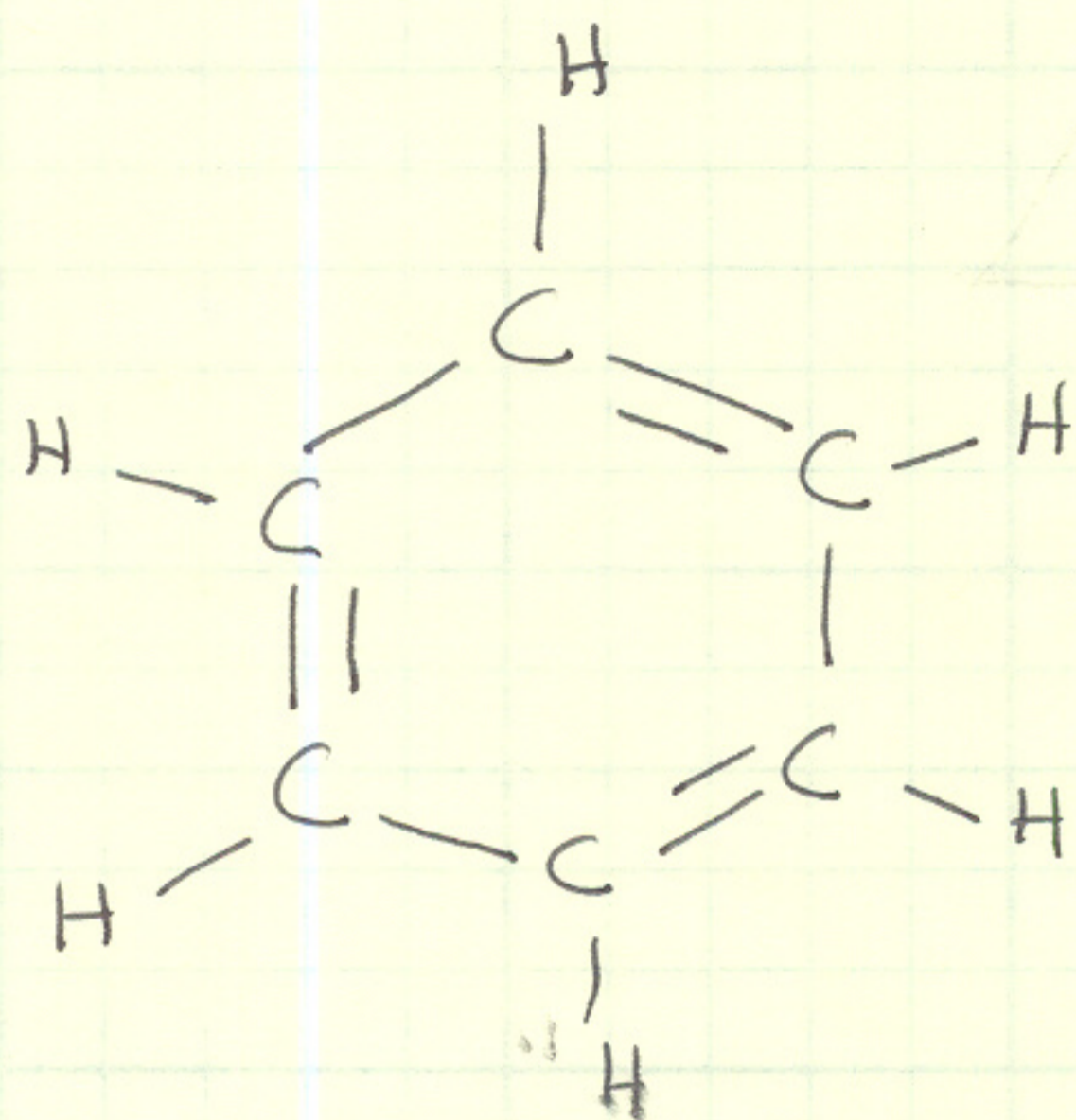
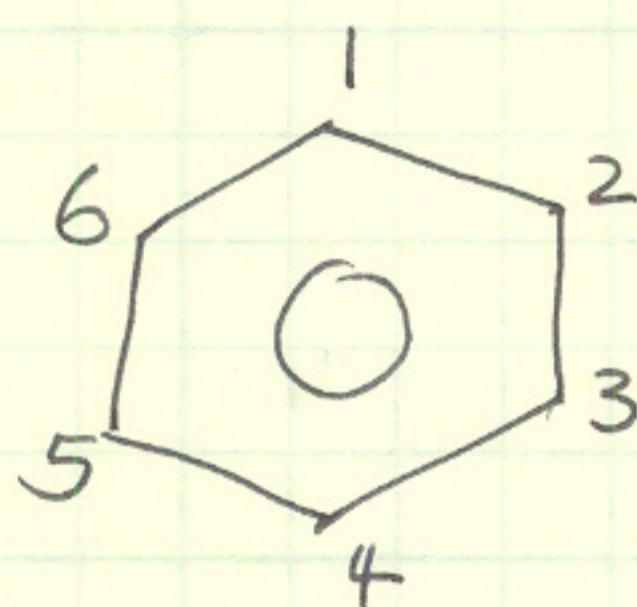


