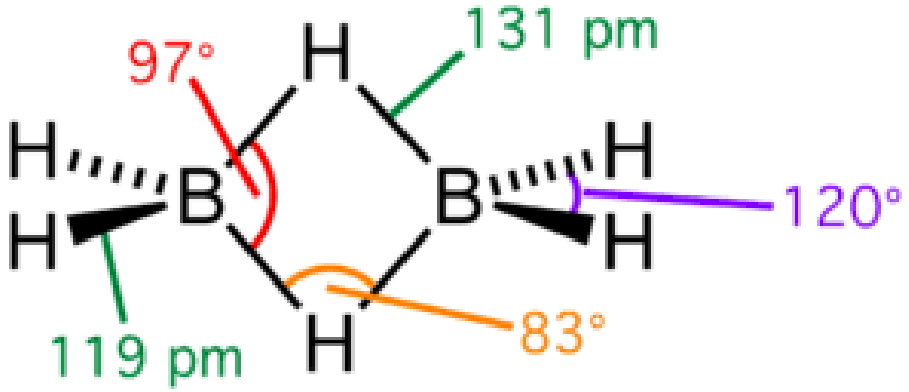


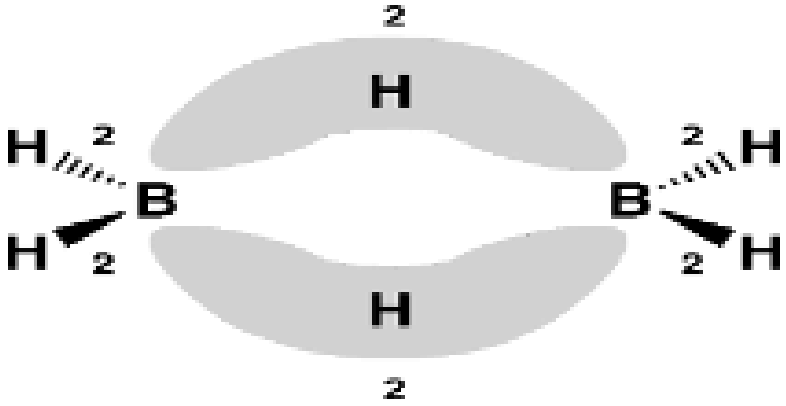
M. Eraković, D. Cinčić, K. Molčanov, V. Stilinović, *Angew. Chem. Int. Ed.* 2019, 58, 15702.

Banane i palačinke

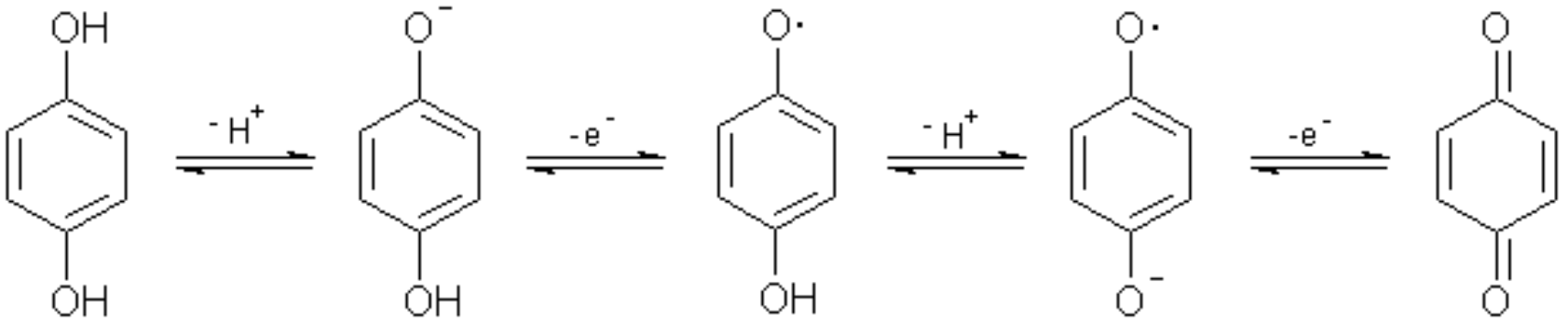
Kratak pogled u svijet policentričnih veza

3c, 2e – '*Banana Bond*'



