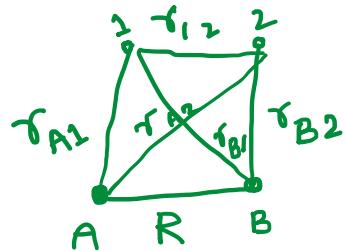


H_2 molecule (2 electrons)



$$\hat{H} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_{A1}} - \frac{1}{r_{A2}} - \frac{1}{r_{B1}} - \frac{1}{r_{B2}} + \frac{1}{r_{12}} + \frac{1}{R}$$

This term makes the problem impossible to solve exactly

$$\hat{H}\psi = E\psi$$

Trial/guess wavefn

$$\tilde{\Phi}_{MO}(\bar{r}_1, \bar{r}_2) \text{ or } \tilde{\Phi}_{VB}(\bar{r}_1, \bar{r}_2)$$

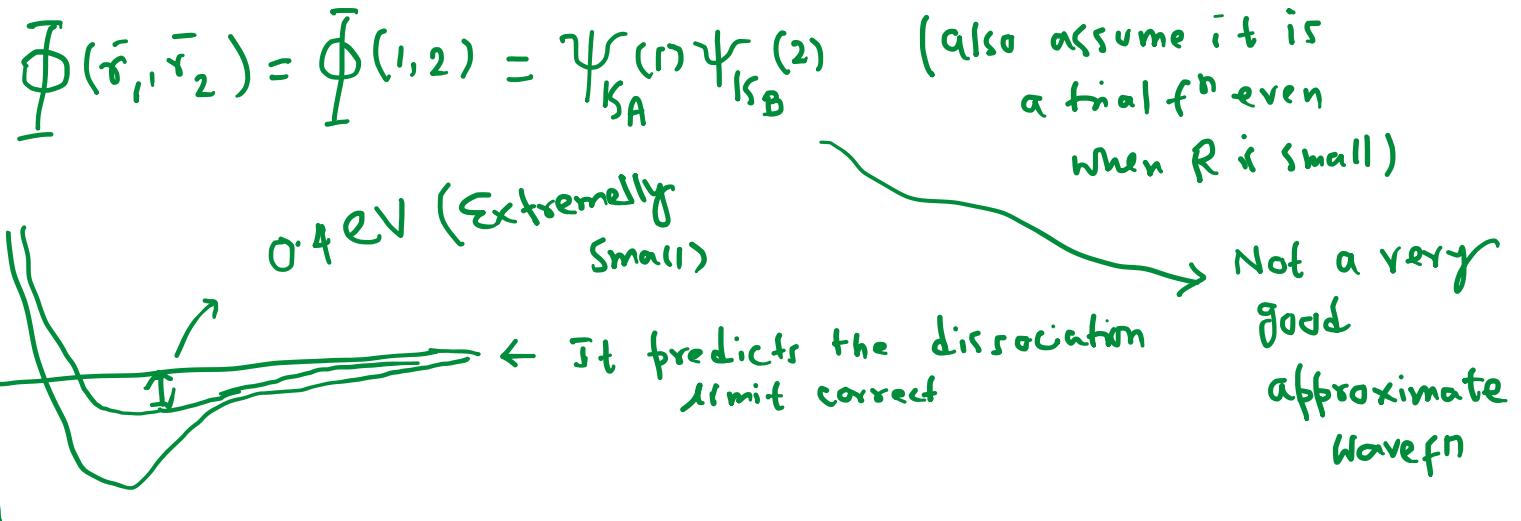
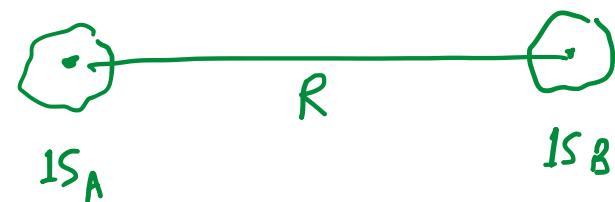
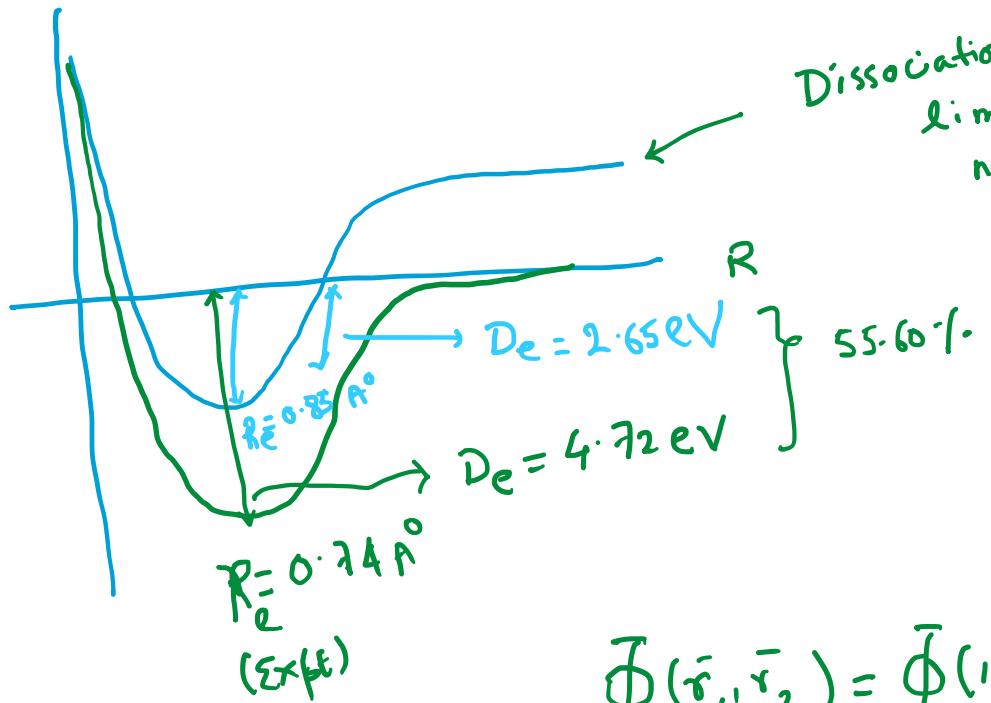
$$\psi_{IS_A}(\tau_2)$$

Suppose there is no $\frac{1}{r_{12}}$ term
es only feel nuclei

$$\tilde{\Phi}_{MO}(\bar{r}_1, \bar{r}_2) = \underbrace{\sigma_{g_{1S}}(\tau_1) \sigma_{g_{1S}}(\tau_2)}_{\substack{\downarrow \\ \downarrow}} \rightarrow \frac{1}{\sqrt{2(1+s)}} \left(\frac{e^{-\tau_{A1}}}{\sqrt{\pi}} + \frac{e^{-\tau_{B1}}}{\sqrt{\pi}} \right)$$

$$E = \frac{\int \tilde{\Phi}_{MO}^*(\bar{r}_1, \bar{r}_2) \hat{H} \tilde{\Phi}_{MO}(\bar{r}_1, \bar{r}_2) d\tau_1 d\tau_2}{\int \tilde{\Phi}_{MO}^*(\bar{r}_1, \bar{r}_2) \tilde{\Phi}_{MO}(\bar{r}_1, \bar{r}_2) d\tau_1 d\tau_2}$$

Quite involved calculation



When the distance (R) is small

e_2 may be found/associated with nucleus A

e_1

"

