

$$E_k = \alpha + 2\beta \cos \frac{2k\pi}{N} \quad N \text{ even, } k=0, \pm 1, \dots, \frac{N}{2} \quad N \text{ odd, } k=0, \pm 1, \dots, \pm \frac{N-1}{2}$$

(a) Benzene:  $N=6$

$k=0$	$E = \alpha + 2\beta$	
$\pm 1$	$\alpha + 2\beta \cos \frac{2\pi}{6} = \alpha + \beta$	(2-fold degeneracy)
$\pm 2$	$\alpha - \beta$	(2-fold degeneracy)
3	$\alpha - 2\beta$	

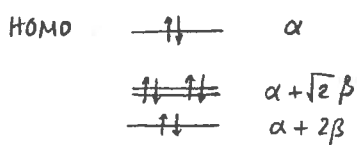


Binding energy:  $2(\alpha + 2\beta) + 4(\alpha + \beta) = 6\alpha + 8\beta$

Comparing to  $6(\alpha + \beta)$ ,  
delocalization energy is  $2\beta$ .

Cyclooctatetraene:  $N=8$

$k=0$	$E = \alpha + 2\beta$	
$\pm 1$	$\alpha + 2\beta \cos \frac{2\pi}{8} = \alpha + \sqrt{2}\beta$	(2-fold degeneracy)
$\pm 2$	$\alpha + 2\beta \cos \frac{4\pi}{8} = \alpha$	" "
$\pm 3$	$\alpha + 2\beta \cos \frac{6\pi}{8} = \alpha - \sqrt{2}\beta$	" "
4	$\alpha - 2\beta$	



Binding energy:  $2(\alpha + 2\beta) + 4(\alpha + \sqrt{2}\beta) + 2\alpha$   
 $= 8\alpha + 4(1 + \sqrt{2})\beta$

Comparing to  $8(\alpha + \beta)$ ,  
delocalization energy is  $4(\sqrt{2} - 1)\beta \approx 1.64\beta$