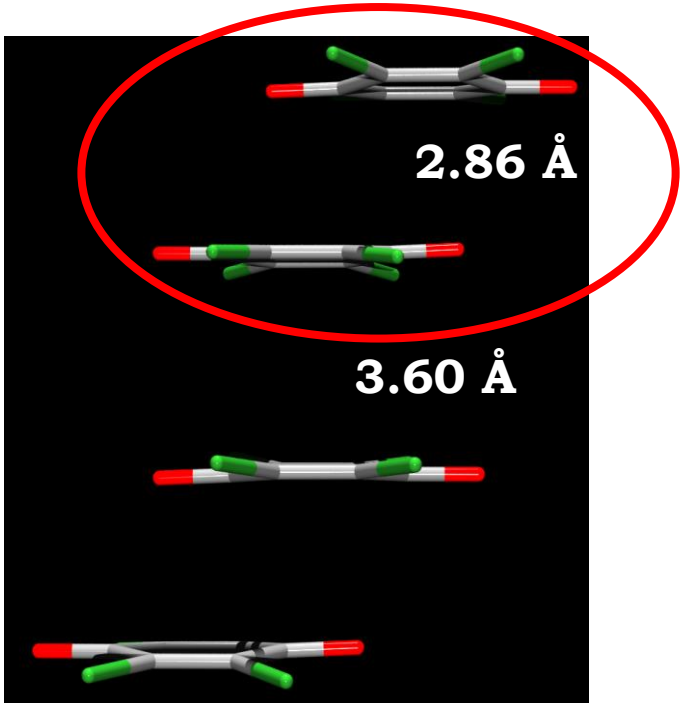


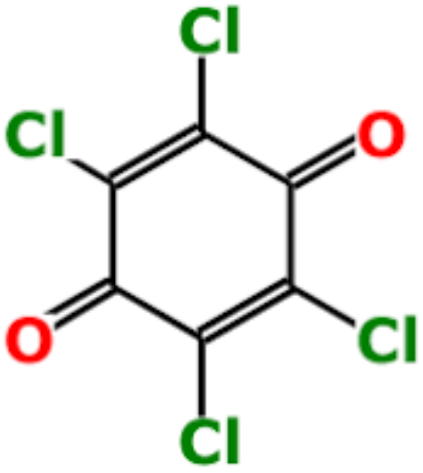
Višecentrične veze? semikinonski radikal-anioni



hidrokinon | fenoksidni anion | fenoksilni radikal | semikinonski radikal-anion | kinon

24c, 2e – '*Pancake Bond*'





