O‘zbekiston Respublikasi Sog‘liqni saqlash vazirligi
TOSHKENT FARMATSEVTIKA INSTITUTI
NOORGANIK, FIZIK VA KOLLOID KIMYO KAFEDRASI

3-MA’RUZA:

KIMYOVIY BOG’LANISH VA MOLEKULA TUZILISHI. VALENT BOG’LANISHLAR (VB) USULI.

MOLEKULYAR ORBITALLAR (MO) USULI

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TOSHKENT-2022

REJA:

Mavzuning ma’ruza davomida yoritiladigan qismlari:

1. Kimyoviy bog’lanish tushunchasi;
2. Oktetlar qoidasi;
3. Gipervalentlik;
4. Molekulyar orbitallar metodi;
5. Molekulalararo ta’sir.

Mavzuning talaba mustaqil o’zlashtirishi lozim bo’lgan qismlari:

1. Kovalent bog’lanish;
2. Valent bog’lanishlar usuli;
3. Kovalent bog’lanish tavsiflari;
4. Ion va metall bog’lanish.
5. Gibridlanish.

ASOSIY ADABIYOTLAR:

1. X.R.Tuxtayev, A.T.Sharipov, S.N.Aminov. Noorganik kimyo. Darslik. – Toshkent.: “Fan va texnologiya”,2018, 560 bet.

2. Shriver and Atkins, Inorganic Chemisrty, Fifth Edition, 2010/ P.W.Atkins, T.L.Owerton, J.P. Rourke, M.T. Weller and F.A. Armstrong, W.H. Freeman and Company, New York. 2010. P. 825.

3. Э.Т.Оганесян, В.А.Попков, Л.И.Щербакова, А. К. Брель; под ред. Э. Т. Оганесяна. — М. : Юрайт, 2019. — 447 с. — Серия: Специалист.

4. Общая и неорганическая химия для фармацевтов: учебник и и практикум для СПО/ под общ.ред. В.В.Негребецкого, И.Ю.Белавина, В.П.Сергеевой.-Издательство Юрайт, 2019.-357 с.-Серия: профессиональное образование.

5. Шрайвер Д., Эткинс П. Неорганическая химия. В 2-х т. Т 1/ Перевод с англ. М.Г.Розовой, С.Я. Истомина, М.Е.Тамм-Мир, 2004.-679 с.

6. Шрайвер Д., Эткинс П.. Неорганическая химия. В 2-х т. Т 2/ Перевод с англ. А.И.Жирова, Д.О.Чаркина, С.Я. Истомина, М.Е.Тамм-Мир, 2004.-486 с.

7. Thomas R. Gilbert - Chemistry_ The Science in Context-Norton (2017)

Insonlar orasidagi munosabatlar

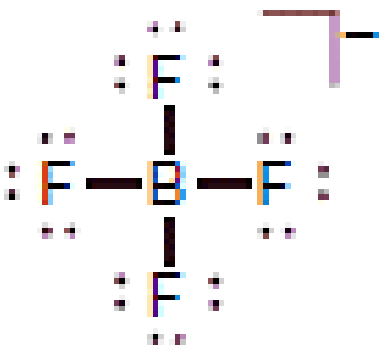
1. Kimyoviy bog'lanish

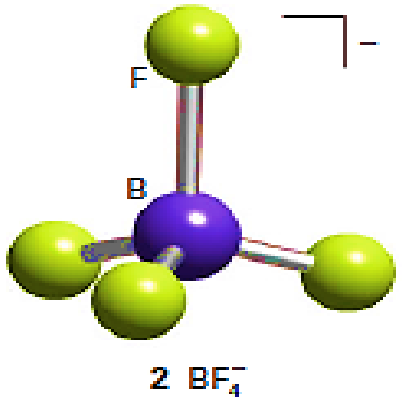
"Bog'lanish - bu ikki yoki undan ortiq komponentlarni (atomlar, molekulalar yoki ionlar) birga ushlab turadigan atomlararo, molekulalararo yoki ionlararo tortishish turi".

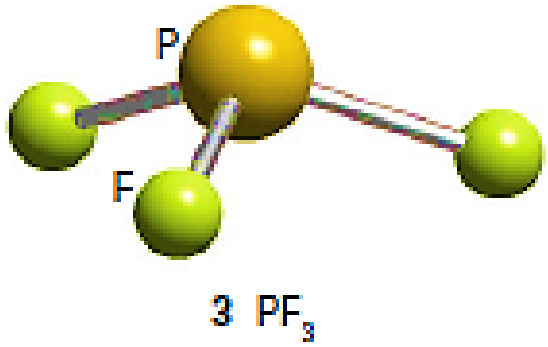
2. Oktet qoidasi

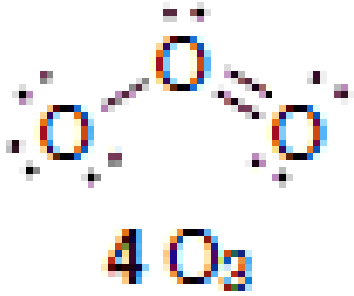
Bo'lingan juftliklar (duplet hamda oktetlar qoidasi) 1916 yilda G. N. Lyuis tomonidan tasvirlangan.

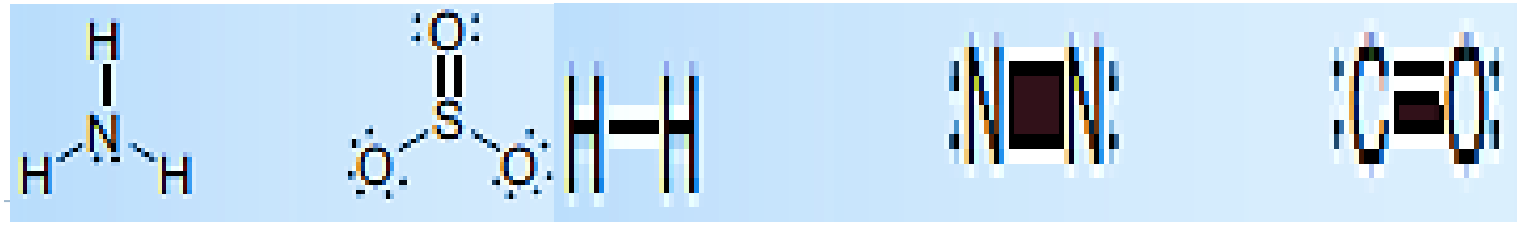
Oktet qoidalari: har bir atom sakkiz elektronli to'liq valentlik qobig'iga erishish uchun qo'shni atom bilan bo'linadi.