" B

$$\Phi_{(1,2)} = c_1 \psi_{1s_A}^{(1)} \psi_{1s_B}^{(2)} + c_2 \psi_{1s_A}^{(2)} \psi_{1s_B}^{(1)}$$

"Take a linear combination"

One can calculate c_1 & c_2 $c_1 = c_2 = \frac{1}{\sqrt{2(1+S^2)}}$ (can be shown!!)

ground state —

$$\underline{\Phi}_{VBT}^{\text{ground}} = \frac{1}{\sqrt{2(1+S^2)}} (\psi_{1s_A}^{(1)} \psi_{1s_B}^{(2)} + \psi_{1s_A}^{(2)} \psi_{1s_B}^{(1)})$$

$$\underline{\Phi}_{VBT}^{\text{excited}} = \frac{1}{\sqrt{2(1-S^2)}} (\psi_{1s_A}^{(1)} \psi_{1s_B}^{(2)} - \psi_{1s_A}^{(2)} \psi_{1s_B}^{(1)})$$

One can calculate E

Can not take only

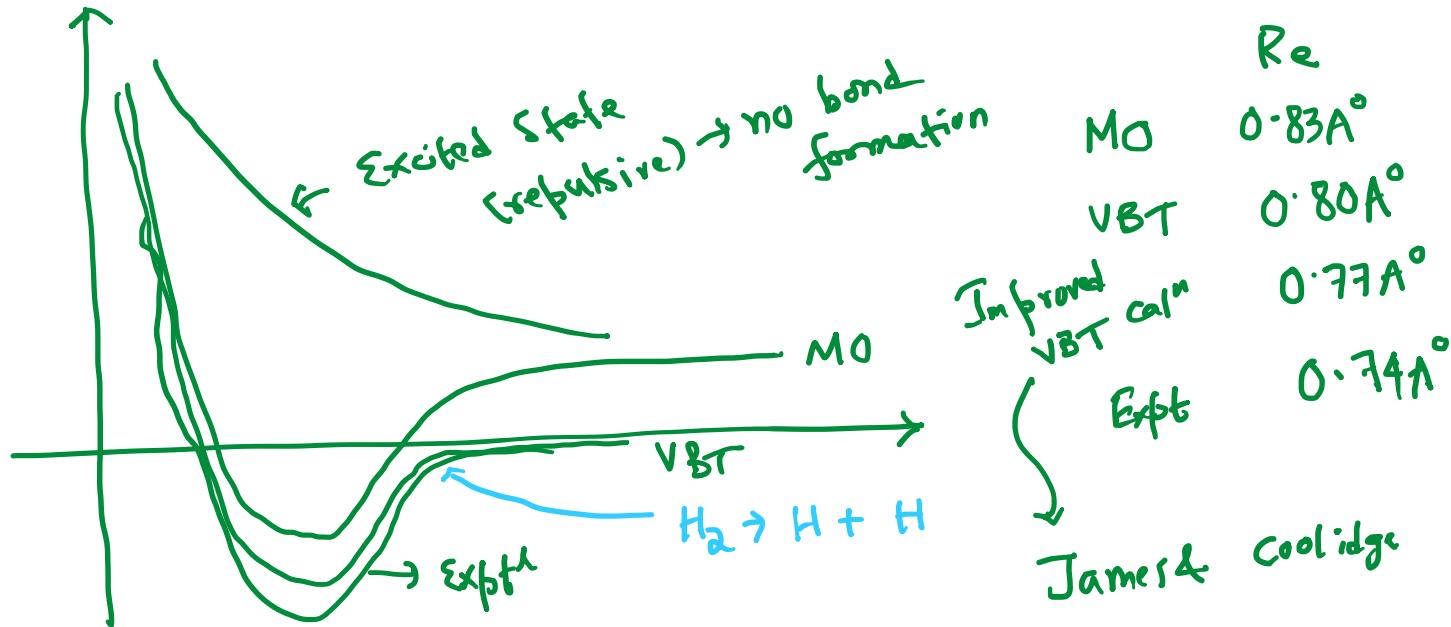
$$\psi_{1s_A}^{(1)} \psi_{1s_B}^{(2)}$$

one should also consider

$$\psi_{1s_A}^{(2)} \psi_{1s_B}^{(1)}$$

→ "Valence Bond" theory
VB theory

VBT



D_e	2.65 eV	
	3.16 eV	→ Weinbaum
	4.00 eV	
	4.72 eV	
"nuclear charge"		
James & Coolidge		

→ Variation parameter "

Why MO gives totally wrong dissociation limit?

$$\begin{aligned}
 \Phi_{MO} &= \sigma_g^{1s(1)} \sigma_g^{1s(2)} = \left(\frac{1}{\sqrt{2(1+s)}} \right)^2 \{ \psi_{1s_A}^{(1)} + \psi_{1s_B}^{(2)} \} \{ \psi_{1s_A}^{(2)} + \psi_{1s_B}^{(1)} \} \\
 &= \frac{1}{2(1+s)} \{ \underbrace{\psi_{1s_A}^{(1)} \psi_{1s_A}^{(2)} + \psi_{1s_B}^{(1)} \psi_{1s_B}^{(2)}}_{H^- H^+} + \underbrace{\psi_{1s_A}^{(1)} \psi_{1s_B}^{(2)} + \psi_{1s_B}^{(1)} \psi_{1s_A}^{(2)}}_{H^+ H^-} \}
 \end{aligned}$$

"Structures" $H^- H^+$ $H^+ H^-$ $H + H$ ν_{covalent}

VBT terms

Include Spin

$$\Phi_{\text{MO}}(1,2) \times \frac{1}{\sqrt{2}} (\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

Symmetric
Antisymmetric

$\Phi_{VBT}^{(1,2)}$

But one can design an experiment
 How to fix your VBT so that $\text{H}_2 \rightarrow \text{H}^+ + \text{H}^-$ is predicted

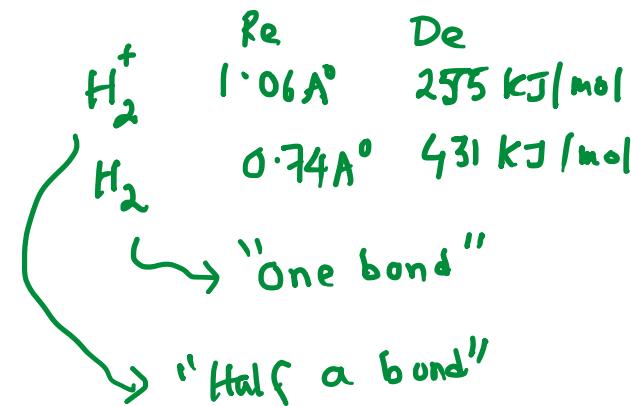
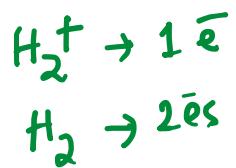
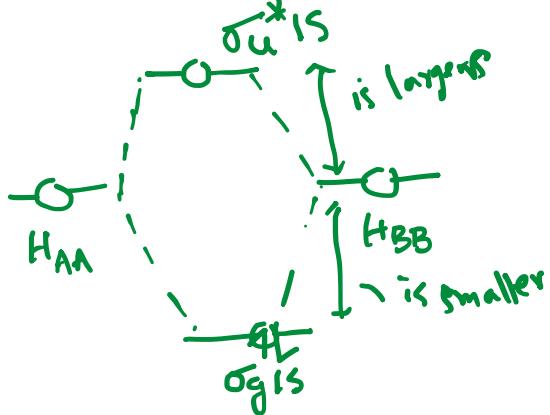
$$\Phi_{improved}^{(1,2)} = c_2 \Phi_{H;H} + c_1 \left(\Phi_{H^+H^+} + \Phi_{H^+H^-} \right)$$

$$\text{H}:\text{H}$$

Covalent \rightarrow 2 \times s are equally shared by the nuclei A & B



c_1, c_2 are variational parameters



$$\text{Bond order} = \frac{1}{2} \left(\# \text{ of } \bar{e} \text{ in bonding MO} - \# \text{ of } \bar{e} \text{ in Antibonding MO} \right)$$

$$\begin{bmatrix} H_{AA} - \epsilon & H_{AB} - \epsilon S \\ H_{AB} - \epsilon S & H_{BB} - \epsilon \end{bmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = 0$$