# Hückel theory applied to benzene



aromatic hydrocarbon



Total wavefunction 
$$\psi = c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3 + c_4 \phi_4 + c_5 \phi_5 + c_6 \phi_6$$

$\phi_1, \phi_2, \dots$  etc. represent the unhybridized  $2p$  orbital on each C that is used for  $\pi$  bonding.

Secular determinant:

$H_{11} - ES_{11}$	$H_{12} - ES_{12}$	$H_{13} - ES_{13}$	$H_{14} - ES_{14}$	$H_{15} - ES_{15}$	$H_{16} - ES_{16}$
$H_{21} - ES_{21}$	$H_{22} - ES_{22}$	$H_{23} - ES_{23}$	$H_{24} - ES_{24}$	$H_{25} - ES_{25}$	$H_{26} - ES_{26}$
$H_{31} - ES_{31}$	$H_{32} - ES_{32}$	$H_{33} - ES_{33}$	$H_{34} - ES_{34}$	$H_{35} - ES_{35}$	$H_{36} - ES_{36}$
$H_{41} - ES_{41}$	$H_{42} - ES_{42}$	$H_{43} - ES_{43}$	$H_{44} - ES_{44}$	$H_{45} - ES_{45}$	$H_{46} - ES_{46}$
$H_{51} - ES_{51}$	$H_{52} - ES_{52}$	$H_{53} - ES_{53}$	$H_{54} - ES_{54}$	$H_{55} - ES_{55}$	$H_{56} - ES_{56}$
$H_{61} - ES_{61}$	$H_{62} - ES_{62}$	$H_{63} - ES_{63}$	$H_{64} - ES_{64}$	$H_{65} - ES_{65}$	$H_{66} - ES_{66}$

= 0

Using Hückel approximations

$$\begin{vmatrix} \alpha - E & \beta & 0 & 0 & 0 & \beta \\ \beta & \alpha - E & \beta & 0 & 0 & 0 \\ 0 & \beta & \alpha - E & \beta & 0 & 0 \\ 0 & 0 & \beta & \alpha - E & \beta & 0 \\ 0 & 0 & 0 & \beta & \alpha - E & \beta \\ \beta & 0 & 0 & 0 & \beta & \alpha - E \end{vmatrix} = 0$$

Expanding this determinant and solving the equation gives the following solutions.