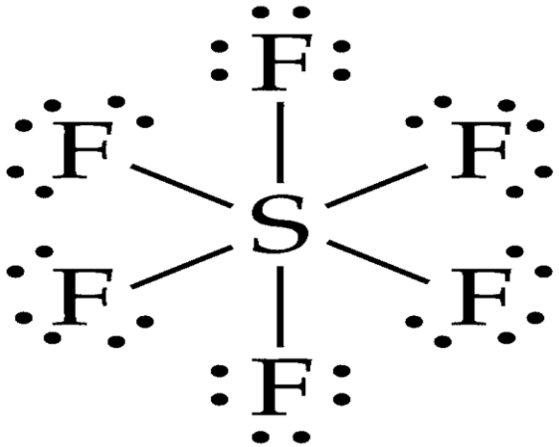
3. Gipervalentlik

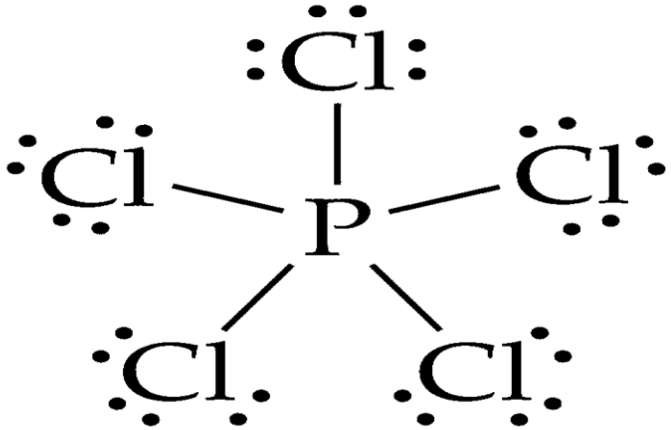
Oktetadagi valentlik elektronlar sonidan ortiq elektronlarning bo'lishi GIPERVALENTLIK deb ataladi.

Markaziy atomlar bilan bog'lanishda ishtirok etadigan elektronlari soni 8 dan ortiq bo'lgan atomlar *gipervalent atomlar* deb ataladi.

Bu hodisa *kengaygan oktet* deb ataladi va asosan 2 davr elementlaridan keyin keladigan elementlarda uchraydi.

Masalan, SF_6 molekulasida markaziy atom bilan bog`lanishda 12 ta elektron ishtirok etadi. Bunda qo'shimcha elektronlarni joylashtirish uchun bo'sh d-orbitallarning mavjudligi hisobga olinadi.





Turli bog’lardagi ion bog’lanish hissasi

Bog’	C-I	C-H	C-Cl	C-F
Ion bog’ hissasi, %	0	4	6	40
Bog’	H-Cl	H-F	Be-F	Li-F
Ion bog’ hissasi, %	18	45	80	89

C-I bog’idan C-F bog’iga o’tgan sari bog’ning ionlilik darajasi ortadi.

4. Molekulyar orbitallar metodi

VBU usuli kamchiliklari:

- **- ba'zi moddalarda elektron juftlar yordamisiz bog'lanish hosil bo'lishi. XIX asrning oxirida J.Tomson (H_2^+).**
- **- tarkibida toq elektronlar bo'lgan moddalargina magnitga tortiladi (suyuq yoki qattiq O_2).**
- **- erkin radikallar tarkibida ham juftlashmagan elektronlar bo'ladi.**
- **- benzolga o'xshash aromatik uglevodorodlarning tuzilishini VBU tushuntirib bera olmaydi.**
- **- toq elektronlarning rolini ko'rsatadigan nazariya 1932 yilda Xund va Malliken yaratgan, bu nazariya molekulyar orbitallar (MO) nazariyasi.**

Molekulada elektronning holati ikkita yadro va bitta elektron ta'sirida tasvirlanadi, keyin elektronning harakati to'lqin funksiyasi bilan ifodalanadi:

Bog'lovchi simmetrik funksiya:

$$\omega_1 = C_1 \varphi_1 + C_2 \varphi_2$$

Bo'shashtiruvchi antisimmetrik funksiya:

$$\omega_2 = C_1 \varphi_1 - C_2 \varphi_2$$

C_1, C_2 - koeffitsientlar;

φ_1, φ_2 - ayni elektronning birinchi va ikkinchi yadrolariga oid to'lqin funksiyalari;

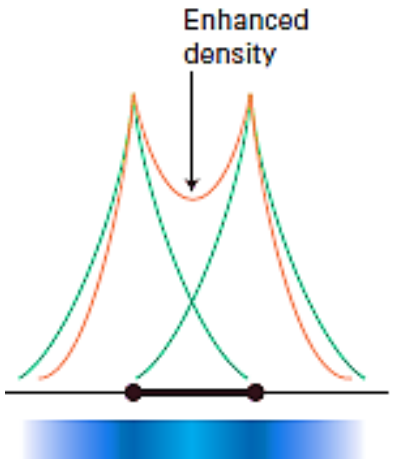
ω_1 - simmetrik funksiya;

ω_2 - antisimmetrik funksiya.

Molecular orbital theory

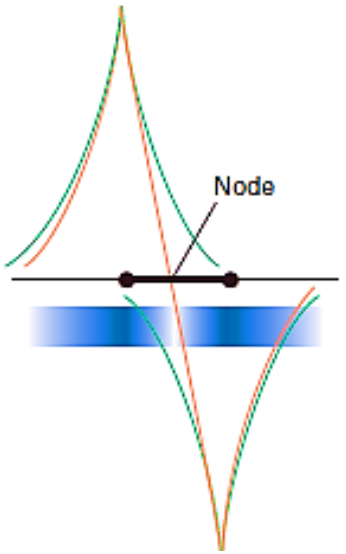
$$\psi = c_A\chi_A + c_B\chi_B \qquad \psi_* = \chi_A \pm \chi_B$$

Bog'lovchi orbitallar



the atomic orbitals on neighbouring atoms.

Bo'shashtiruvchi orbitallar



nodal surface in an antibonding molecular orbital.

MO da molekula tarkibidagi elektronlarning o'zaro ta'siri e'tiborga olinmaydi.

AO ning s, p, d, f orbitallari bor.

MO da ham σ, π, λ va φ molekular orbitallar.

AO elektronning energiyasi bosh va orbital kvant sonlarga bog'liq bo'lib, magnit kvant songa bog'liq emas.