$\epsilon = H_{AA} \text{ or } H_{BB}$

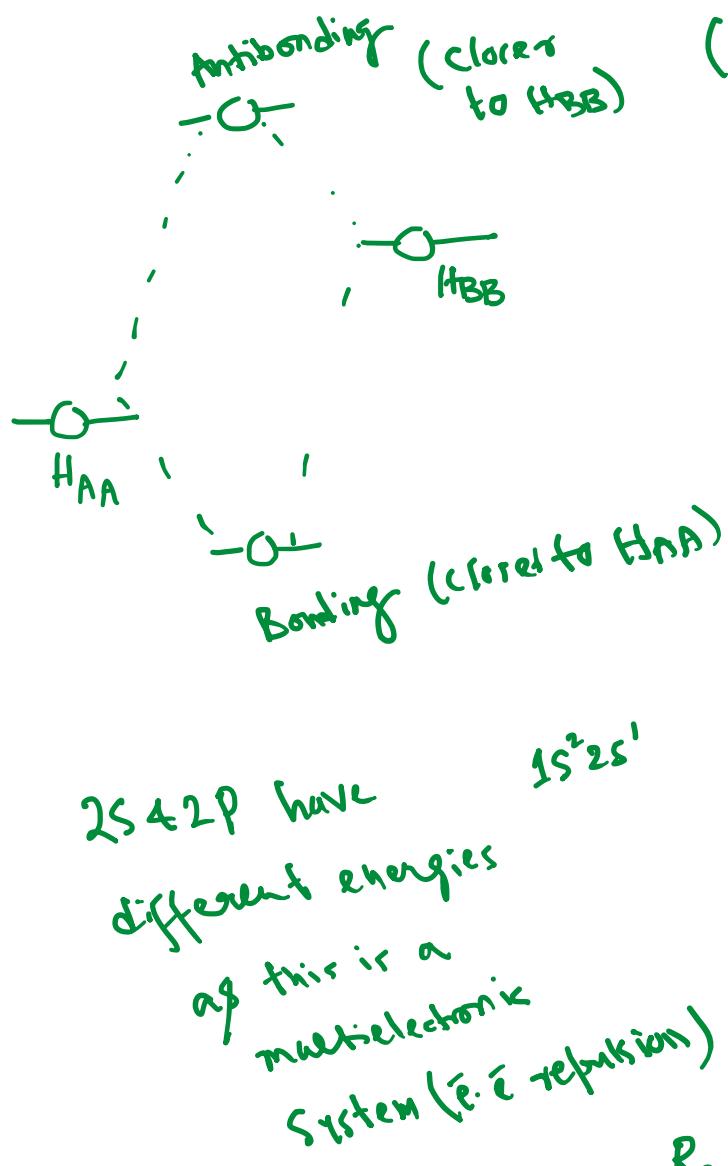
$$\text{H}_2 \rightarrow \frac{1}{2}(2-0) = 1$$

$$\text{H}_2^+ \rightarrow \frac{1}{2}(1-0) = \frac{1}{2}$$

$$\text{He}_2 \rightarrow \frac{1}{2}(2-\lambda) = 0$$

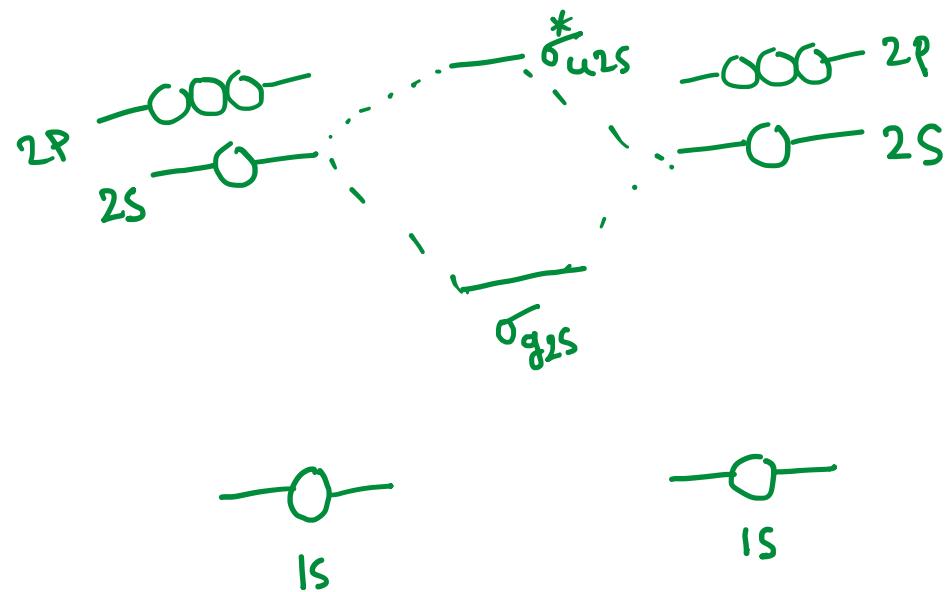
$$\Rightarrow (H_{AA} - \epsilon)(H_{BB} - \epsilon) - (H_{AB} - \epsilon S)^2 = 0$$

Suppose we have a situation where $H_{AB} = 0$ and $S = 0$.
 ↪ No Mixing of AOs → "Resonance Integral" → No bond formation!!
 ↪ overlap integral



(Heteronuclear diatomics)

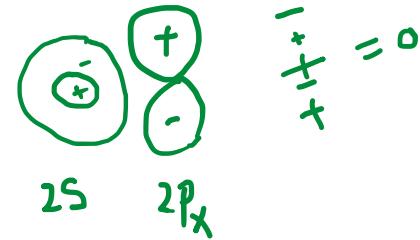
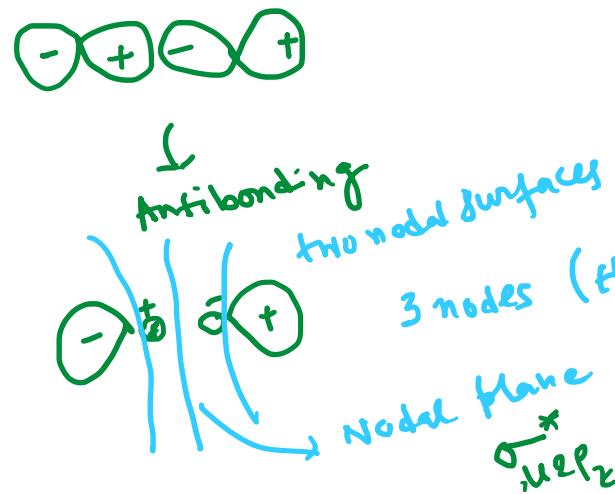
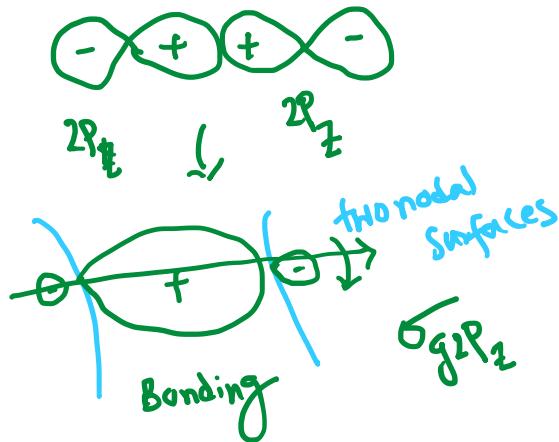
Li_2



