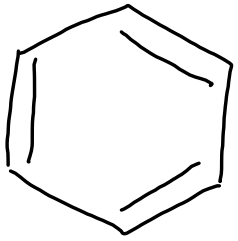
Chpt 15 Aromatics

Benzene - simplest arom cmpd

C_6H_6 

all bonds same length (1.4 Å)

all bond angles are 120°

all C's are sp^2

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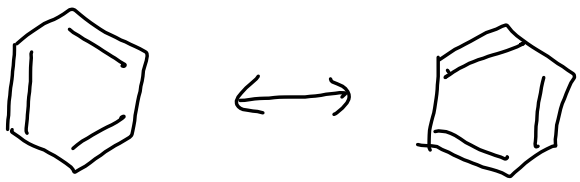
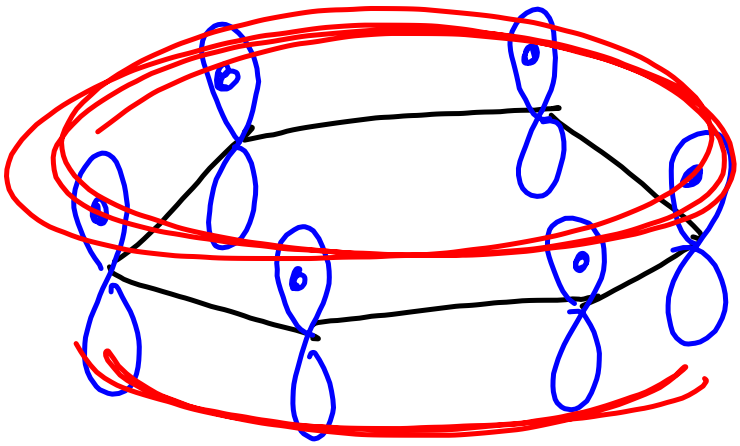
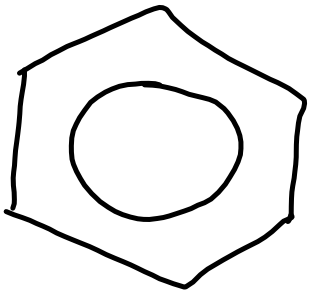
entire molecule is planar

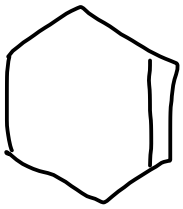




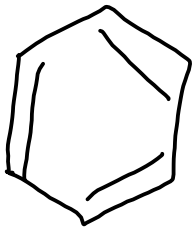
The 6 πe^- over 6 C's delocalize into a donut cloud above & below C ring



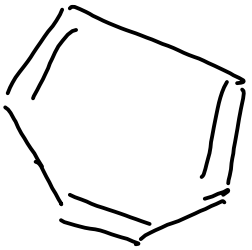
e- delocalization produces a cmpd more stable than a cmpd w/out it



1640



1600

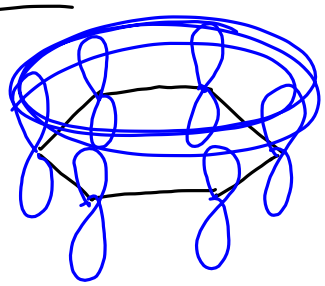


1,3,5-cyclohexa triene (theoretical)

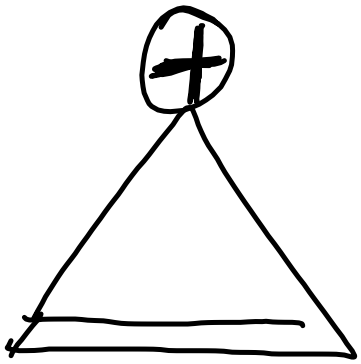
Benzene is more stable than the theoretical by 36 kcal

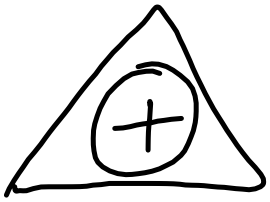
Criteria for a ring to be aromatic!