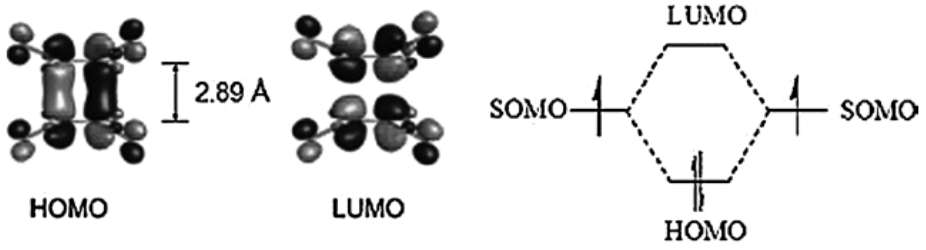
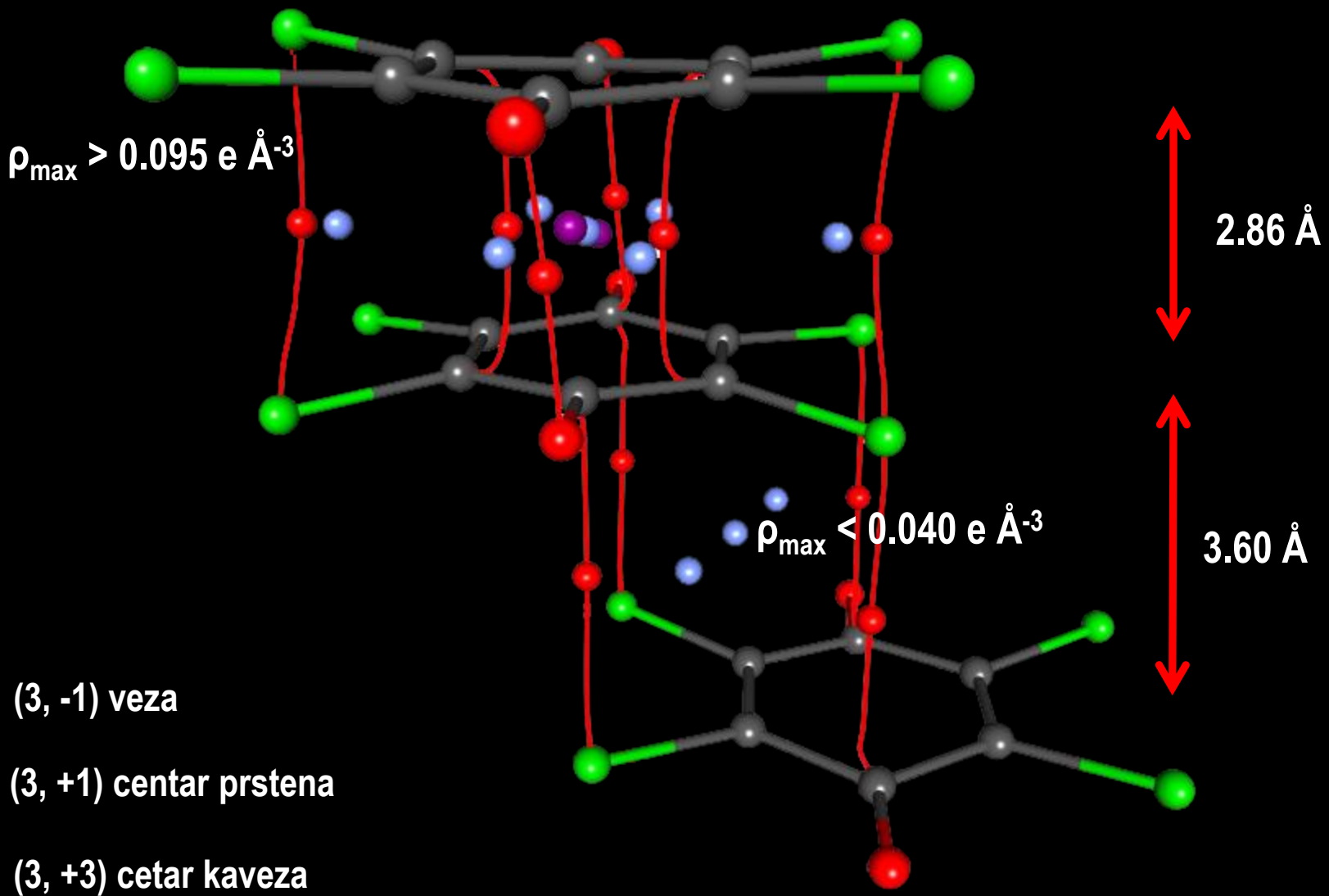