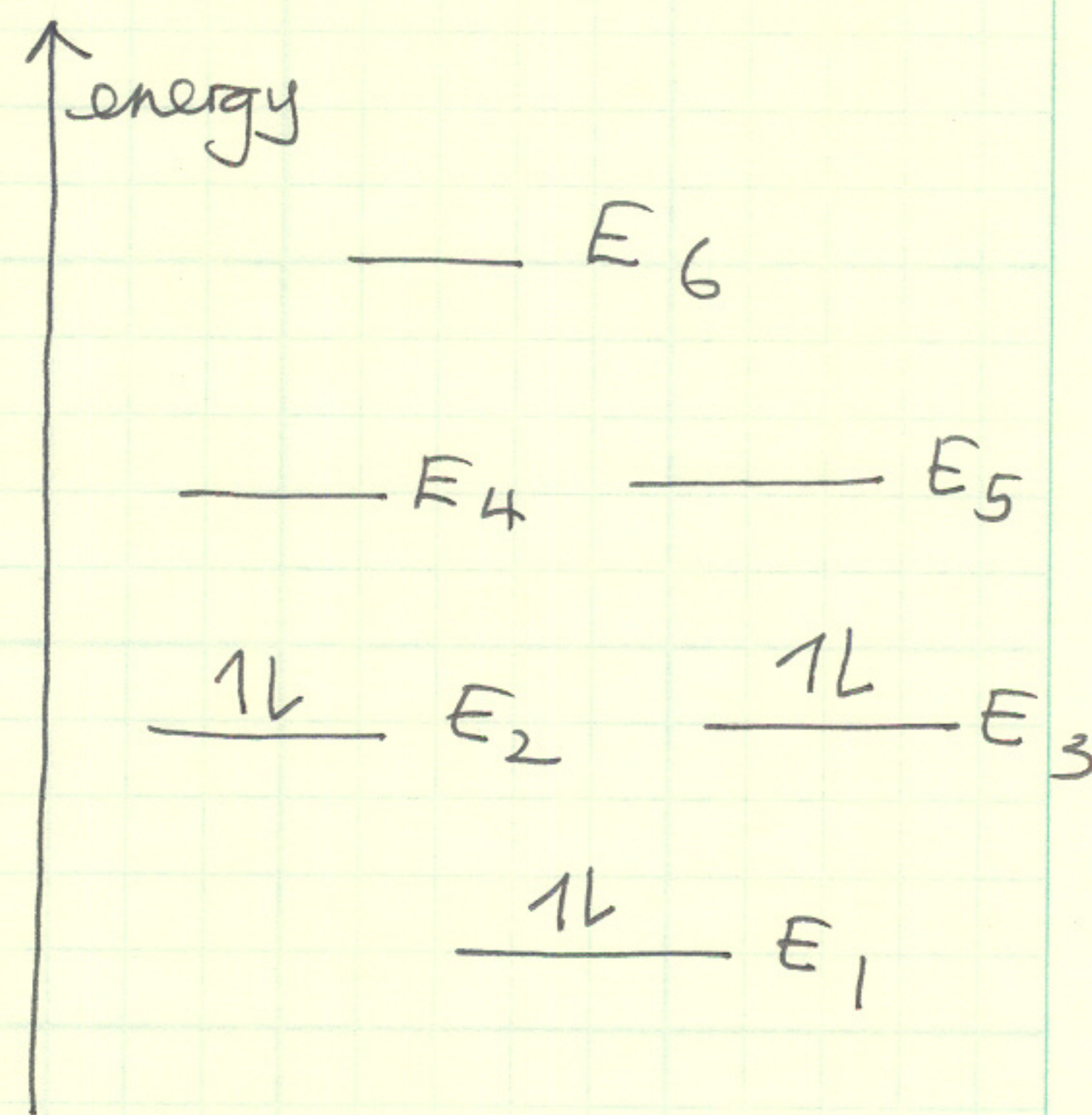
$$E_1 = \alpha + 2\beta$$

$$E_2 = E_3 = \alpha + \beta$$

$$E_4 = E_5 = \alpha - \beta$$

$$E_6 = \alpha - 2\beta$$

$$(\beta < 0)$$



$$\begin{aligned} \pi\text{-electron energy for benzene} &= 2(\alpha + 2\beta) + 4(\alpha + \beta) \\ &= 6\alpha + 8\beta \end{aligned}$$