MO da elektronlar energiyasi bosh, orbital va magnit kvant sonlariga bog'liq.

$$BT = \frac{n_{bog'e} - n_{bo'shash\ e}}{2}$$

Если $\lambda = \pm 1$, π - состояние

n bog'.e – bog'lovchi orbitallardagi elektronlar soni;

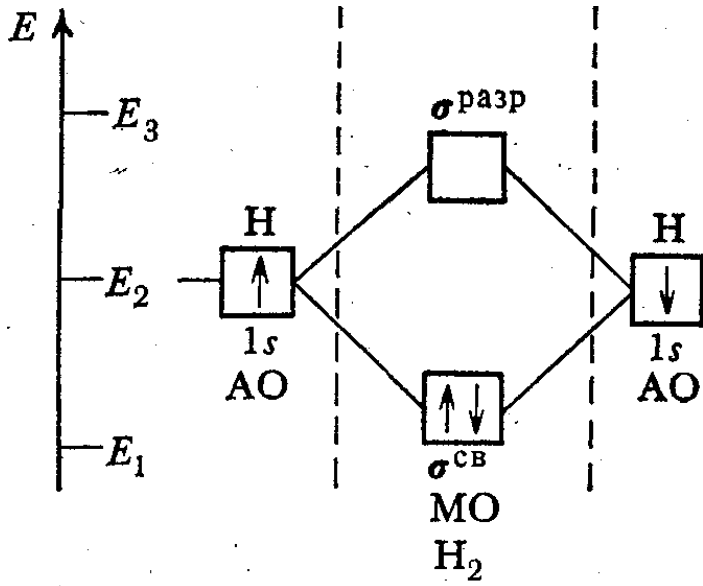
n bo'shash e – antibog'lovchi orbitallardagi elektronlar soni;

$2H(1s^1) \rightarrow H_2[\sigma$ bog'lovchi $1s)^2]$

Bog' tartibi 1 ga teng:

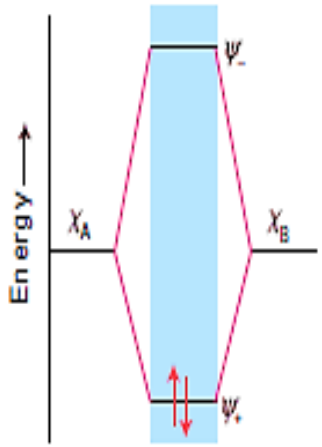
$$BT = \frac{2 - 0}{2} = 1$$

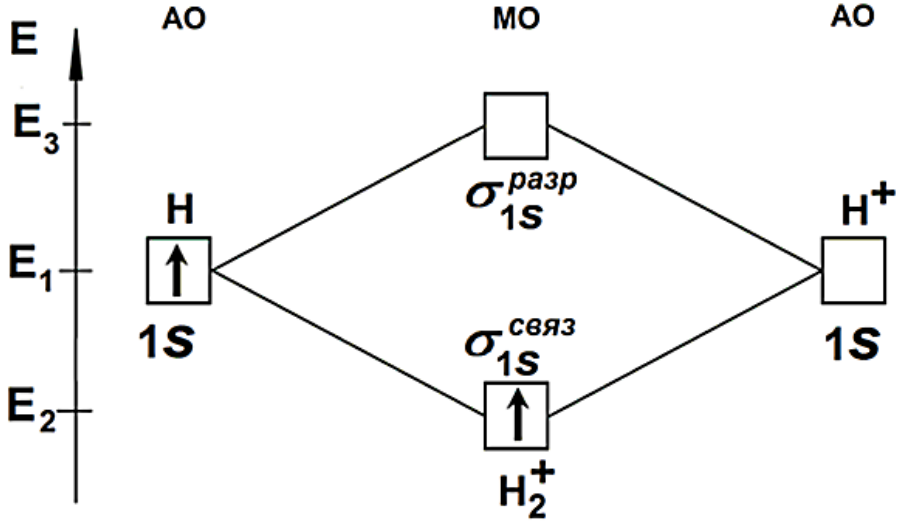
H_2 molekulasi hosil bo'lishida 435 Kj/mol energiya ajralib chiqadi. $2H(1s^1) \rightarrow H_2[\sigma$ bog' $1s)^2]$



(a) Bond order $b = \frac{1}{2}(n - n^*)$

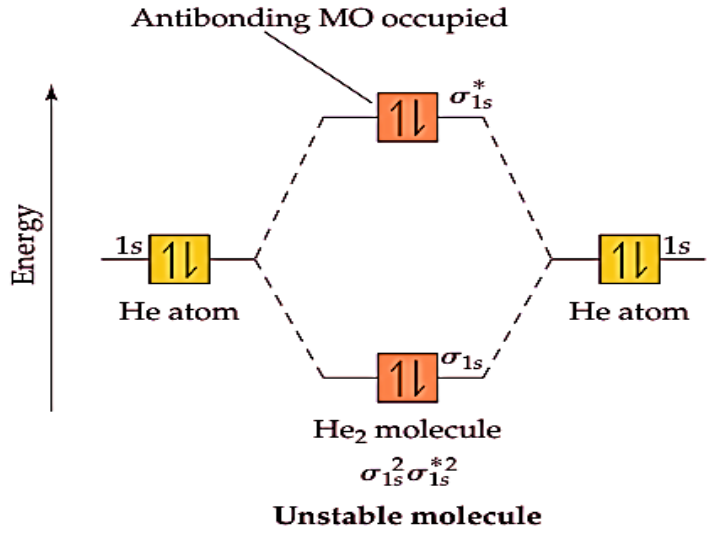
Molekulyar orbitallar usuliga ko’ra, vodorod ioni H_2^+, geliy molekulasi (He_2) hamda geliy ioni (He_2^+)





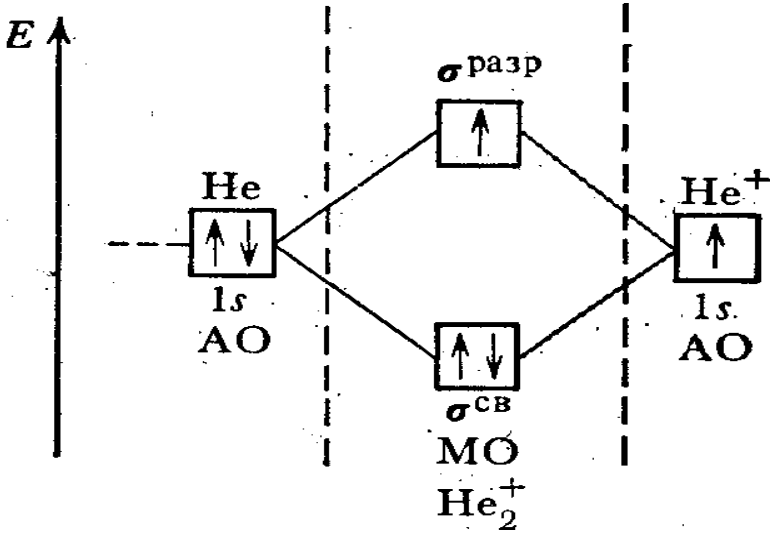
$H(1s^1)+H^+(1s^0)\rightarrow H_2^+$

$[(\sigma\ bog'.\ 1s^1)]$.