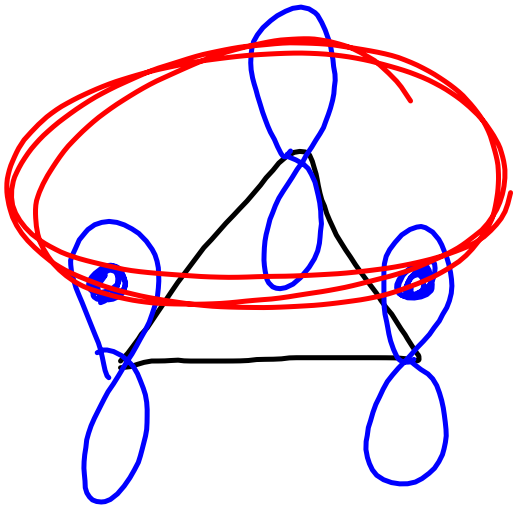
1. must be a ring
2. all atoms in ring must be sp^2
3. the # π e^- in ring must be $(4n+2)$
   where $n = 0, 1, 2 \ldots$
   magic #'s are 2
   6
   10
4. for max overlap of the p-orbs, ring must be flat



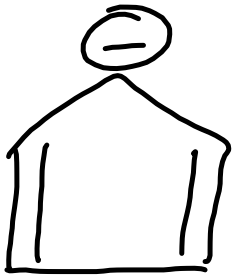
Arom rings w/ 2 πe^-

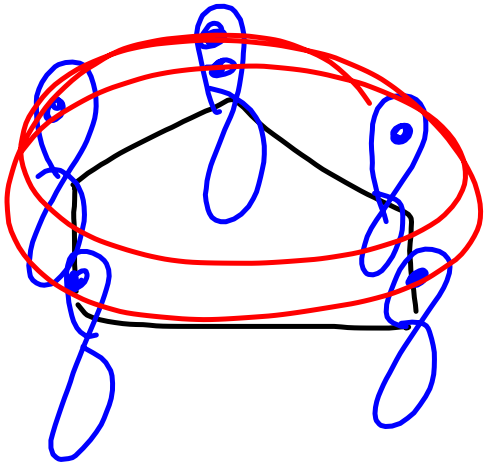


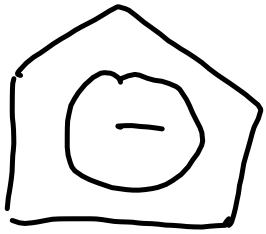


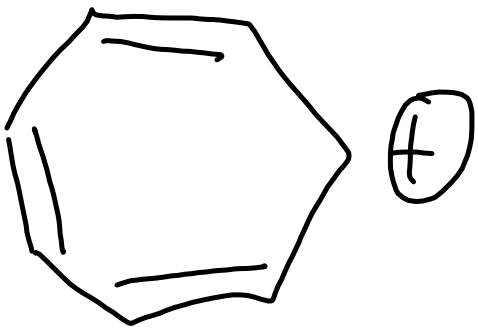


Arom rings w/ 6 π e⁻

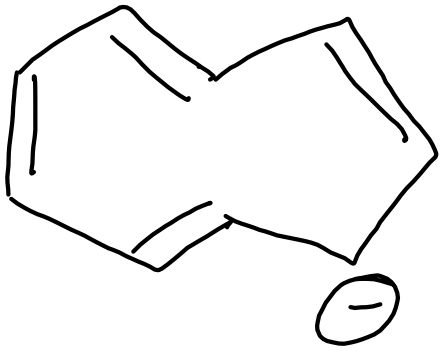


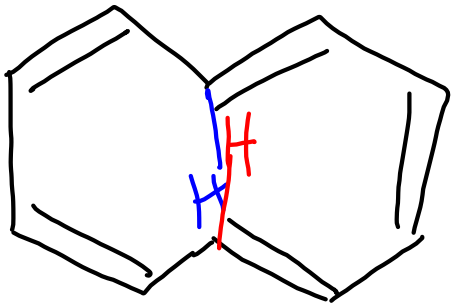






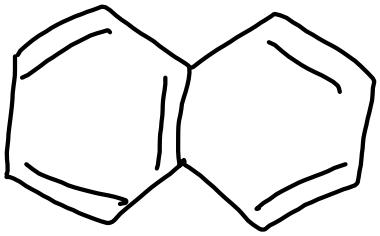
Arom rings w/ 10 πe^-





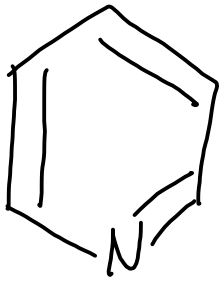
not arom –
not planar

twists to avoid
interactions between H's
(so is actually normal)