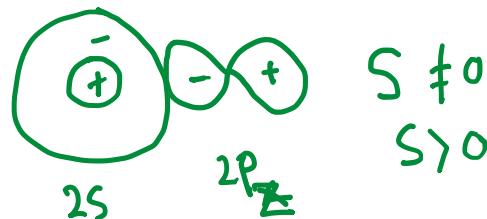
$$R_e = 2.67 \text{ \AA} \quad (\text{1s orbitals do not interact/mix much})$$

"inert"

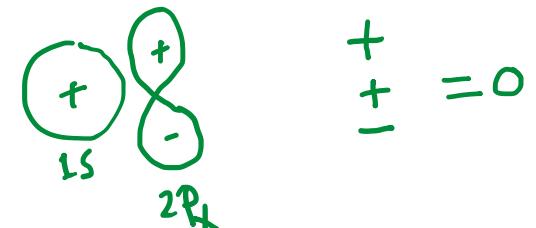
Internuclear distance is along Z



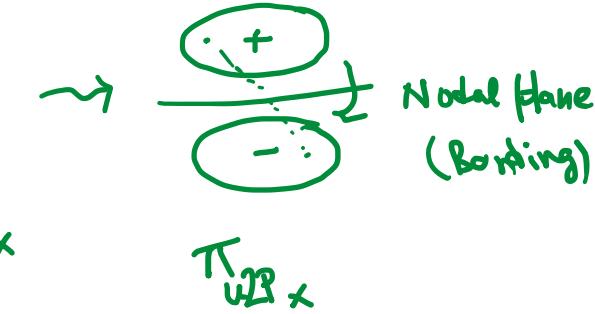
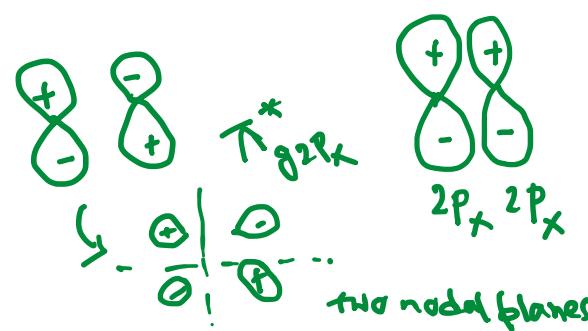
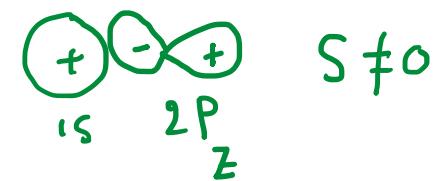
$$S = \int \psi_{2S}^* \psi_{2P_x} d\tau = 0$$



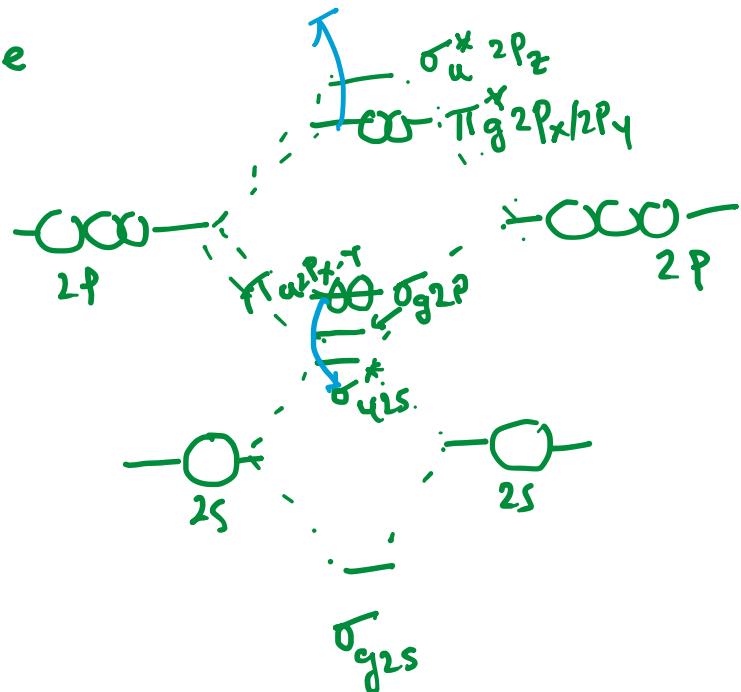
(they will mix, form
MOS)



$\int \psi_{1S}^* \psi_{2P_x} d\tau = 0$
"Overlap integral
is zero"



General
diatomic
molecule



Is it true for all homonuclear
diatomics?

2s - 2p separation is
large (no. of es is
large)

O, F

B, C → 2s - 2p gap is
small

When 2s-2p separation is small



(Valence MOs)

L_{i_2}

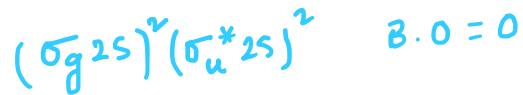


B.O = 1

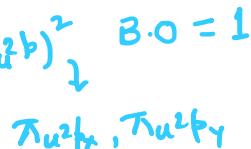
Bond length = 2.67 \AA

B_{e_2}

(Does not exist experimentally verified)



B.O = 0



π_{u2p_x}, π_{u2p_y}

B_{2u}



(No unpaired e⁻)

B.O = 2

(Double bond)

289 kJ/mol

627.6 kJ/mol
 1.31 \AA

C_2

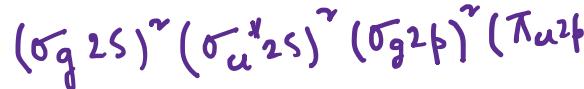


B.O = 3

(Triple bond)

941.4 kJ/mol
 1.01 \AA

N_2



2-unpaired e⁻
(verified using photoelectron spectroscopy)