$He(1s^2)+He(1s^2)\rightarrow He_2$

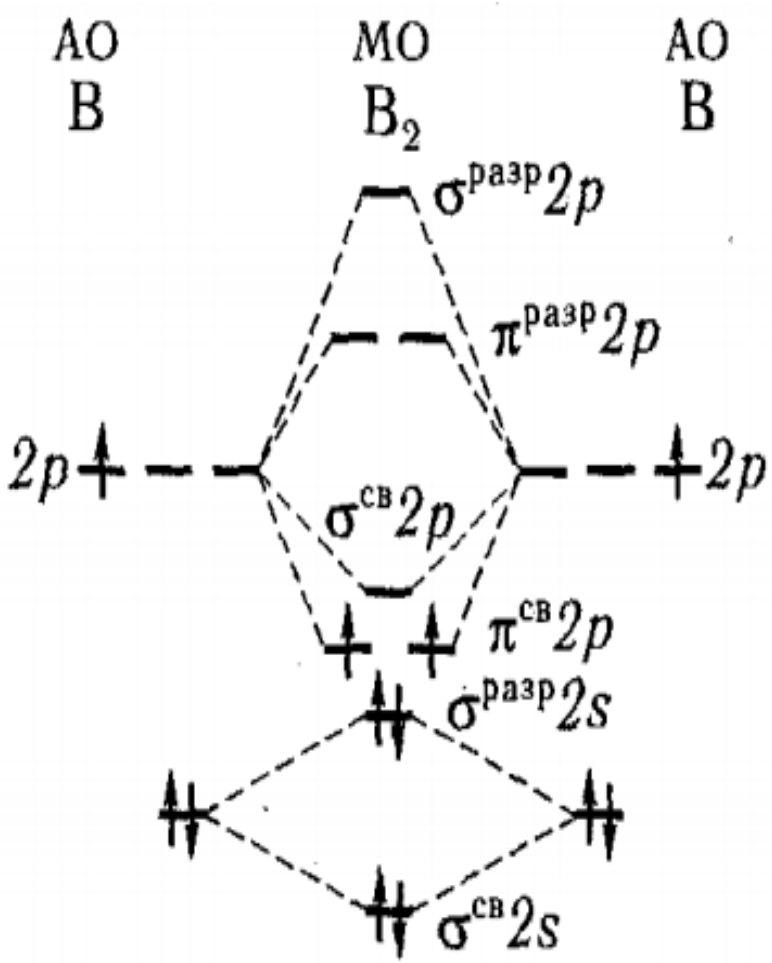
$[(\sigma\ bog'.\ 1s)^2(\sigma\ bo'sh.\ 1s)^2]$.

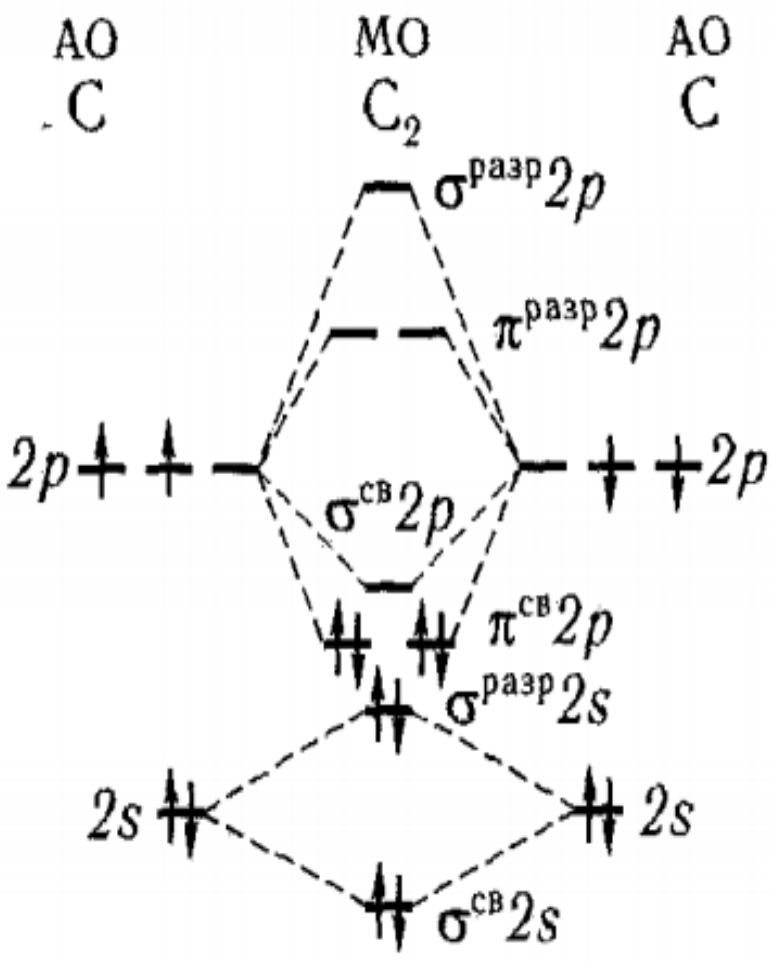


$He(1s^2)+He^+(1s^1)\rightarrow He^{2+}$

$[(\sigma\ bog'.\ 1s)^2(\sigma\ bo'sh.\ 1s)^1]$.

