# Ch 16

Note Title 2/10/2006

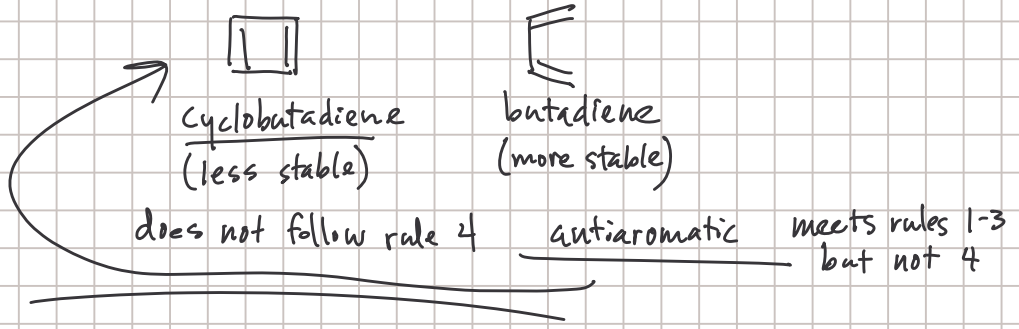
## Aromatic compounds

1) cyclic, w/ conj. double bonds

2) each atom in ring needs unhybridized p orbital
(sp² already have one - carbocations / carbanions)


3) p orbitals must be parallel (to overlap)
(ring must be planar)

4) delocalization of π electrons must lower energy





**Nonaromatic** doesn't meet rules 1-3

## Hückel's Rule — for predicting which compounds are aromatic or antiaromatic

★ to qualify, cpd must have continuous ring of overlapping p orbitals (rules 1-3)

# π electrons $(4N+2)$ : aromatic 2, 6, 10, 14, 18 π e⁻

$N = 0, 1, 2, 3, \ldots$

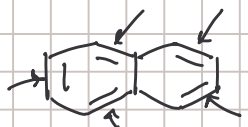
$(4N)$ : antiaromatic 4, 8, 12, ... π e⁻

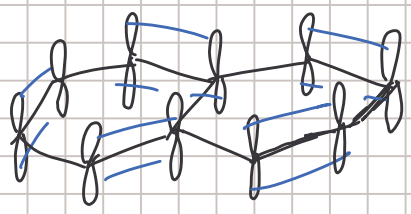
$4N+2$ π e⁻ has all paired e⁻, all in bonding MOs

$4N$ π e⁻, has 2 unpaired e⁻, in nonbonding MOs

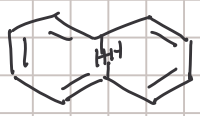

6 π electrons  $6 = 4N+2$ where $N=1$


4 π electrons  $4 = 4N$ where $N=1$


naphthalene

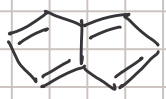

10 π e⁻ = $4N+2$ where $N=2$

aromatic!

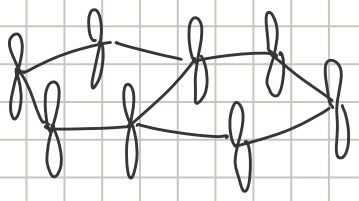

not planar!  NON aromatic

(cannot apply Hückel's rule)

similar energy to 



Pentalene



$8\ \pi e^-$ = $4N$ where $N = 2$

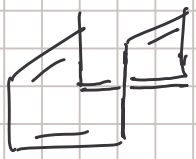
antiaromatic

less stable than 

cyclooctatetraene

COT antiaromatic if planar

actually

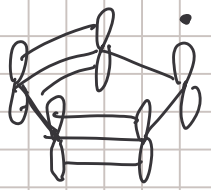


non planar conformation is better

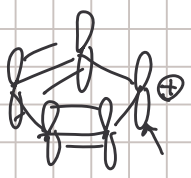
(not planar)

NONaromatic is more stable than antiaromatic

## Aromatic ions



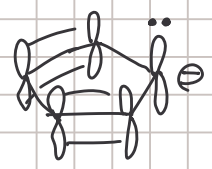
$5\ \pi e^-$ = radical nonaromatic



= 

$4\ \pi e^-$ antiaromatic

will never exist



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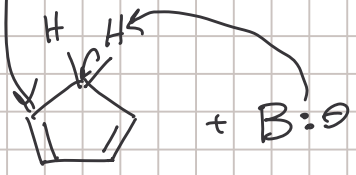
$6\ \pi e^-$ = aromatic

extra-stable carbanion

nonaromatic



cyclopentadiene (acid)

relatively strong acid

cyclopentadienyl anion

(extra stable) aromatic