B.O = 2

O_2

O_2 is paramagnetic

O_2^+ B.O = 2.5
 1.1227 \AA

O_2^- B.O = 1.5
 1.26 \AA

F_2

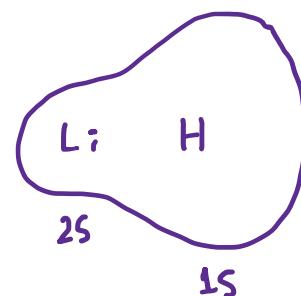
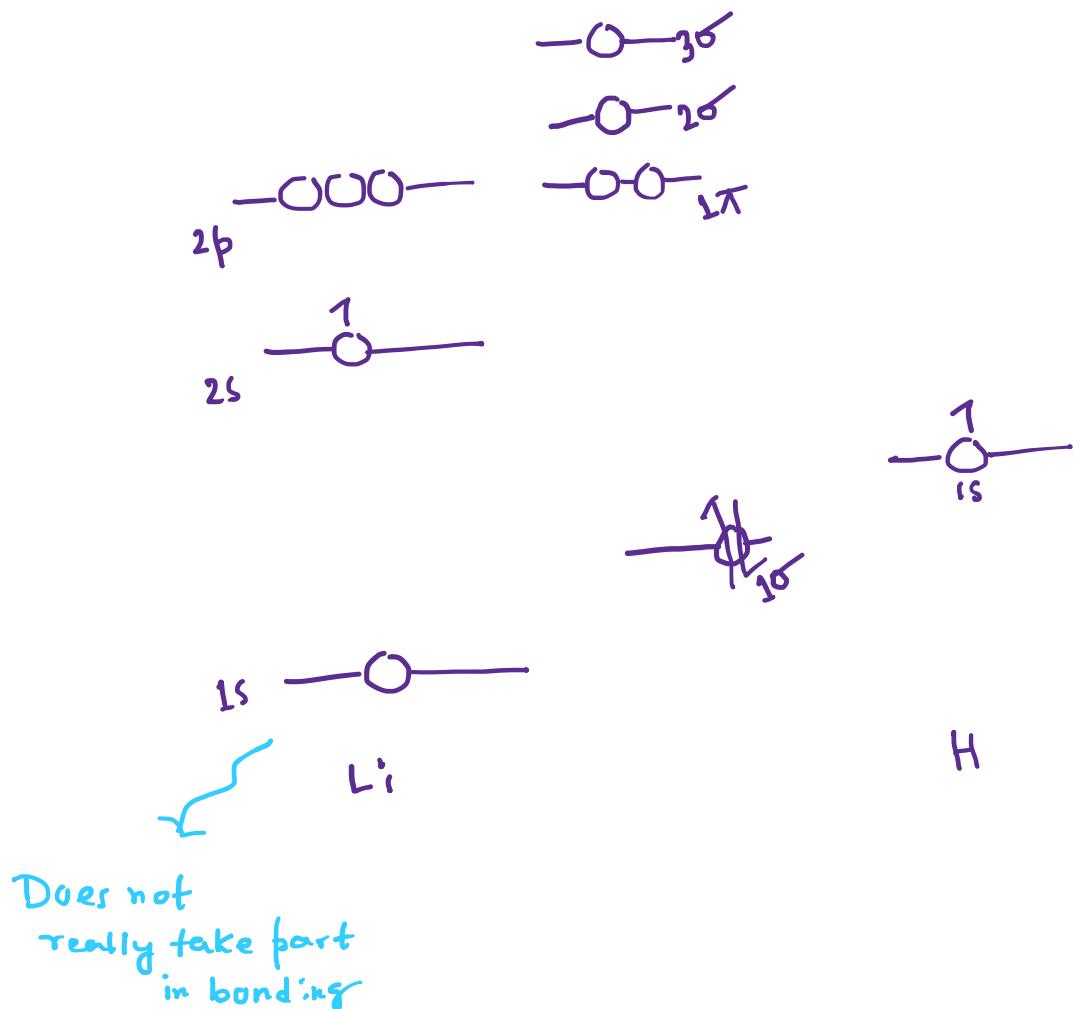
..... $(\pi_g^* 2p)^4$
B.O = 1

No unpaired electron 151 kJ/mol

1.21 \AA

493.7 kJ/mol

Heteronuclear Diatomic



charge density is more on hydrogen



ionic character ~ 80%

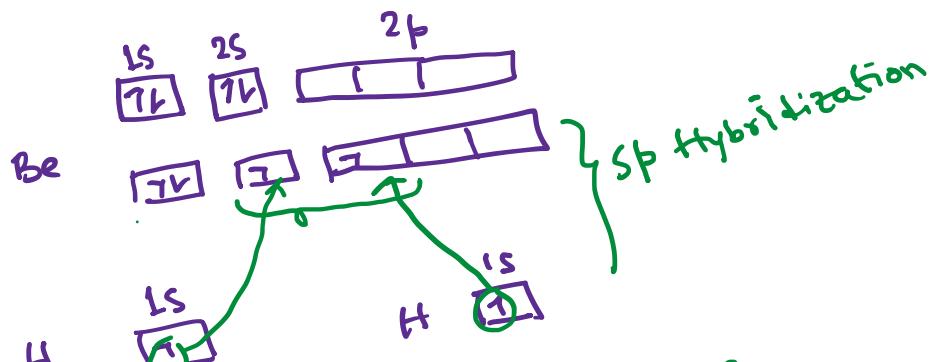
Dipole moment = 5.9 Debye

- Hybridization -



$1s^2 2s^2$ (closed shell)

$1s^2 2s^1 2p^1$ (two unpaired electrons)



Equivalent orbitals
Linus Pauling

On Be atom

$$\begin{aligned}\phi_1 &= \alpha_1 2s + b_1 2p \\ \phi_2 &= \alpha_2 2s + b_2 2p\end{aligned}\} \text{ "hybrid orbitals"}$$

are normalized

$$\int d\tau 2s^2 = 1$$

$$\int \phi_i^* \phi_i d\tau = \int \phi_i^* d\tau = 1$$

$$\alpha_1 \alpha_2 + b_1 b_2 = 0$$

$$\alpha_1^2 + b_1^2 = 1$$

$$\begin{aligned}\int \phi_i^* d\tau &= \int d\tau (\alpha_1 2s + b_1 2p)^2 = \int d\tau \alpha_1^2 2s^2 + \int d\tau b_1^2 2p^2 \\ \int \phi_i^* \phi_j d\tau &= \alpha_1 \alpha_2 \int d\tau [s^2 + b_1 b_2 \cancel{\int 2p^2 d\tau}] + \dots = 0\end{aligned}$$

α_1^2

+ $\int d\tau 2\alpha_1 b_1 2s 2p = 1$
 \downarrow
 α_1 (orthogonal)

Two hybrid orbitals are equivalent \Rightarrow Contribution of 2s in ϕ_1 = Contribution of 2s in ϕ_2

$$a_1^2 + b_1^2 = 1$$

-total contribution of 2s
 $= 1$

$$a_1^2 + a_2^2 = 1$$

$$2a_1^2 = 1 \Rightarrow a_1^2 = \frac{1}{2} = a_2^2$$

total contribution of 2p = 1

$$b_1^2 + b_2^2 = 1 \Rightarrow b_1^2 = \frac{1}{2} = b_2^2$$

$$a_1^2 = a_2^2$$

Contribution of 2p in ϕ_1 = Contribution of 2p in ϕ_2

$$b_1^2 = b_2^2$$

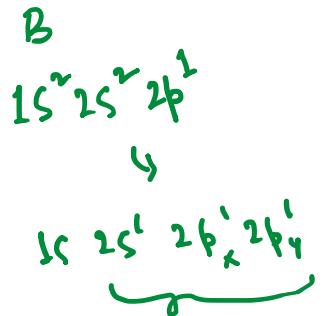
$$a_1 = \frac{1}{\sqrt{2}}, \quad a_2 = \frac{1}{\sqrt{2}}$$

$$b_1 = \frac{1}{\sqrt{2}}, \quad b_2 = -\frac{1}{\sqrt{2}}$$

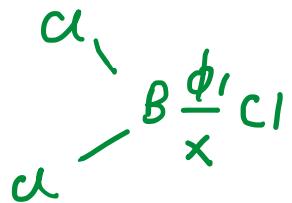
$$\phi_1 = \frac{1}{\sqrt{2}} (2s + 2p_z)$$

$$\phi_2 = \frac{1}{\sqrt{2}} (2s - 2p_z)$$

} Hybrid orbitals



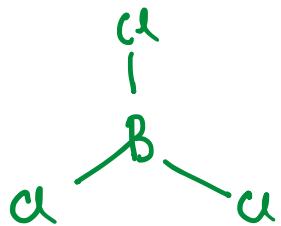
For ϕ_1 is along x axis



$c_1 = 0$ (no contribution from $2p_y$)