Molekulyar orbitallar usuliga ko'ra, B_2 va C_2 molekulalari hosil bo'lishining energitik tuzilishi



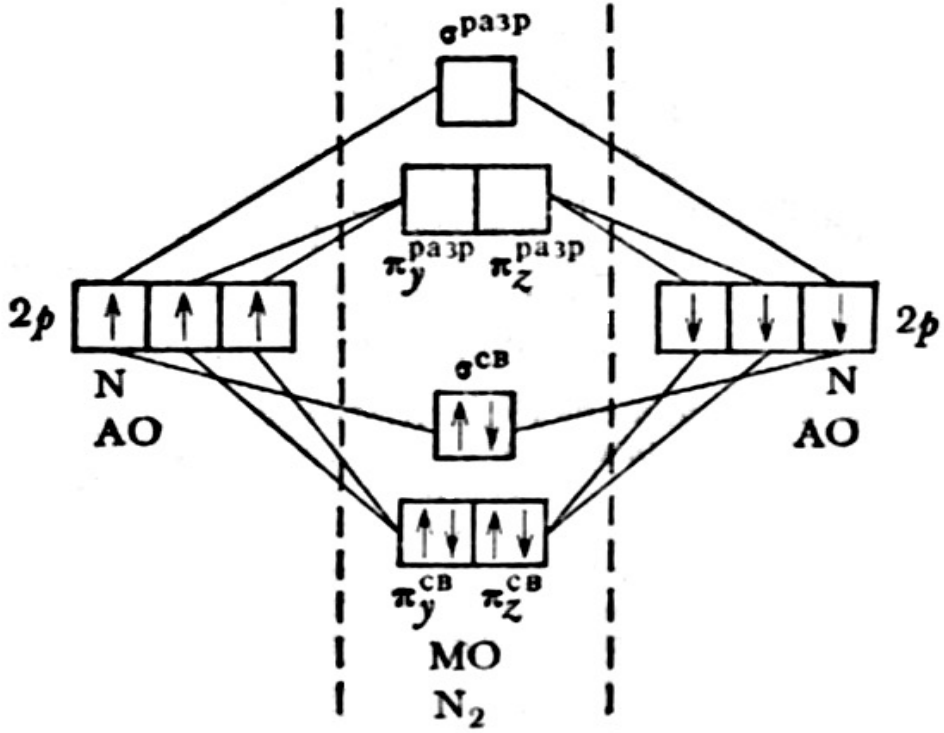


Molekulyar orbitallar usuliga ko’ra, azot va kislorod molekulalari tuzilishi

$N(2s^2 2p^3) + N(2s^2 2p^3) \rightarrow N_2$

$[(\sigma\ bog'.2p)^2(\pi\ bog'.2p^2)2\ (\sigma\ bo'sh.2p^o)^2(\pi\ bo'sh.2p^o)^2]$

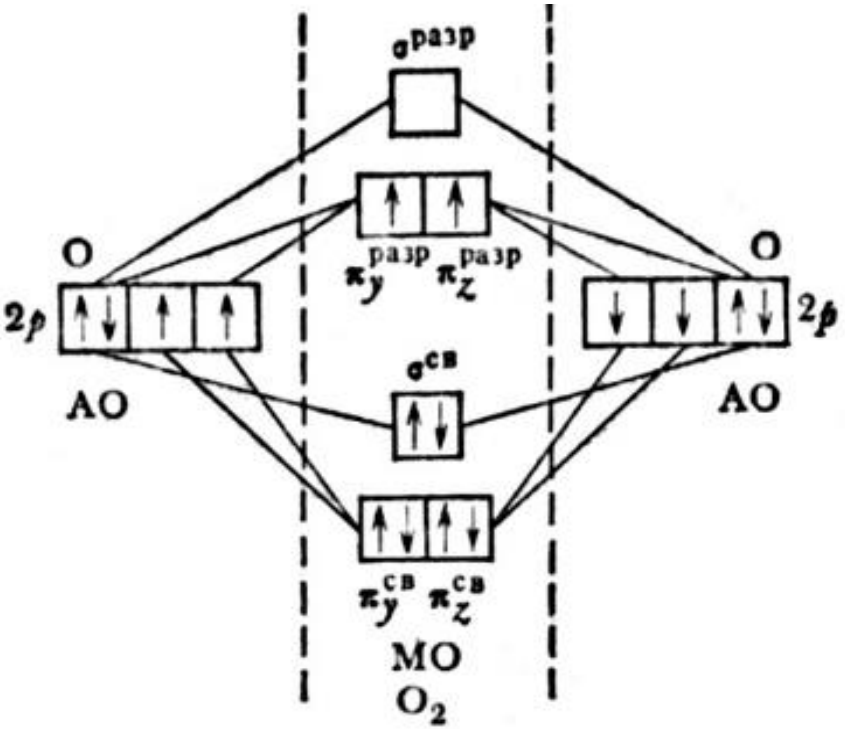
BT = 6-0/2=3



$O(2s^2 2p^4) + O(2s^2 2p^4) \rightarrow O_2$

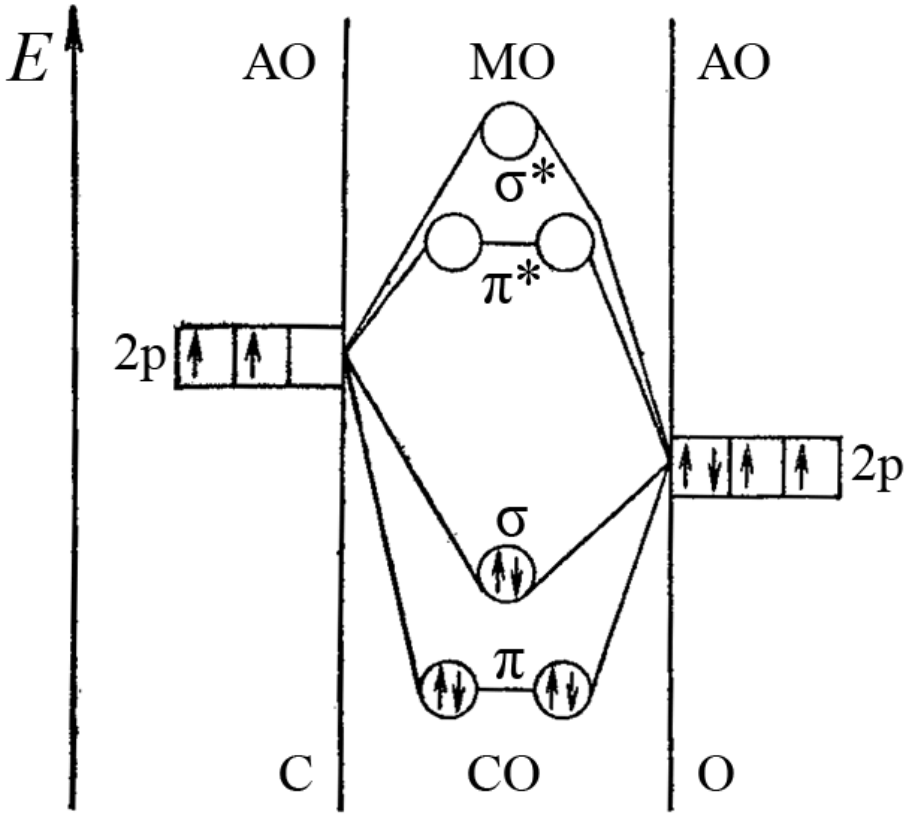
$[(\sigma\ bog'.2p)^2(\pi\ bog'.2p^2)2\ (\sigma\ bo'sh.2p^0)^2(\pi\ bo'sh.2p^2]$