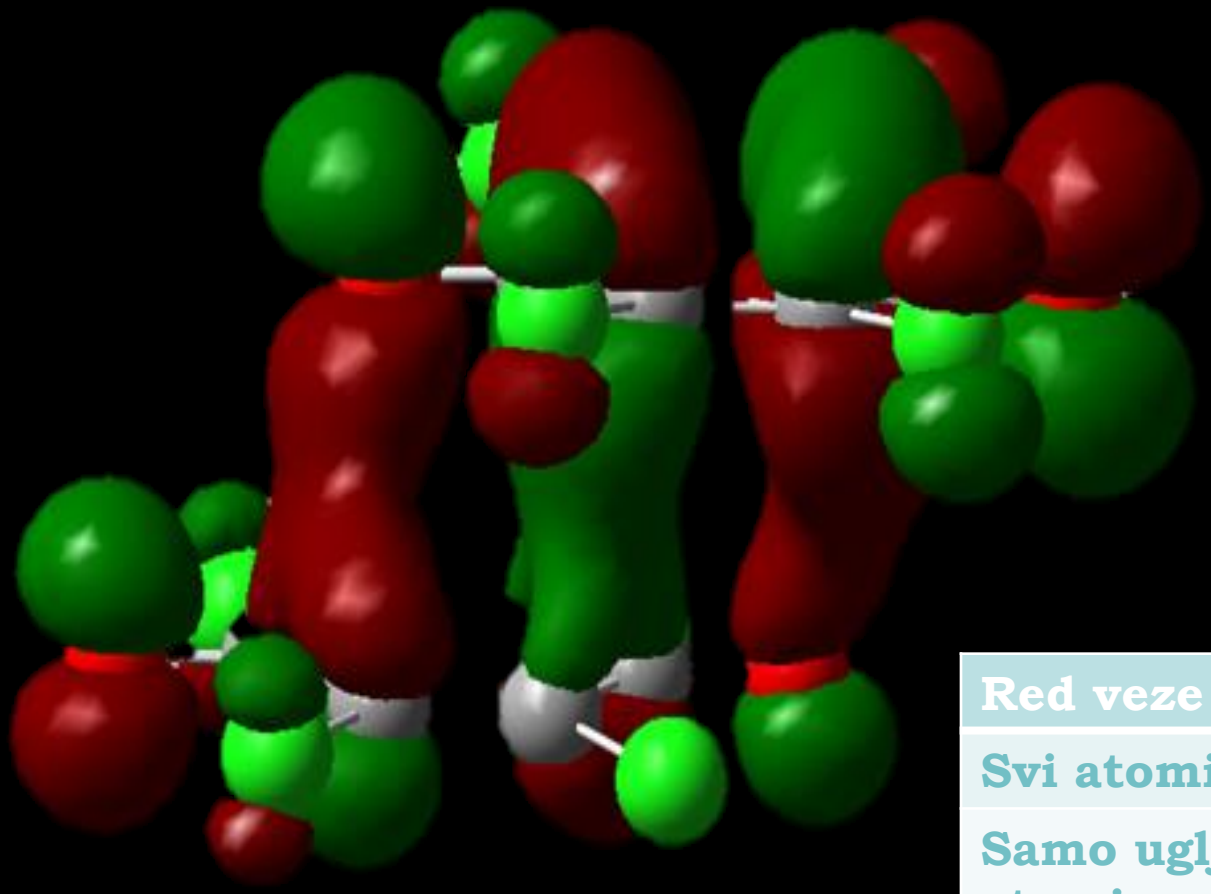