ϕ_1, ϕ_2 are ϕ_3 equivalent

BCl₃



Three equivalent bonds

Three hybrid orbitals

$$\phi_1 = a_1 2s + b_1 2p_x + c_1 2p_y$$

$$\phi_2 = a_2 2s + b_2 2p_x + c_2 2p_y$$

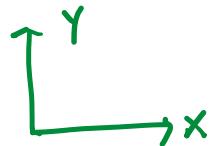
$$\phi_3 = a_3 2s + b_3 2p_x + c_3 2p_y$$

$$\int \phi_1^2 dr = 1 = a_1^2 + b_1^2 = 1 ; \int \phi_2^2 dr = a_2^2 + b_2^2 = 1$$

$$\int \phi_3^2 dr = a_3^2 + b_3^2 = 1$$

(Total contribution of 2s)
 $a_1^2 + a_2^2 + a_3^2 = 1 \Rightarrow a_i^2 = \frac{1}{3}$

$$a_1^2 = a_2^2 = a_3^2 \quad (\text{contribution of } 2s \text{ in } \phi_1 = \dots \phi_2 = \dots \phi_3) \quad a_i = \frac{1}{\sqrt{3}}$$



$$a_1^r + b_1^r = 1 \Rightarrow \frac{1}{3} + b_1^r = 1 \Rightarrow b_1^r = \frac{2}{3} \Rightarrow b_1 = \sqrt{\frac{2}{3}}$$

$$\int d\tau \phi_1 \phi_2 = 0 = \int d\tau \left(\frac{1}{\sqrt{3}} 2s + \sqrt{\frac{2}{3}} 2p_x \right) \left(\frac{1}{\sqrt{3}} 2s + b_2^2 p_x + c_2^2 p_y \right)$$

$$= \frac{1}{3} \int d\tau 2s^2 + \sqrt{\frac{2}{3}} \cdot b_2 \int 2p_x^2 \quad (\text{all other cross terms are zero})$$

$$\Rightarrow \frac{1}{3} + \sqrt{\frac{2}{3}} b_2 = 0$$

$$b_2 = -\frac{1}{3} \cdot \sqrt{\frac{3}{2}} = -\frac{1}{\sqrt{6}}$$

Similarly $\int d\tau \phi_1 \phi_3 = 0 \Rightarrow b_3 = -\frac{1}{\sqrt{6}}$ (check th.s)

$$a_2^r + b_2^r + c_2^r = 1 \Rightarrow \left(\frac{1}{\sqrt{3}}\right)^r + \left(-\frac{1}{\sqrt{6}}\right)^r + c_2^r = 1 \Rightarrow \frac{1}{3} + \frac{1}{6} + c_2^r = 1$$

$$c_2^r = \frac{1}{2} \Rightarrow c_2 = \frac{1}{\sqrt{2}}$$

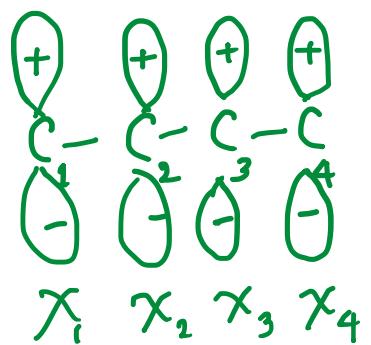
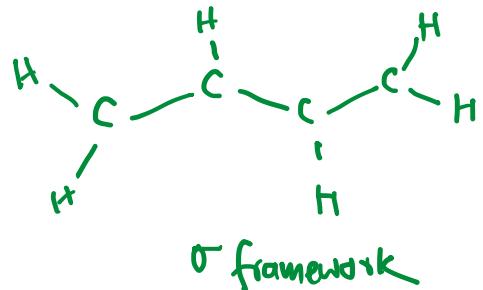
$$\left. \begin{aligned} \phi_1 &= \frac{1}{\sqrt{3}} 2s + \sqrt{\frac{2}{3}} 2p_x \\ \phi_2 &= \frac{1}{\sqrt{3}} 2s - \frac{1}{\sqrt{6}} 2p_x + \frac{1}{\sqrt{2}} 2p_y \\ \phi_3 &= \frac{1}{\sqrt{3}} 2s - \frac{1}{\sqrt{6}} 2p_x - \frac{1}{\sqrt{2}} 2p_y \end{aligned} \right\}$$

Sp² hybrid orbitals

$$\overbrace{a_3^r + b_3^r + c_3^r = 1}^{\text{check th.s.}} \Rightarrow c_3^r = \frac{1}{2} \Rightarrow c_3 = -\frac{1}{\sqrt{2}}$$

Hückel MO Theory

for Conjugated molecules



sp^2 hybridized



butadiene

on each carbon \rightarrow 1 unhybridized π orbital

they form π bonds

Molecular Orbital description

$$c_1 \chi_1 + c_2 \chi_2 + c_3 \chi_3 + c_4 \chi_4$$

Do a variational calculation

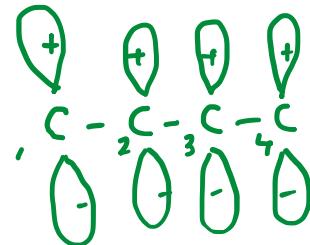
$$\underset{\pi}{\mathcal{E}}(c_1, c_2, c_3, c_4)$$

Calculate

$$\frac{\partial E}{\partial c_1} = 0; \frac{\partial E}{\partial c_2} = 0; \frac{\partial E}{\partial c_3} = 0; \frac{\partial E}{\partial c_4} = 0$$

4 equations in this case

$$\begin{pmatrix} H_{11}-\epsilon & H_{12}-\epsilon S_{12} & H_{13}-\epsilon S_{13} & H_{14}-\epsilon S_{14} \\ H_{21}-\epsilon S_{21} & H_{22}-\epsilon & H_{23}-\epsilon S_{23} & H_{24}-\epsilon S_{24} \\ H_{31}-\epsilon S_{31} & H_{32}-\epsilon S_{32} & H_{33}-\epsilon & H_{34}-\epsilon S_{34} \\ H_{41}-\epsilon S_{41} & H_{42}-\epsilon S_{42} & H_{43}-\epsilon S_{43} & H_{44}-\epsilon \end{pmatrix}_{4 \times 4} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0$$



$$S_{14} = \int d\tau X_1^* X_4 \approx 0 \quad (\text{far away})$$

$$H_{14} = \int d\tau X_1^* \hat{H} X_4 \approx 0 = H_{13}$$

↓
Resonance $H_{12} = H_{23} = H_{34} = \beta$
Integral (neighbors)

$$H_{11} = \int d\tau X_1^* \hat{H} X_1 = \alpha$$

↓ Coulomb integral

$$H_{22} = H_{33} = H_{44} = \alpha$$

All the overlap integrals = 0
 $S_{12} = 0$ (Assumption \rightarrow Hückel)

$$\frac{1}{\beta} \begin{pmatrix} \alpha - \epsilon & \beta & 0 & 0 \\ \beta & \alpha - \epsilon & \beta & 0 \\ 0 & \beta & \alpha - \epsilon & \beta \\ 0 & 0 & \beta & \alpha - \epsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0$$

$$\begin{bmatrix} \frac{\alpha - \epsilon}{\beta} & 1 & 0 & 0 \\ 1 & \frac{\alpha - \epsilon}{\beta} & 1 & 0 \\ 0 & 1 & \frac{\alpha - \epsilon}{\beta} & 1 \\ 0 & 0 & 1 & \frac{\alpha - \epsilon}{\beta} \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0$$