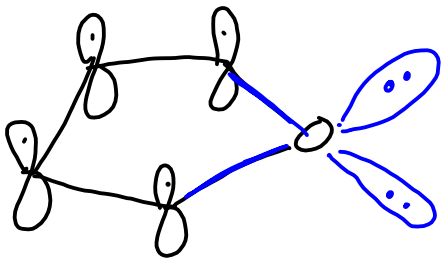
naphthalene
is
aromatic

Other arom rings can contain N, O, S called heterocycles

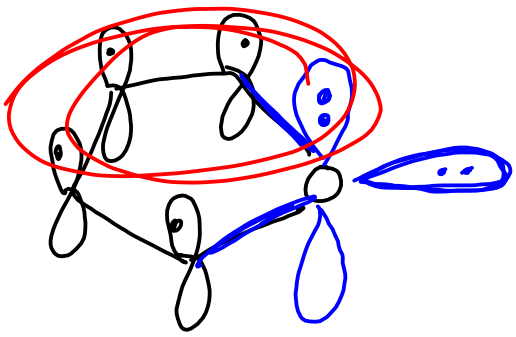


6 π e⁻ arom

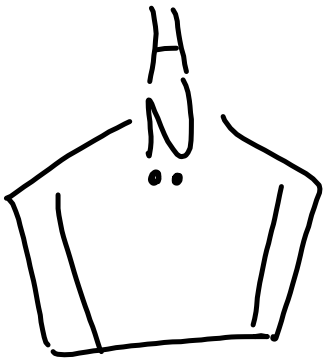
Oran is aromatic



sp^3 O



sp^2 O



4 e- from double bonds

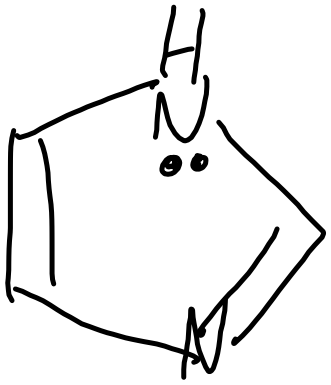
+ 2 e- from lp on N

6

4 πe^- in double bonds

