Resonance and Orbitals
Week 2 Problem Set
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Patterns:
a. Lone pair next to the π bond (double or triple)
b. Lone pair next to the charge
c. π Bond next to the charge
d. π Bond between two atoms where one is very EN
e. Alternating π bond in a ring

Relative Importance of Contributing Structures:
(1) Maximize octets
(2) Minimize charge
(3) Negative charge on more EN element

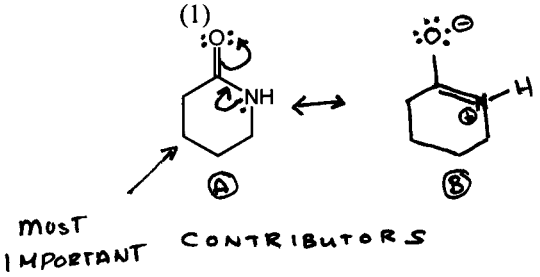
A. Define *resonance.*
THE ~~DISTRIBUTION~~ Delocalization OF CHARGE AND/OR ELECTRON DENSITY IN A MOLECULE.

B. Define *resonance hybrid.*
THE REALISTIC PICTURE OF WHAT A MOLECULE LOOKS LIKE. THE SUM OF ALL RESONANCE CONTRIBUTORS.

C. Why is it incorrect to use '⟷' when describing resonance structures.
THE RESONANCE CONTRIBUTORS DO NOT HAVE ELECTRON DENSITY GOING BACK AND FORTH FROM ONE STRUCTURE TO ANOTHER. THEY ARE NOT IN EQUILIBRIUM.

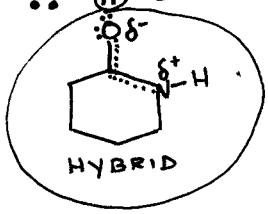
D. Draw *all* possible reasonable resonance contributors and resonance hybrids. Indicate which contributor is most important. If there are no other contributors *explain why.*

(1)

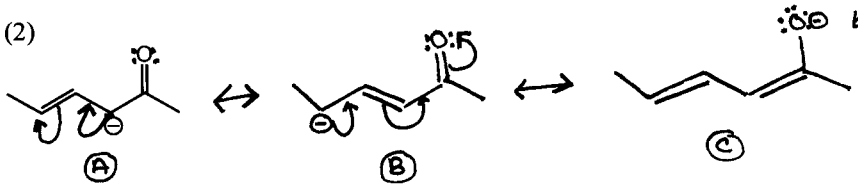


MOST IMPORTANT CONTRIBUTORS

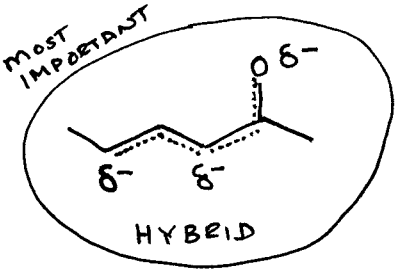
RESONANCE CONTRIBUTORS Ⓐ & Ⓑ HAVE FULL OCTETS ON EACH ATOM.
Ⓑ HAS CHARGE SEPARATION, Ⓐ DOES NOT.
∴ Ⓐ IS A GREATER CONTRIBUTOR THAN Ⓑ



(2)