Simplest possible system

Ethene



$$\phi = c_1 \chi_1 + c_2 \chi_2$$

$$\begin{bmatrix} x & 1 \\ 1 & x \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0$$

Let us take $\frac{\alpha - \epsilon}{\beta} = x$ Hückel Matrix

$$\begin{bmatrix} x & 1 & 0 & 0 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 0 & 0 & 1 & x \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0$$

$\rightarrow \boxed{\quad} = 0 \rightarrow 4 \text{ solutions}$

$\sim x^4 \text{ eqn} \rightarrow 4 \text{ roots}$
Secular Determinant

$$\boxed{| = 0 \rightarrow x^2 - 1 = 0} \quad x = +1 \text{ or } -1$$

two allowed energies

$$x = -1$$

$$-1 = \frac{\alpha - \epsilon}{\beta} \Rightarrow \epsilon_1 = \alpha + \beta$$

$$x = +1$$

$$+1 = \frac{\alpha - \epsilon}{\beta} \Rightarrow \epsilon_2 = \alpha - \beta$$

$$x = -1$$

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0$$

$$\Rightarrow \begin{cases} -c_1 + c_2 = 0 \\ c_1 - c_2 = 0 \end{cases} \quad c_1 = c_2$$

$$\phi_1 = \frac{1}{\sqrt{2}} (x_1 + x_2)$$

$$\text{Put } x = 1 \quad \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0 \Rightarrow c_1 = -c_2$$

$$\phi_2 = \frac{1}{\sqrt{2}} (x_1 - x_2)$$

~~$\epsilon_2 = \alpha - \beta$~~ α, β both are negative

~~$\epsilon_1 = \alpha + \beta$~~

(Bonding MO)

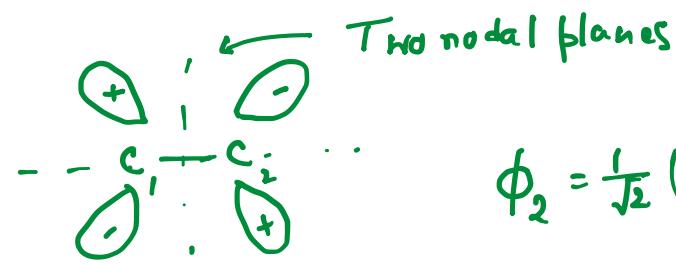
1 on each carbon

$$\begin{aligned} \phi_1 &= c_1 x_1 + c_2 x_2 \\ &= c_1 (x_1 + x_2) \end{aligned}$$

$$\int d\tau \phi_1^2 = c_1^2 \int (x_1 + x_2)^2 d\tau = 1$$

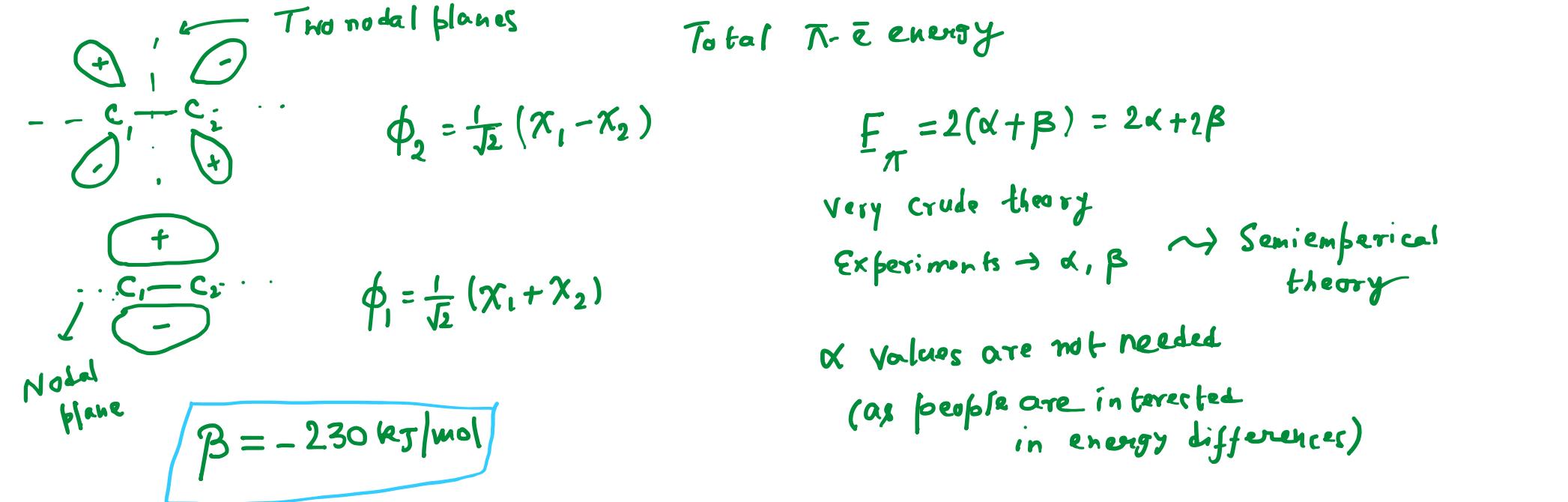
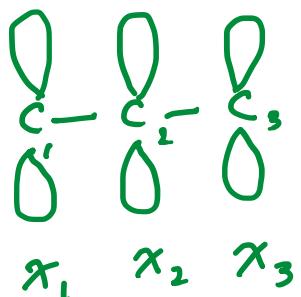
$$\begin{aligned} &= c_1^2 \left[x_1^2 \int d\tau + c_1^2 \left[x_2^2 \int d\tau + c_1^2 \left[2x_1 x_2 \int d\tau \right] \right] \right] \\ &\quad \downarrow \quad \downarrow \quad \downarrow \\ &= c_1^2 + c_1^2 = 2c_1^2 = 1 \end{aligned}$$

$$\Rightarrow c_1 = \frac{1}{\sqrt{2}}$$



$$\beta = -230 \text{ kJ/mol}$$

Three carbon atom system



allyl (radical | cation | anion)

Hückel Matrix

$$\begin{bmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \quad \begin{vmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{vmatrix} = 0$$

$$x(x^2 - 1) - 1(x - 0) + 0 = 0$$

$$x^3 - 2x = 0$$

$$\Rightarrow x(x^2 - 2) = 0 \quad x=0, x=-\sqrt{2}, +\sqrt{2}$$

$$x = \sqrt{2}$$

$$\epsilon_3 = \alpha - \sqrt{2}\beta$$

Antibonding

$$x = 0$$

$$\epsilon_2 = \alpha$$

Non-bonding

$$x = -\sqrt{2}$$

$$\epsilon_1 = \alpha + \sqrt{2}\beta$$

Bonding

Cation

$$\phi_3 = \frac{1}{2} (x_1 - \sqrt{2}x_2 + x_3)$$

$$\phi_2 = \frac{1}{\sqrt{2}} (x_1 - x_3)$$

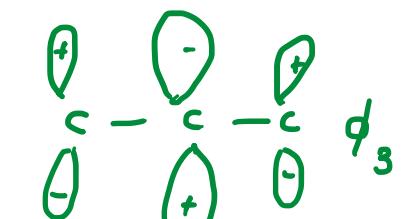
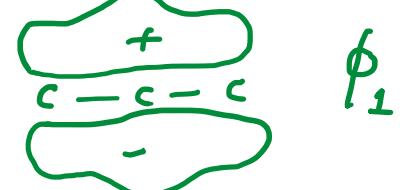
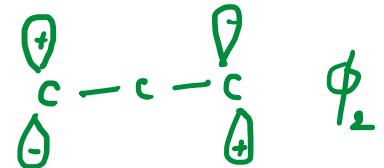
$$\phi_1 = \frac{1}{2} (x_1 + \sqrt{2}x_2 + x_3)$$