+ 2 πe^- from one lp on S

6



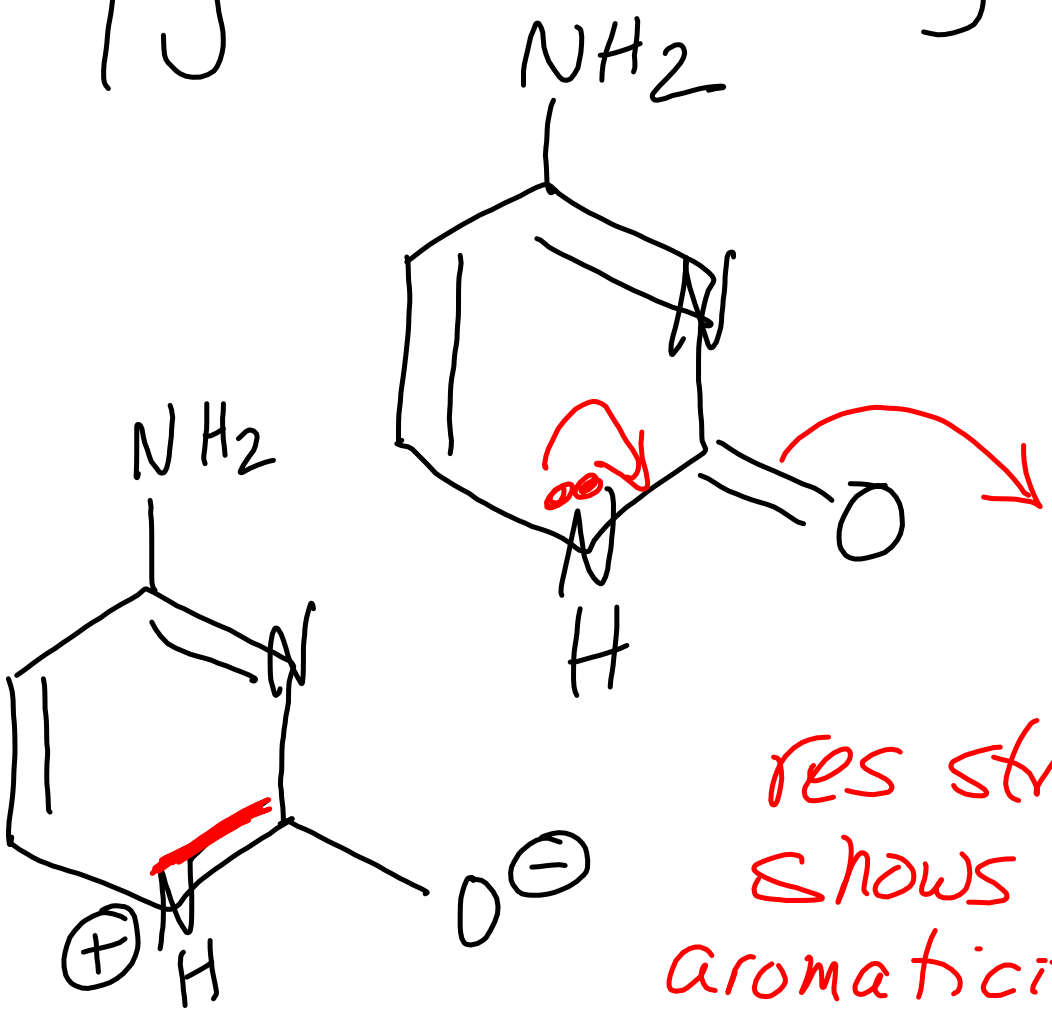
4 π e- from double bonds

2 π e- from lp on N

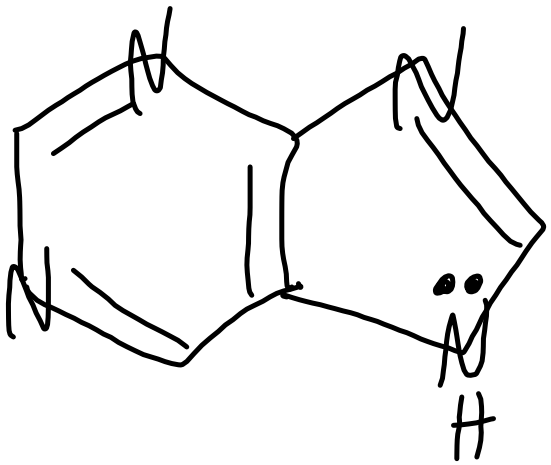
imidazole

6

Cytosine is a Pyrimidine ring



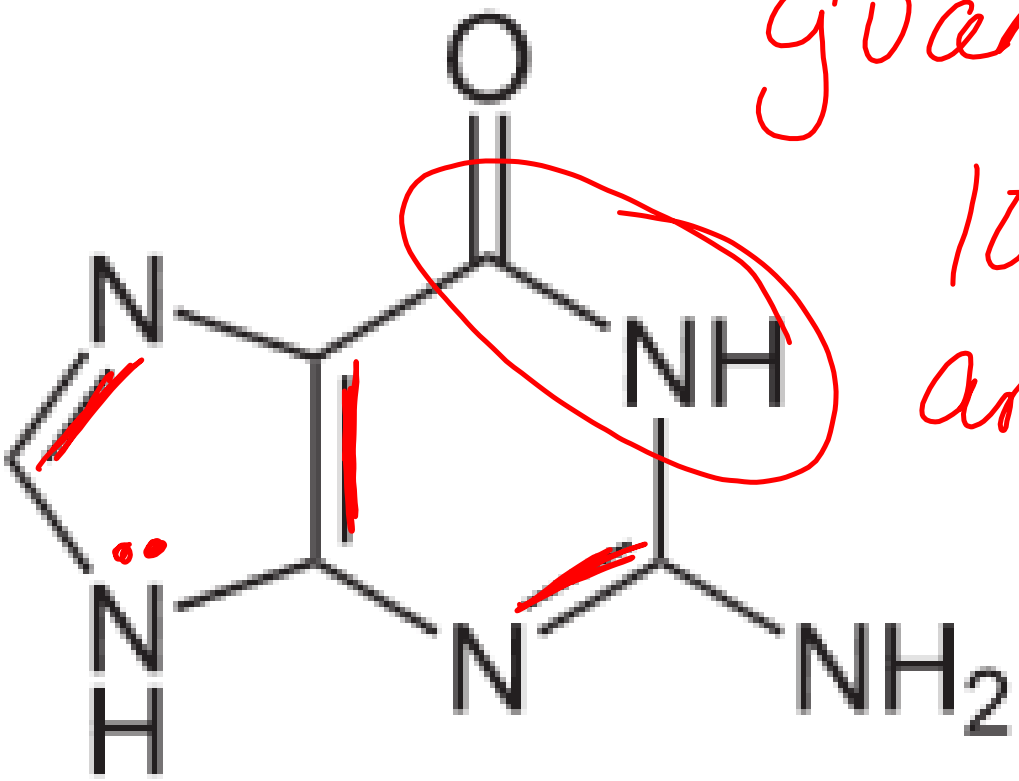
res str shows the aromaticity



8 π e⁻ from double bonds

+ 2 π e⁻ from lp on N

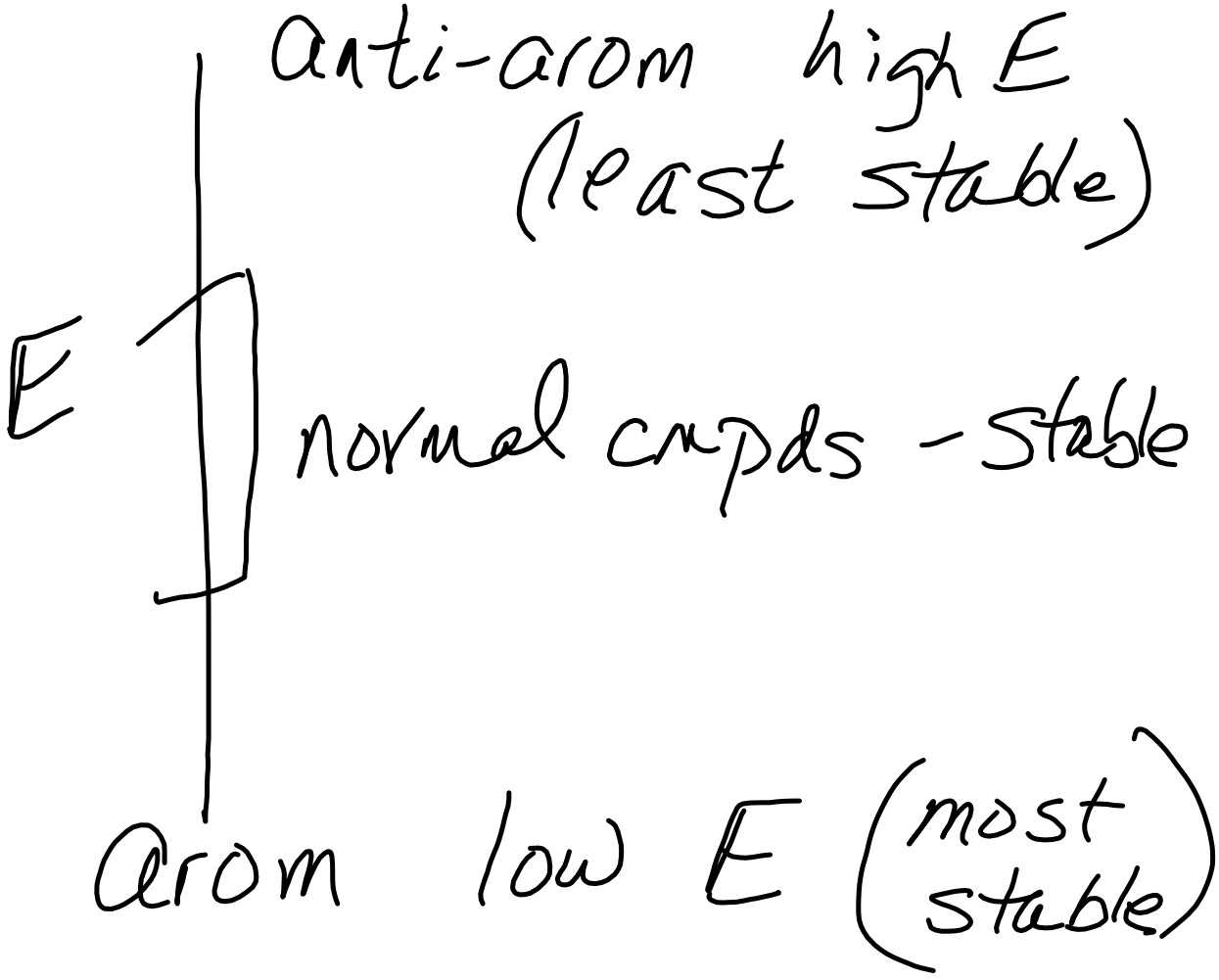
10



guanine