BT = 6-2/2=2

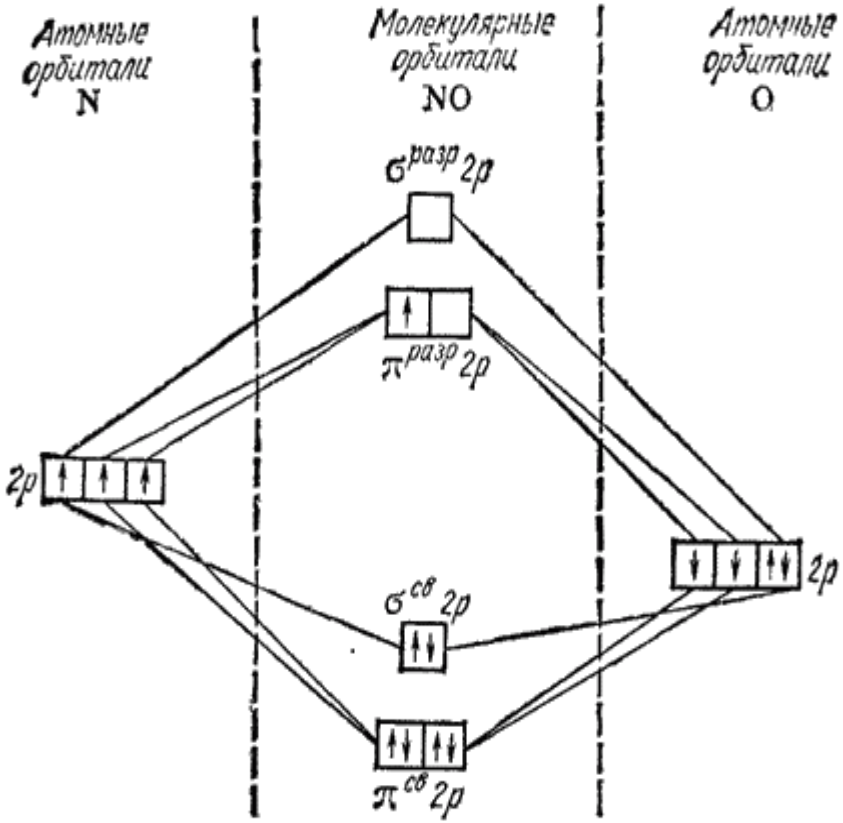


Molekulyar orbitallar usuliga ko’ra, CO va NO molekulalari tuzilishi

BT = 6-0/2=3



BT = 6-1/2=2,5

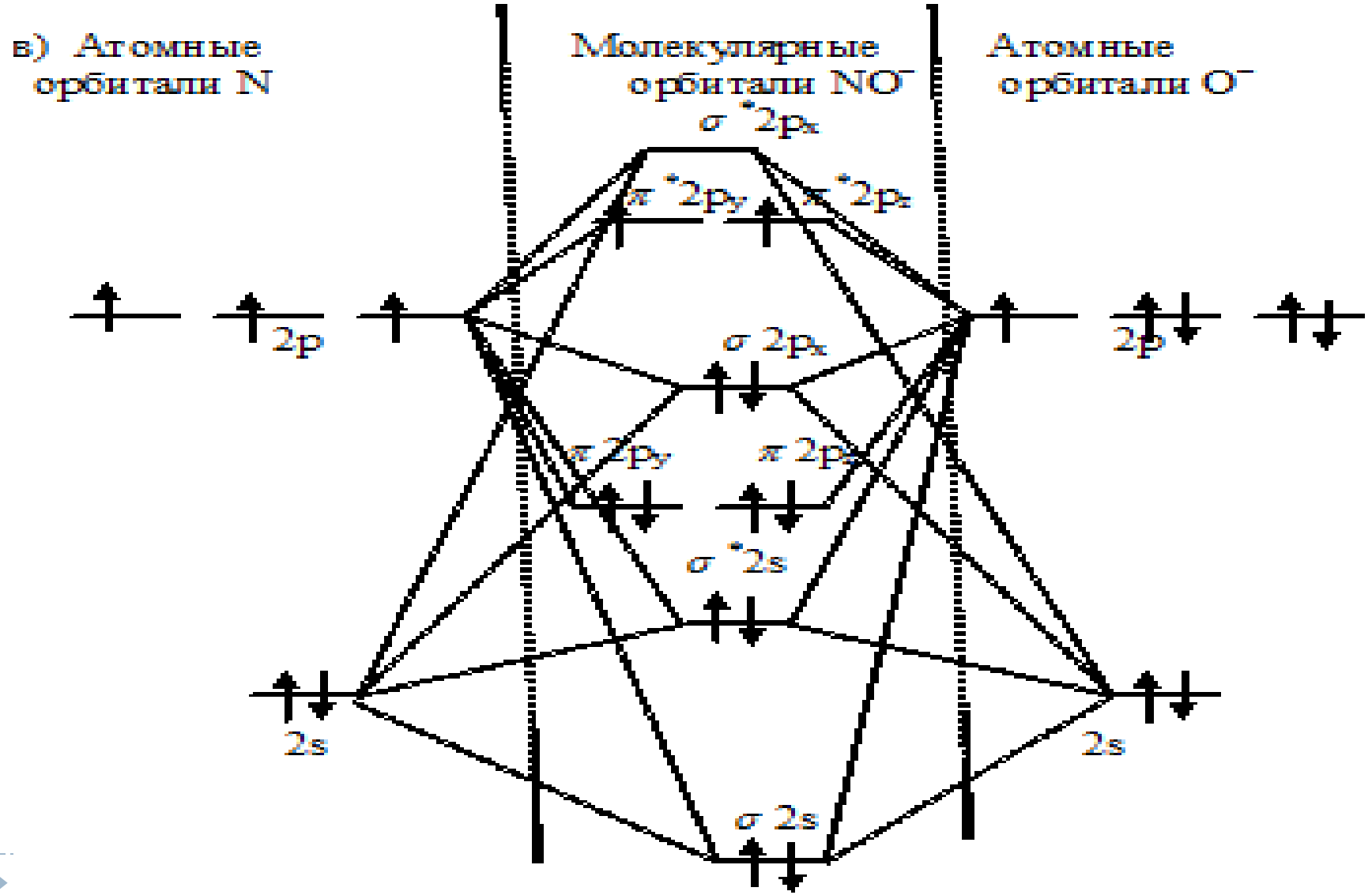


Molekulyar orbitallar metodining afzalliklari:

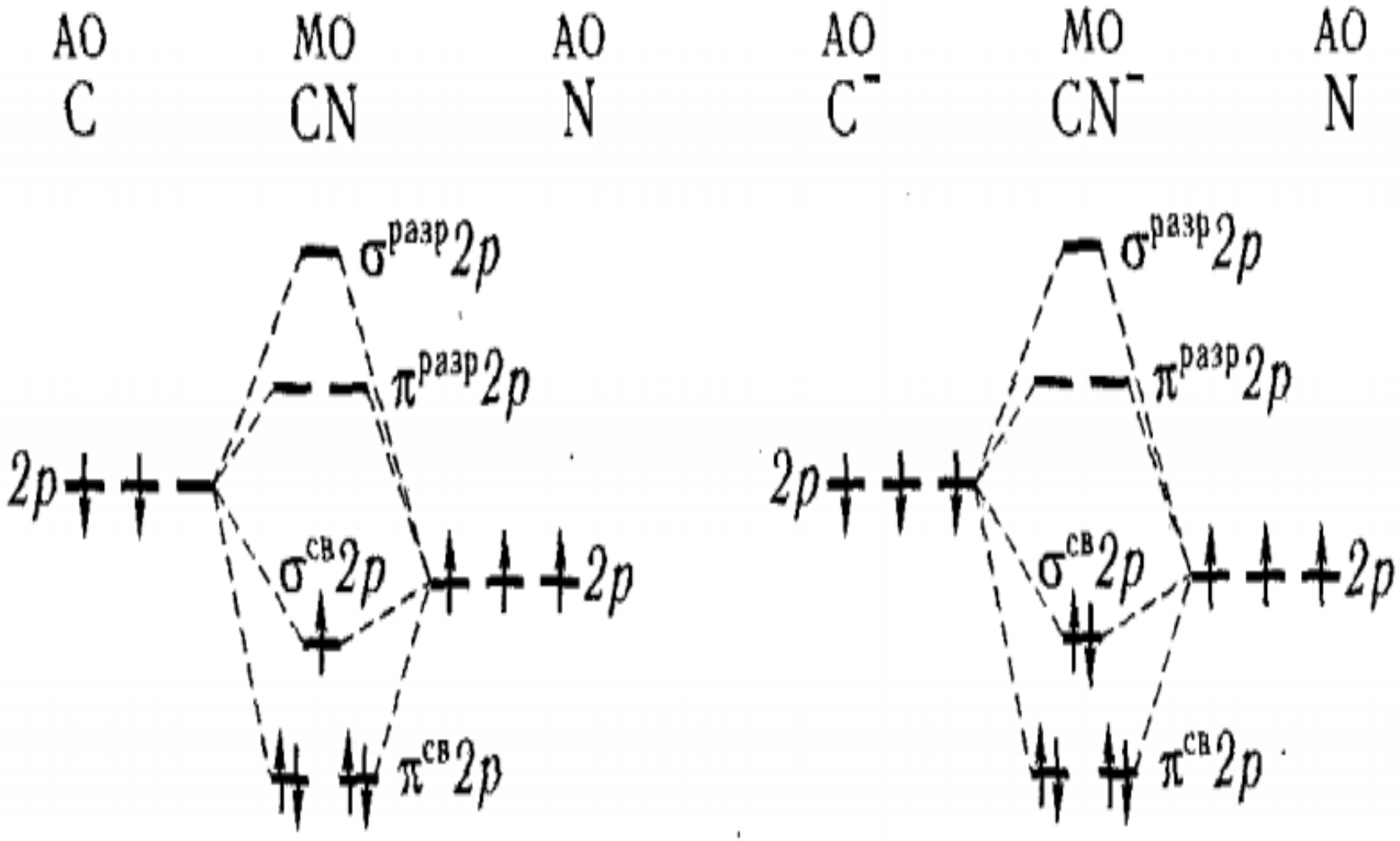
- **- MO usuli har qanday yadro tizimi va elektronlarning barqarorligini tushuntiradi;**
- **- MO usuli molekulalarning va kompleks birikmalarning magnit va optik xossalarini to'liq tushuntiradi;**
- **- molekuladagi har bir elektronning holatini baholaydi.**

BeH_2	BH_2	CH_2	NH_2	OH_2
180°	131°	136°	103°	105°

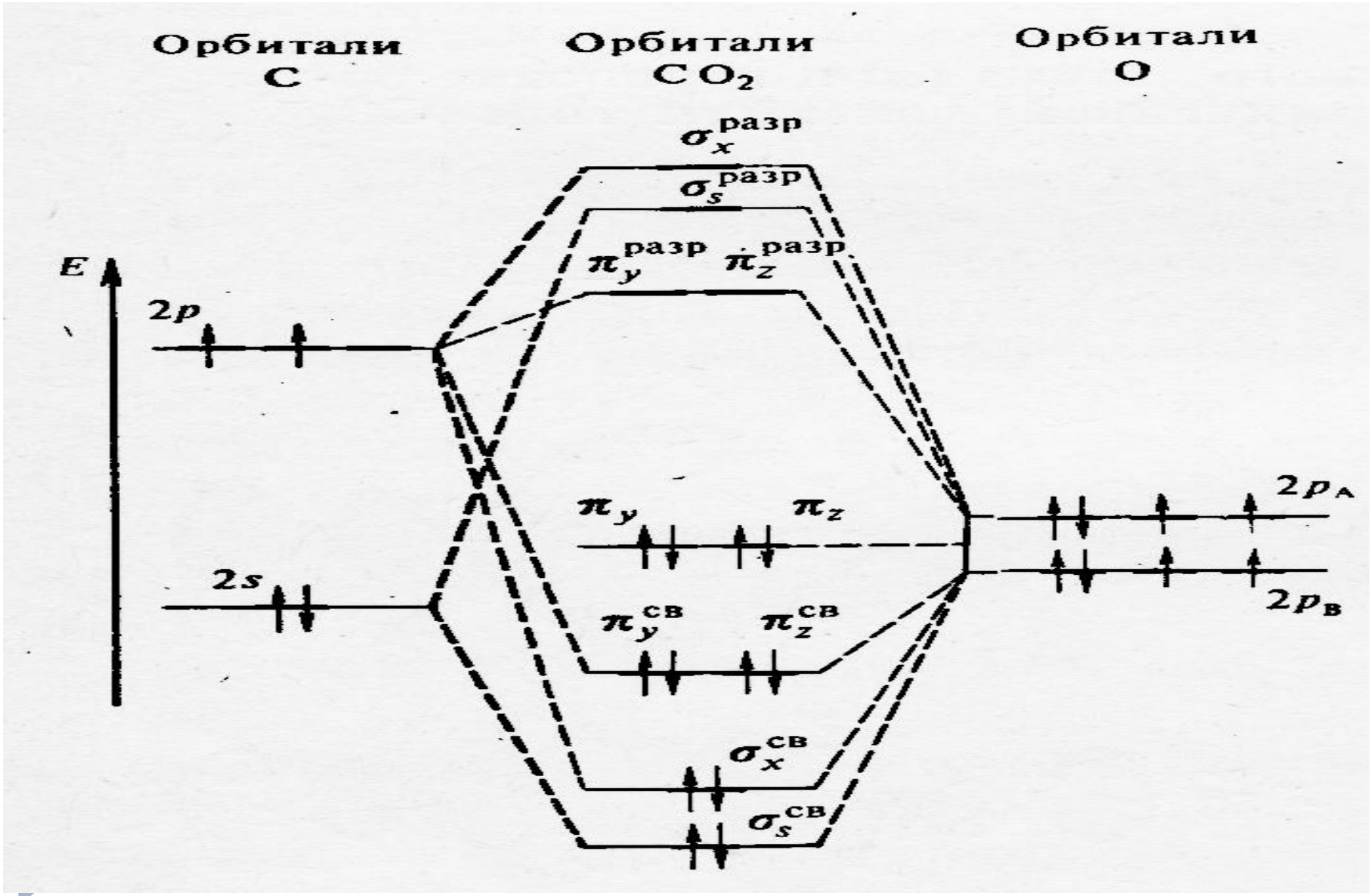
Molekulyar orbitallar usuliga ko'ra, NO-molekulalari hosil bo'lishining energitik tuzilishi