Figure 1. Illustration of the bonding (b_{3u}) and antibonding (b_{2g}) combinations of the two SOMOs in $TCNE_2^{2-}$ as obtained by using Hartree–Fock (HF) calculations. The energy level diagram is on the right.

Topologija elektronske gustoće u dimerima



HOMO orbitala dimera

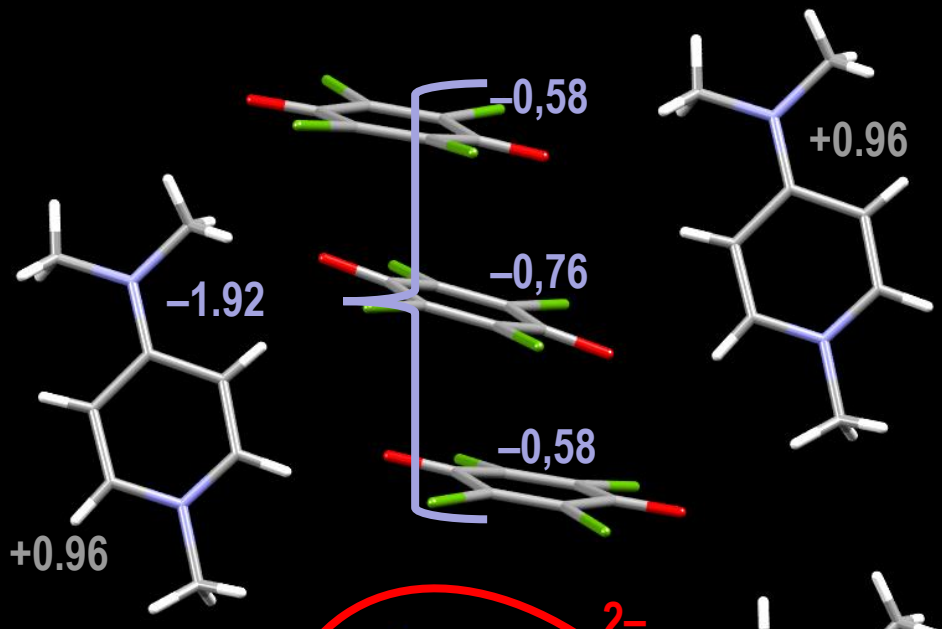


Red veze	
Svi atomi	0.80
Samo ugljikovi atomi	0.27

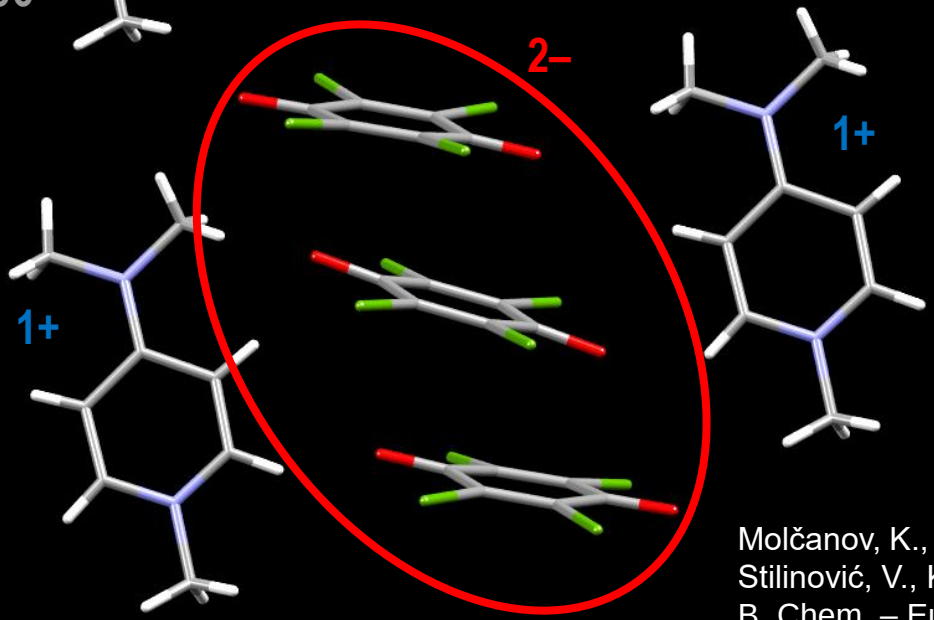
Energija veze (kovalentni doprinos): –39.4 kJ mol^{-1}

36c, 2e – [*N*-Me-4-$(Me)_2$NPy]$_2$($Cl_4Q)_3$

Naboji iz elektronske gustoće:

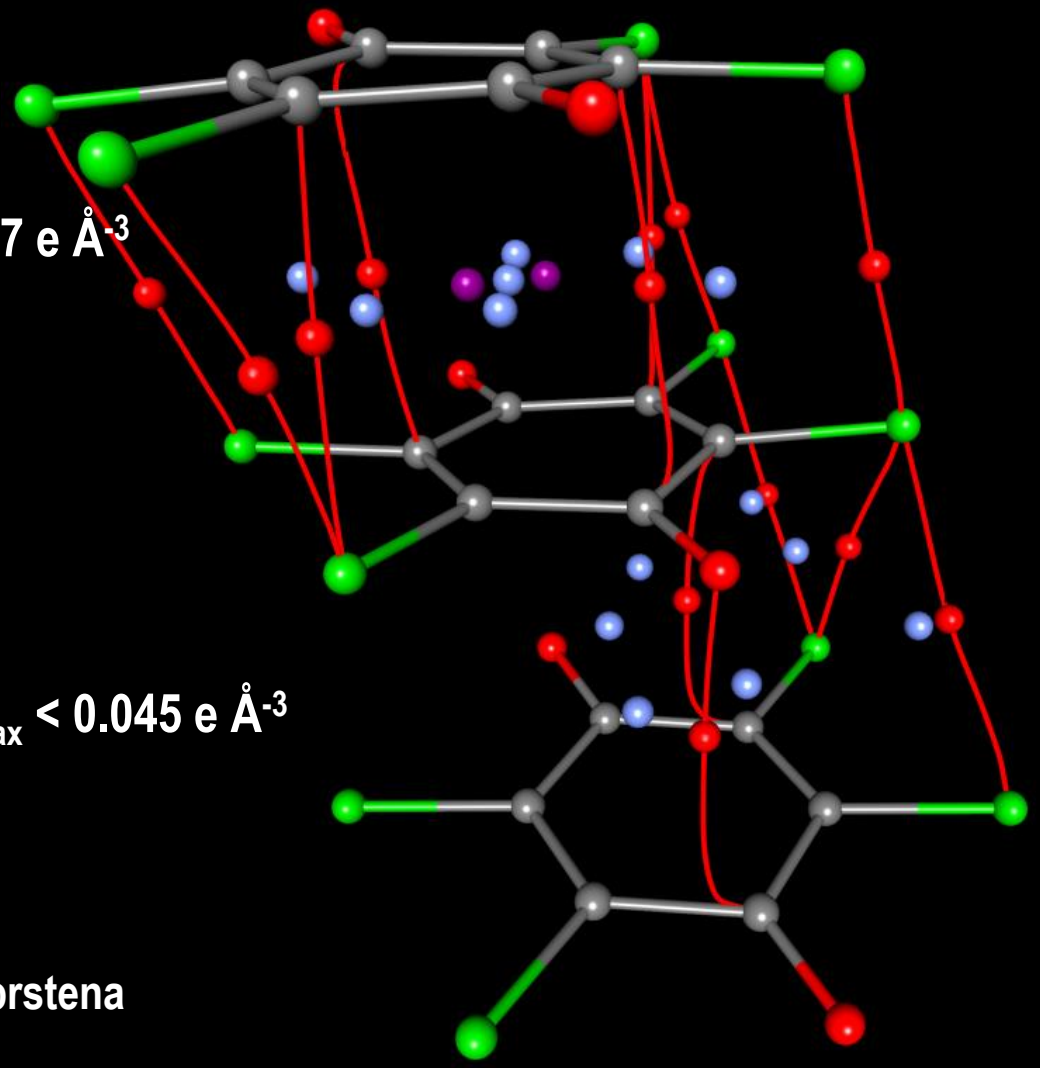


Naboji po kemijskom smislu:



Molčanov, K., Milašinović, V., Ivić, N., Stilinović, V., Kolarić, D., Kojić-Prodić, B. Chem. – Eur. J., 2018, 24(33), 8292.

