Arrange the following with respect to increasing stability due to π-electron delocalization:

- Aromatic
- Anti-aromatic

| A | i < ii < iii |
| B | i < iii < ii |
| C | ii < i < iii |
| D | ii < iii < i |
| E | iii < ii < i |
| F | iii < i < ii |

Aromatic = stabilization due to cyclic delocalization of electrons.

Molecular orbital theory: a review.

An important failure of simple resonance theory is the inability to predict the instability of cyclobutadiene.

Lots of delocalization energy → Instability

An important success of simple molecular orbital theory is the ability to predict the instability of cyclobutadiene.

Does the interaction of two filled molecular orbitals (HOMO-HOMO interaction) result in stability for butadiene? A. yes B. no

Using this model, what is the origin of stability of butadiene?

Are HOMO-LUMO interactions allowed?

HOMO-LUMO interactions are allowed and predict stabilization of benzene by electron delocalization.
The molecular orbitals of benzene

Allow overlap between positions 2 and 3 as well as 1 and 4.

HOMO-LUMO interactions are forbidden because of the symmetry of the molecular orbitals!!!

Can I do these molecular calculations?

http://www.ic.sunysb.edu/Class/orgchem/
Hückel's Rule: Cyclic compounds with $4n + 2$ π-electrons will be stabilized by cyclic delocalization.

Since benzene has 6 π-electrons, Hückel's rule predicts benzene to be stabilized by the cyclic delocalization of electrons.

Does cyclobutadiene obey Hückel's rule?

Chose those compounds predicted by Hückel's Rule to be stabilized by the cyclic delocalization of electrons.

Which order has the following compounds correctly arranged with respect to increasing acidity.

Which of the following molecules would Hückel's rule predict to be stabilized by cyclic delocalization of the π-electrons?
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(A) 1 + 2 + 3  (B) 1 + 3  (C) 2 + 3  (D) 1  (E) 2  (F) 3

Which of the following compounds would you predict to be more basic?

\[ \text{A} \quad \begin{array}{c}
+H^+ \\
\text{pK}_a = 5.21
\end{array} \quad \begin{array}{c}
\text{B} \\
\text{pK}_a = 11.2
\end{array} \]

\[ \Delta \text{pK}_a = (11.2 - 5.21)(5.7 \text{ kJ/mol}) = 18.5 \text{ kJ/mol} \]

Which of the following nitrogen atoms in imidazole would you predict to be more basic?

1. Draw the two cations that are formed by protonating each nitrogen atom.
2. Circle the more acidic cation.
3. Circle the more basic nitrogen atom.

Which has the following compounds correctly classified as aromatic, anti aromatic and non aromatic.

6 π-electrons  8 π-electrons  6 π-electrons

A  aromatic  anti aromatic  non aromatic
B  non aromatic  anti aromatic  aromatic
C  non aromatic  aromatic  anti aromatic
D  anti aromatic  non aromatic  aromatic
What is the correct classification of cyclopentadiene?

A. anti aromatic  
B. non aromatic  
C. aromatic

4 π electrons  
cyclopentadiene  
6 π electrons

Hückel’s Rule: If a cyclic π-system contains 4n + 2 electrons it will be stabilized by cyclic delocalization.