Molekulyar orbitallar usuliga ko’ra, CN и CN- molekulalari hosil bo'lishining energitik tuzilishi



Molekulyar orbitallar usuliga ko'ra, CO_2 molekulalari hosil bo'lishining energitik tuzilishi



5. Molekulalararo ta’sirlar (MT)

Molekulalar o'rtasida orientatsion, dispersion va induksion o'zaro ta'sirlar mavjud.

Dispersion ta’sirlar - qutbsiz molekulalar orasida bir lahzada yuzaga keladigan mikrodipollar hosil bo’lishiga asoslangan.

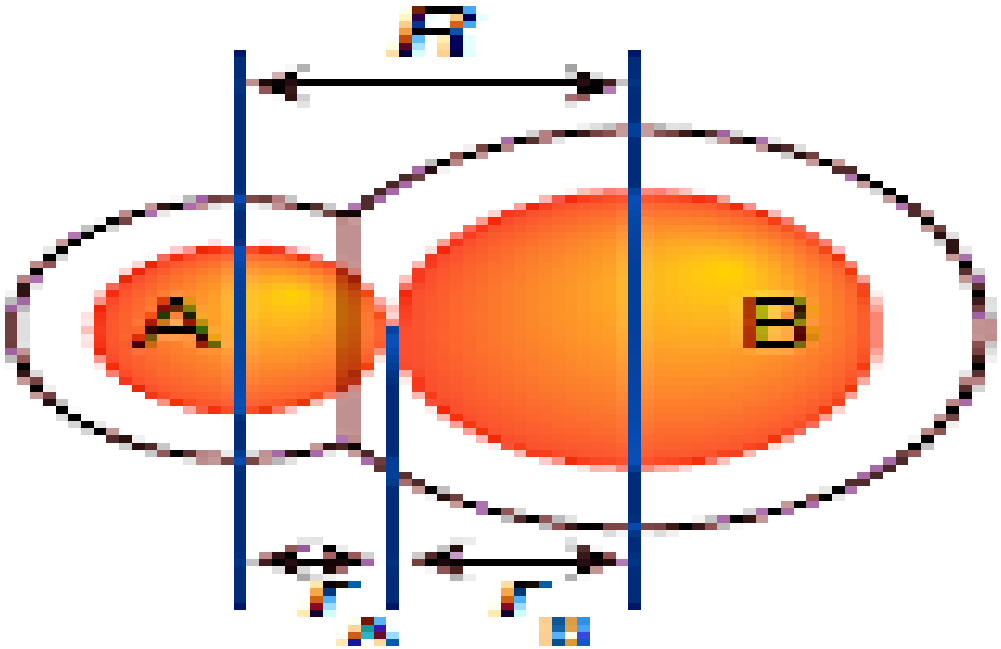
Orientatsion ta’sirlar - qutblangan molekulalar orasida yuzaga keladi. Molekulalarning tartibsiz issiqlik harakati tufayli bir xil zaryadlangan dipollarning uchlari bir-biridan uzoqlashadi, qarama-qarshi zaryadlangan uchlari esa bir-biriga tortiladi. Molekulalar qanchalik qutbli bo'lsa, ular shunchalik kuchliroq tortiladi.

Induksion ta’sirlar - o'zaro ta'sir molekulalarning induksiyalangan dipollari tufayli amalga oshiriladi. Induksion ta’sirlar qanchalik katta bo'lsa, dipolning elektr momenti va molekulaning qutblanishi shunchalik katta bo'ladi.

Induksion ta'sir - qutbli va qutbsiz molekulalar orasida. Qutblangan molekulalar ta'sirida qutblanmagan molekulalar egiladi va unda qoldiq (induktsiyalangan) dipol paydo bo'ladi.

Induksiyalangan dipol o'z navbatida polyar molekulaning elektrik dipol momentini kuchaytiradi.

1. molekulaning qutblanganligiga
2. molekulaning deformatsiyalanishiga.



18 Covalent radius

Elektron berilmasdan yuzaga keladigan ta’sirlar

Elektronlarni atomlarga o'tkazmasdan paydo bo'ladigan molekulalararo o'zaro ta'sir kuchlari *Van-der-Vaals kuchlari* yoki *o'zaro ta'sirlar* deb ataladi.

Van der Vaals kuchlari molekulalarning tortilishi va moddalarning birikishi, gazsimon moddaning suyuqlikka, keyin esa qattiq holatga aylanishiga olib keladi.

Gazsimon xlor sovutilganda kristallar o'rtasida dispersiya kuchlari paydo bo'ladi. Xlor atomlarga parchalanganda 243 kJ/mol ajralib chiqadi.

Xlor kristallarining gazlarga o'tishida sublimatsiya energiyasi 25 kJ/mol ni tashkil qiladi.

E’tiboringiz uchun raxmat!