Topologija elektronske gustoće u trimerima



$\rho_{max} > 0.077$ e Å^{-3}

$\rho_{max} < 0.045$ e Å^{-3}

2.84 Å

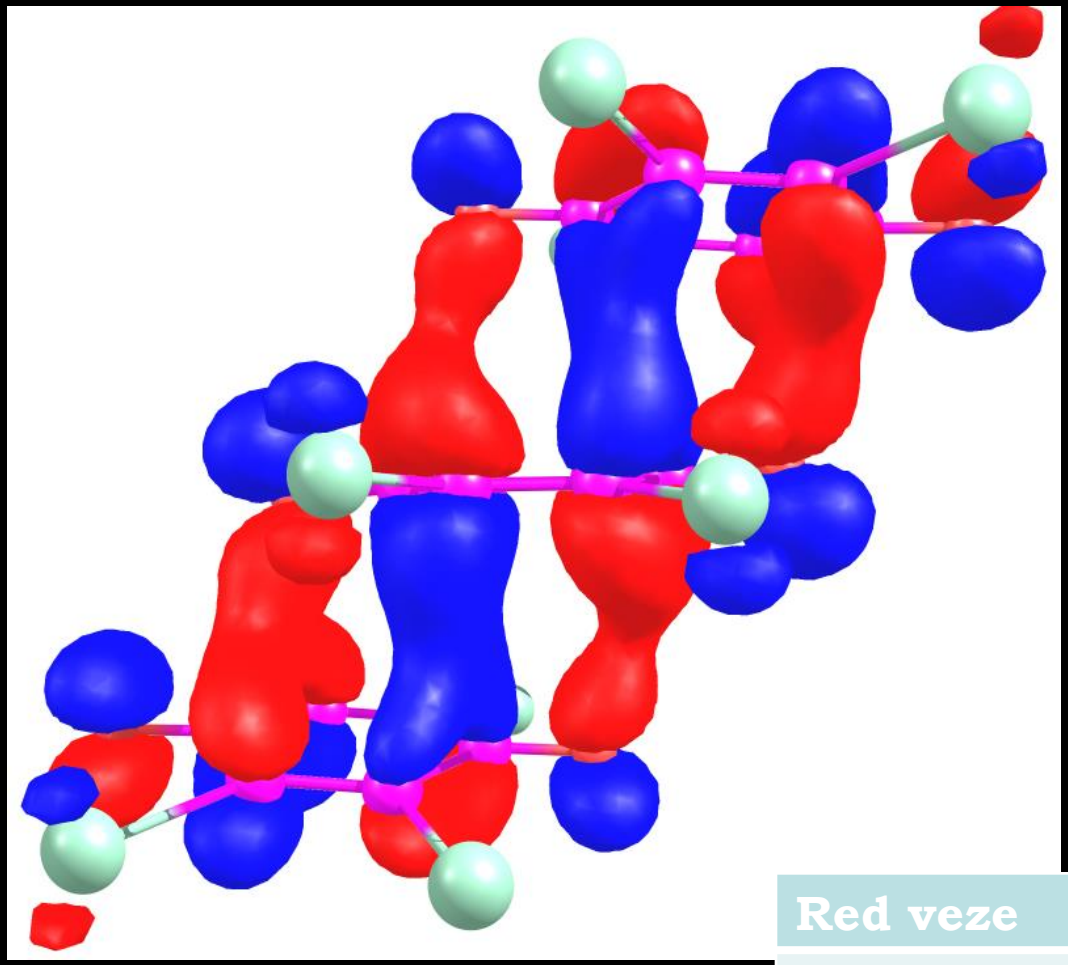
3.59 Å

(3, -1) veza

(3, +1) centar prstena

(3, +3) cetar kaveza

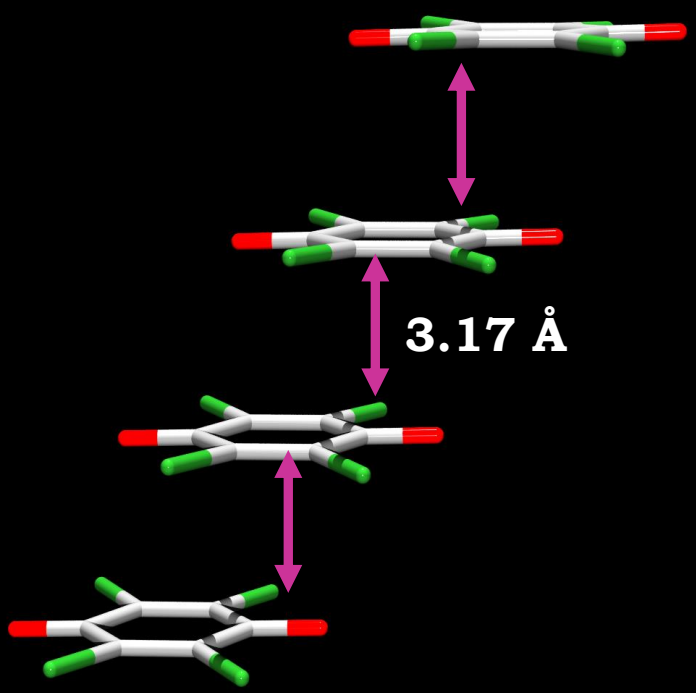
HOMO orbitala trimera

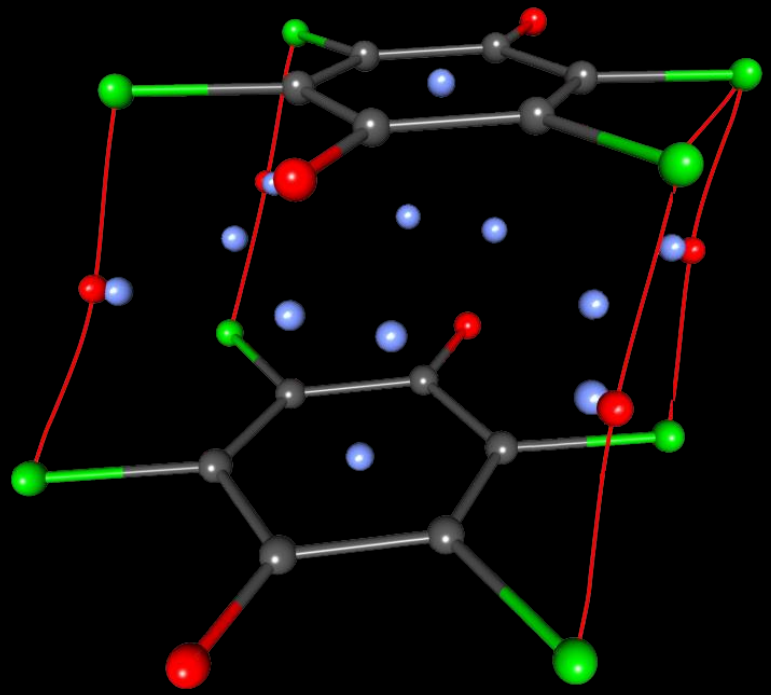


Red veze	
Svi atomi	< 0,71
(vjerojatno oko	0,5