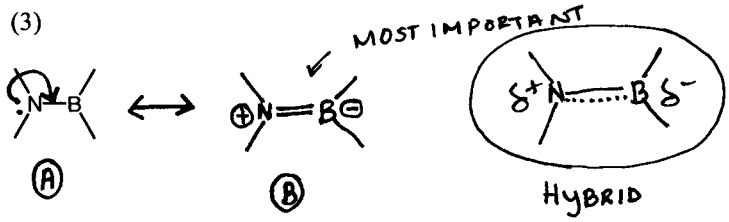


MOST IMPORTANT

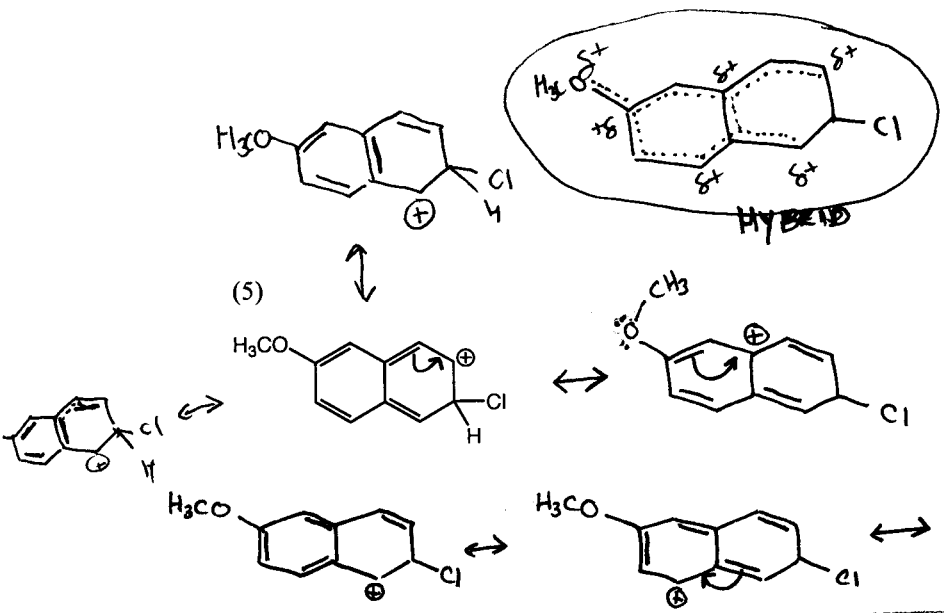


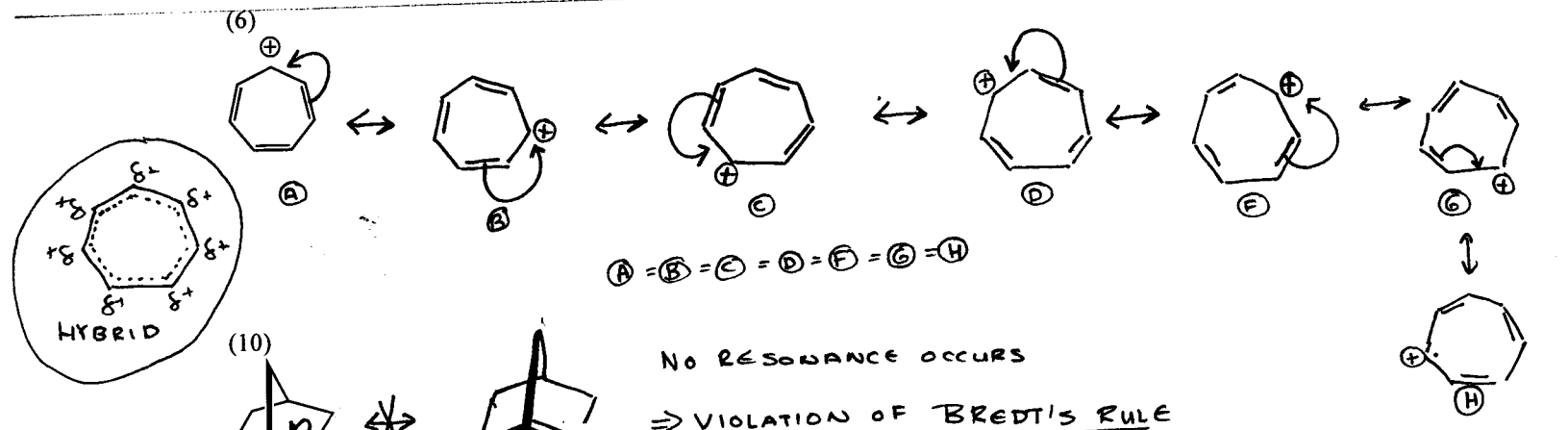
Ⓐ, Ⓑ, Ⓒ ⇒ FULL OCTETS ⇒ SAME
Ⓐ Ⓑ Ⓒ ⇒ MINIMIZE CHARGE SEPARATION ⇒ SAME
Ⓒ ⇒ ELECTRONEGATIVE ATOM HAS NEGATIVE CHARGE.

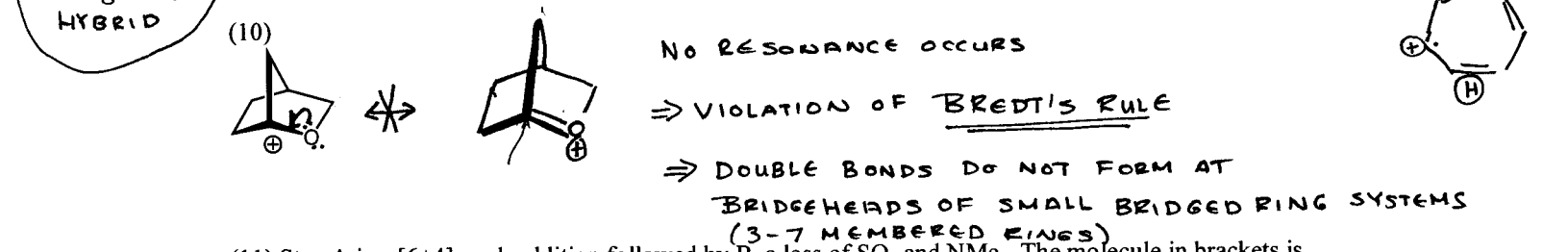
(3)