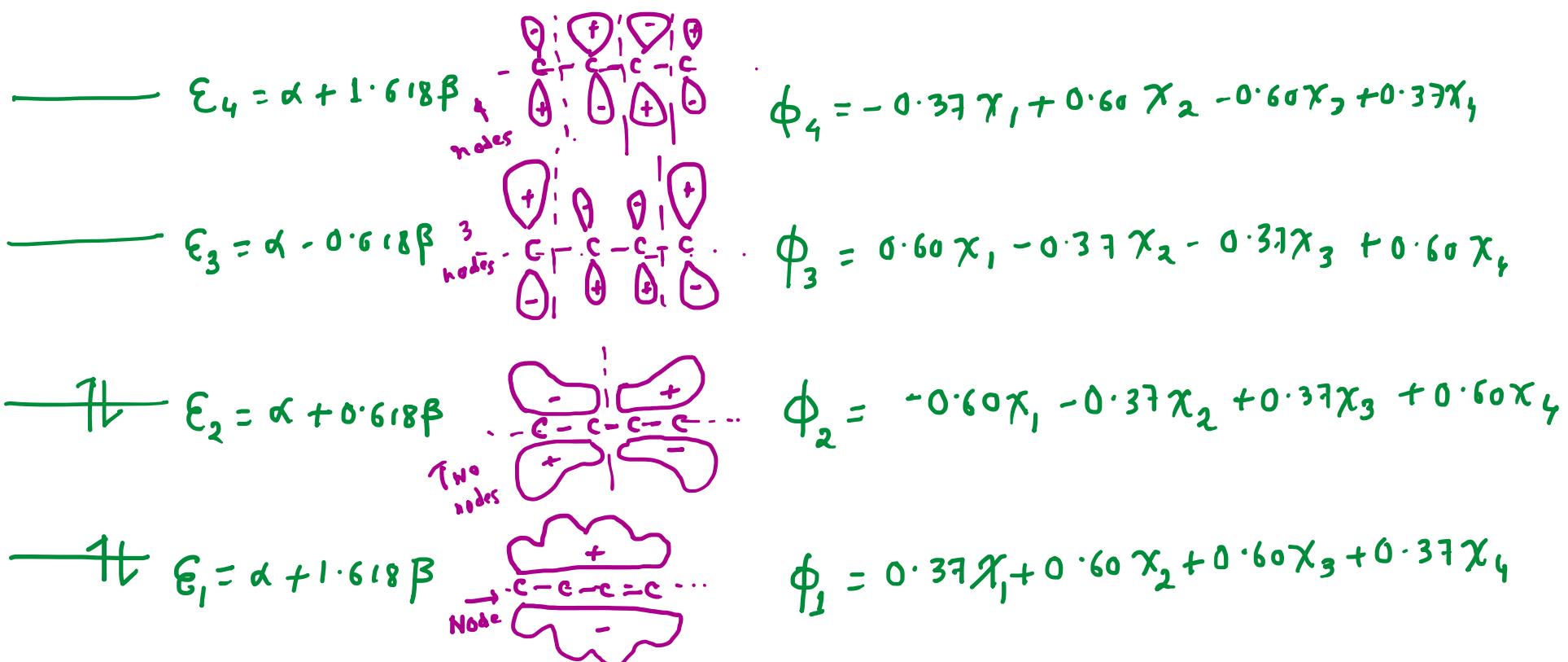
Butadiene

$$\begin{vmatrix} x & 1 & 0 & 0 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 0 & 0 & 1 & x \end{vmatrix} = 0$$

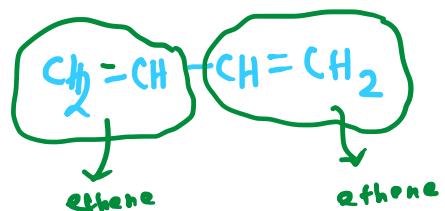
$$x^4 - 3x^2 + 1 = 0$$

$$-1.618, -0.618, 0.618, 1.618$$



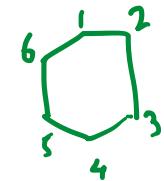


$E_{\pi} = 2(\alpha + 1.618\beta) + 2(\alpha + 0.618\beta) = 4\alpha + 4.472\beta$



$2 \text{ ethene units} \Rightarrow E_{\pi} = (2\alpha + 2\beta) \times 2 = 4\alpha + 4\beta$

Delocalization energy (DE) = $-0.472\beta \approx -110 \text{ kJ/mol}$

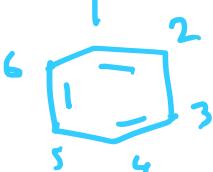


Benzene

$$\begin{bmatrix} x & 1 & 0 & 0 & 0 & 1 \\ 1 & x & 1 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 0 & 1 & x & 1 \\ 1 & 0 & 0 & 0 & 1 & x \end{bmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{pmatrix} = 0$$

$$E_{\pi} = 2(\alpha + 2\beta) + 4(\alpha + \beta)$$

$$E_{\pi} = 6\alpha + 8\beta$$



3 separate ethene
Units

$$E_{\pi} = 3(2\alpha + 2\beta) = 6\alpha + 6\beta$$

$$x = \frac{\alpha - \epsilon}{\beta} \Rightarrow -2 = \frac{\alpha - \epsilon}{\beta} \Rightarrow \epsilon = \alpha + 2\beta$$

$$\epsilon_6 = \alpha + 2\beta$$

$$\epsilon_4, \epsilon_5 = \alpha + \beta$$

$$\epsilon_2, \epsilon_3 = \alpha + \beta$$

$$\epsilon_1 = \alpha + 2\beta$$

$$x^6 - 6x^4 + 9x^2 - 4 = 0$$

$$\Rightarrow (x-2)(x-1)^2(x+1)^2(x+2) = 0$$

$$\left. \begin{array}{lll} x = -2 & x = 1 & x = -1 \\ x = 2 & x = 1 & x = -1 \end{array} \right\} 6 \text{ solutions}$$

Benzene is
very stable
Aromatic

$$\Delta E = +2\beta = 460 \text{ kJ/mol}$$

$$\phi_6 = \frac{1}{\sqrt{6}} (x_1 - x_2 + x_3 - x_4 + x_5 - x_6)$$

π MOs of Benzene

$$\phi_5 = \frac{1}{\sqrt{12}} (x_1 - x_2 + 2x_3 - x_4 - x_5 + 2x_6)$$

$$\phi_4 = \frac{1}{2} (x_1 - x_2 + x_4 - x_5)$$

$$\phi_3 = \frac{1}{2} (x_1 + x_2 - x_4 - x_5)$$

$$\phi_2 = \frac{1}{\sqrt{12}} (x_1 - x_2 - 2x_3 - x_4 + x_5 + 2x_6)$$

$$\phi_1 = \frac{1}{\sqrt{6}} (x_1 + x_2 + x_3 + x_4 + x_5 + x_6)$$