Energija veze (kovalentni doprinos): –17,2 kJ mol^{-1}

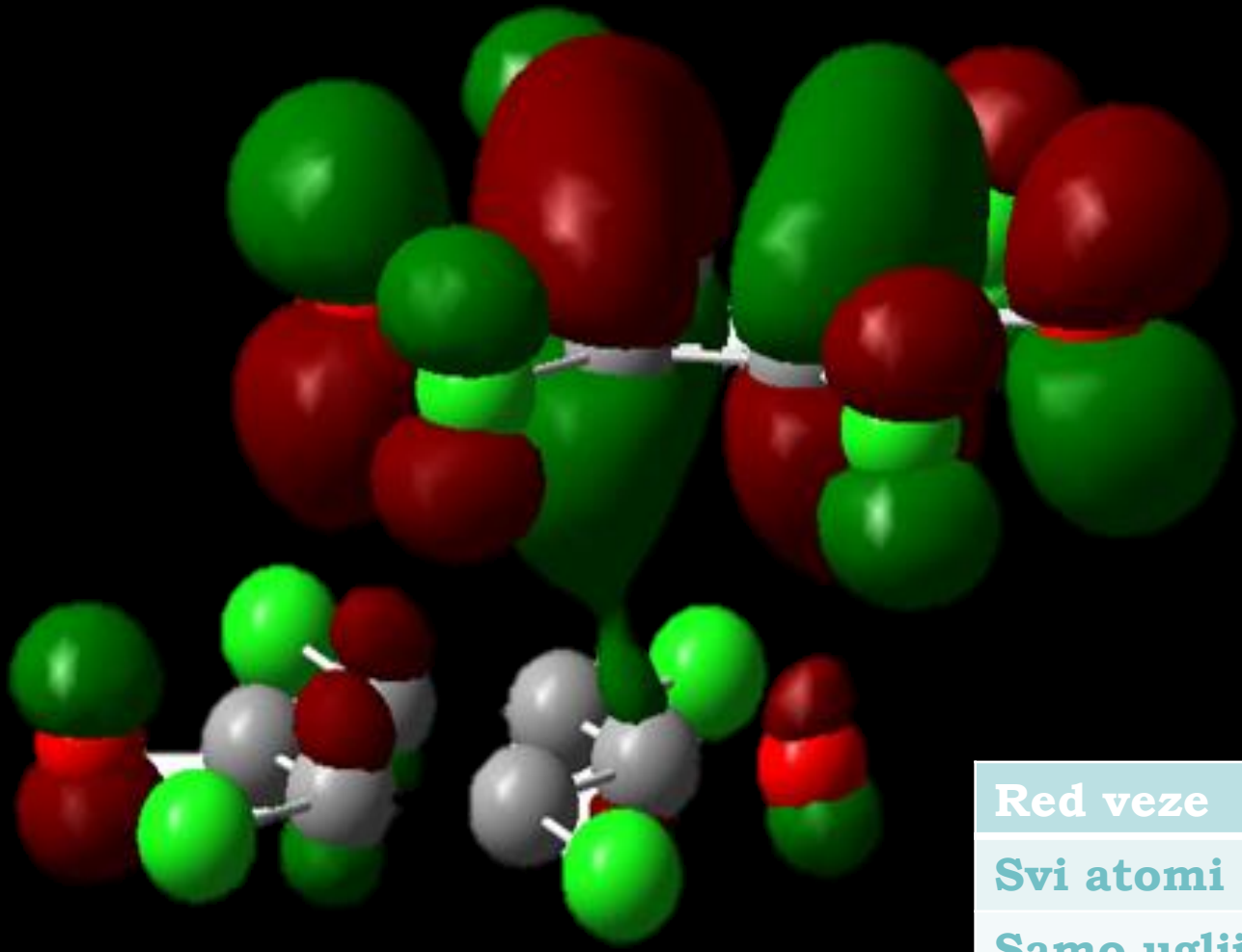
12*n* cc, *n* e – polimer





Molčanov, K., Stilinović, V., Šantić, A., Maltar-Strmečki, N.
Pajić, D., Kojić-Prodić, B. Cryst. Growth Des. 2016, 16, 4777.

HOMO orbitala polimera



Energija veze (kovalentni doprinos): –12,4 kJ mol^{-1}

Red veze	
Svi atomi	0.26
Samo ugljikovi atomi	0.09