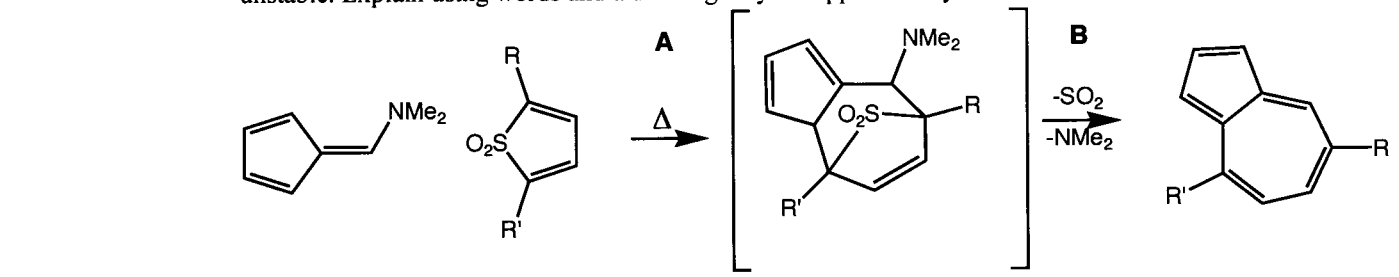
Ⓑ IS MORE IMPORTANT THAN Ⓐ ⇒ FULL OCTETS

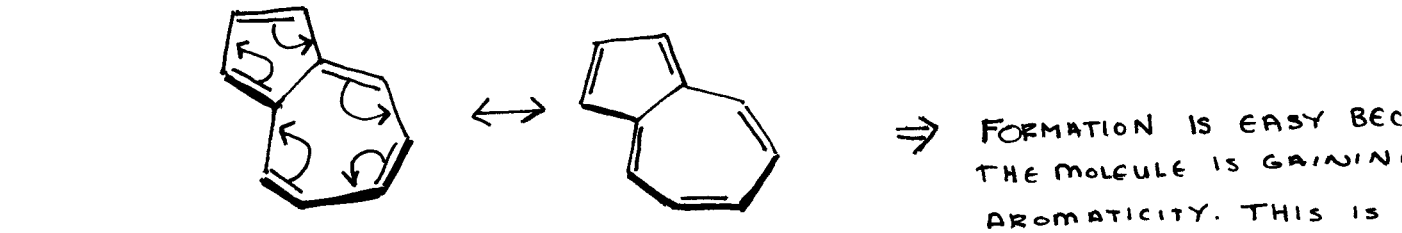




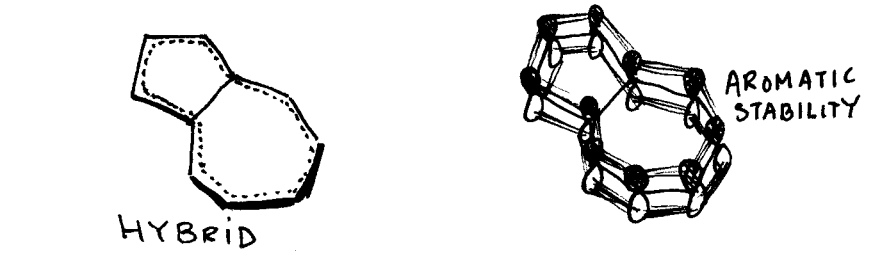


(11) Step A is a [6+4] cycloaddition followed by B, a loss of SO_2 and NMe_2. The molecule in brackets is unstable. Explain using words and a drawing why B happens easily.





⇒ FORMATION IS EASY BECAUSE THE MOLECULE IS GAINING AROMATICITY. THIS IS A SPECIAL STABILIZATION THAT HAPPENS WHEN THERE IS A CYCLIC, PLANAR LOOP OF P-ORBITALS WITH $4n+2$ π ELECTRONS. IN OTHER WORDS, **THINK RESONANCE!**



D. Describe the *hybridization* and the *geometry* of the atom(s) (arrows) in the following molecules.

1.

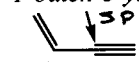
furan

Sp^3 TRIGONAL GEOMETRY

BENT SHAPE

2.

1-buten-3-yne

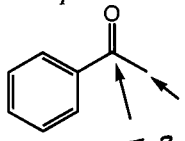


SP3 ; LINEAR

Sp^2 ⇒ TRIGONAL PLANAR

3.

acetophenone



SP3 ; TETRAHEDRAL

Sp^2 ; TRIGONAL PLANAR