10 π e⁻

arom

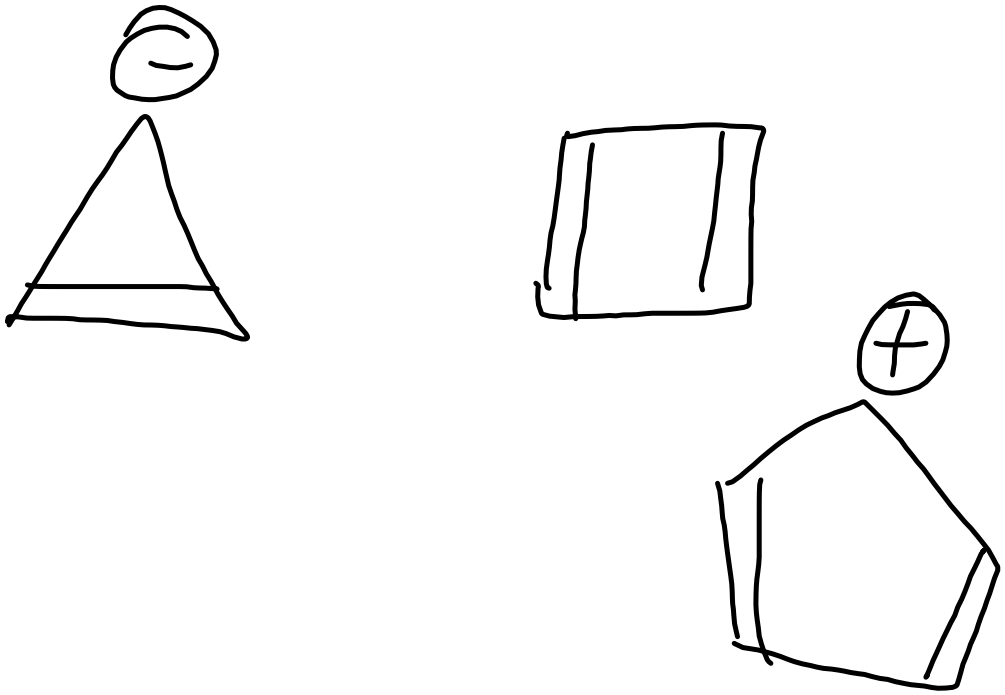

anti-arom high E
(least stable)
E
normal cmpds - stable
arom low E (most stable)

Anti-arom rings:

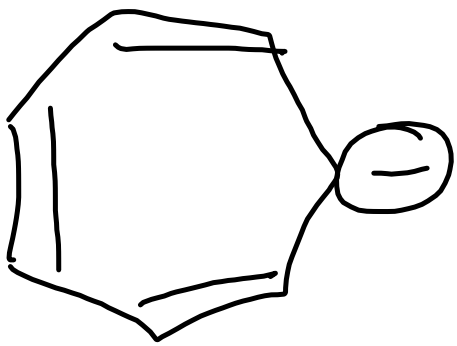
1. must be a ring
2. all atoms in ring must be sp^2
3. ring must be flat
4. # π e^- in donut cloud must be $(4n)$ where $n = 1, 2, 3 \ldots$

Magic #'s are 4, 8, 12

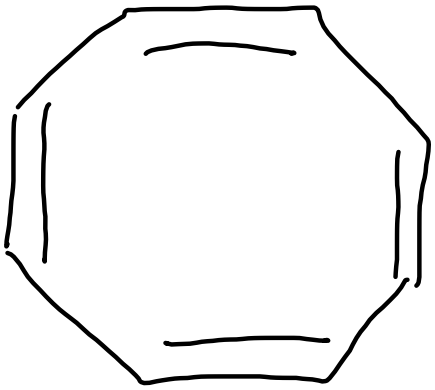
Anti-arom rings w/ 4 π e-



Anti-arom rings w/ 8 π e-



not arom

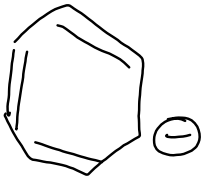


not flat - it bends to gain stability

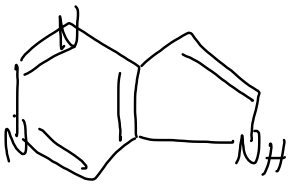
all double bonds are isolated — they do not overlap

aromatic

normal due to sp^3 C in ring



anti-arom



arom

normal

normal due to sp^3 C

arom

anti-arom