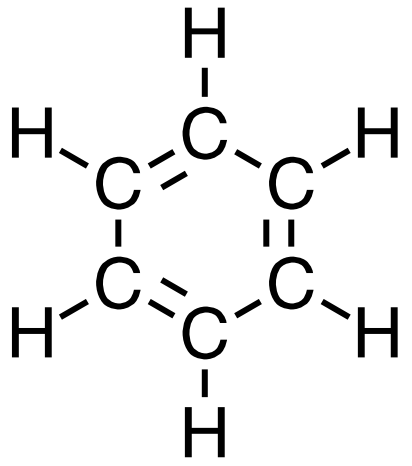
Objective 3

Draw resonance structures,
use curved arrows,
determine extent of delocalization.
Identify major/minor contributor.

Structure ***Should*** Fit Experimental Data

The chemical formula of benzene is C_6H_6.
Experiments show benzene has 6 carbon-carbon bonds of the same length (140 pm).

a. Draw the Lewis structure of benzene.



b. Does this structure fit the experimental data? (C-C single bond = 146 pm, C=C double bond = 134 pm)

“Paper” structure (Lewis structure model) = actual structure.

In some cases, a Lewis structure (model) ≠ actual structure based on experimental data, e.g., x-ray structure.

If not, use two or more **Resonance Structures**.

Lewis structure = localized electrons (shared between 2 atoms)
Resonance structures = ***de***localized electrons (shared between 3 or more atoms) ==> “resonance stabilization”.

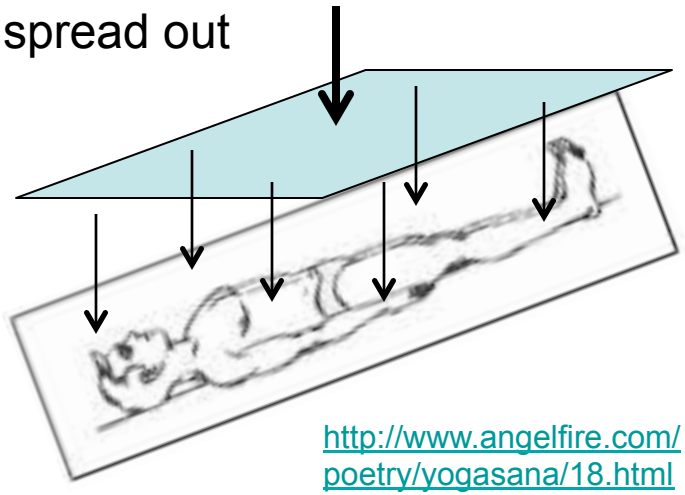
“Localized” vs. “Delocalized”

concentrated

“ow!”

http://www.clipartguide.com/_pages/0511-1007-1912-0911.html

spread out



http://www.angelfire.com/poetry/yogasana/18.html

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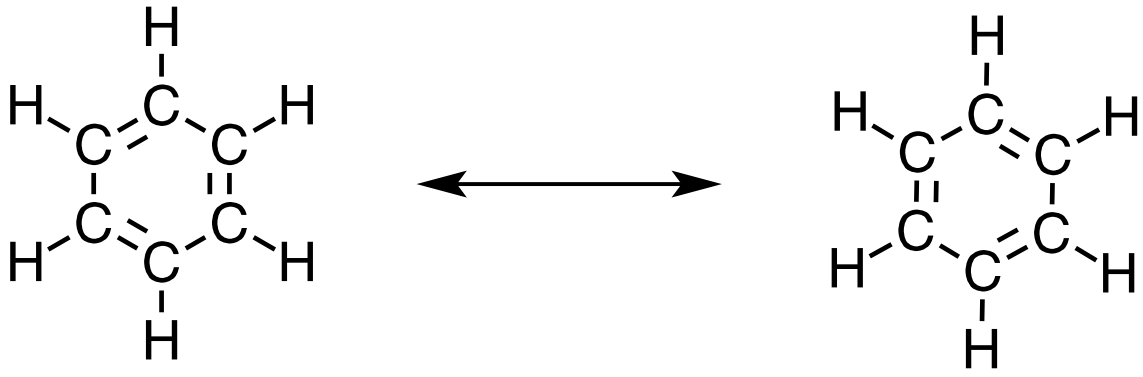

C-C single bond = 146 pm, C=C double bond = 134 pm
Note the alternating C-C and C=C bonds in ring.
Bond order of C-C bonds in benzene = *1.5*

Structure ***Should*** Fit Experimental Data

The chemical formula of benzene is C_6H_6.
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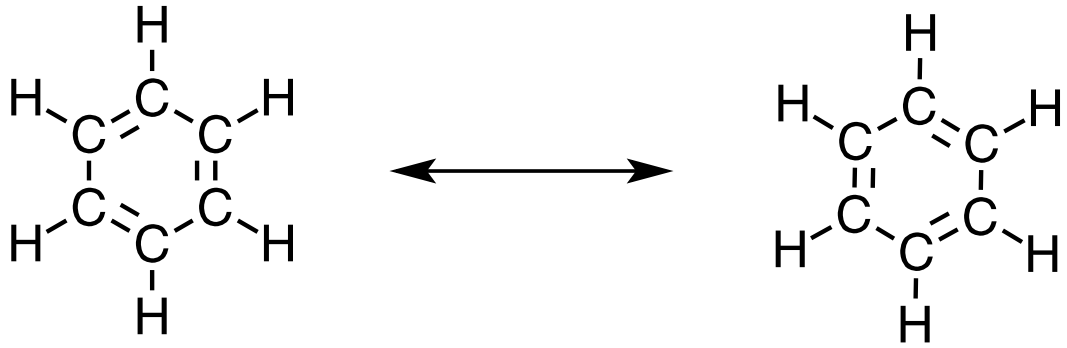


IR:

C=C for alkenes	1680-1600 cm^{-1}
C=C for aromatics	1600-1400 cm^{-1}
C-H for alkanes	3000-2850 cm^{-1}
C-H for aromatics	3150-3050 cm^{-1}

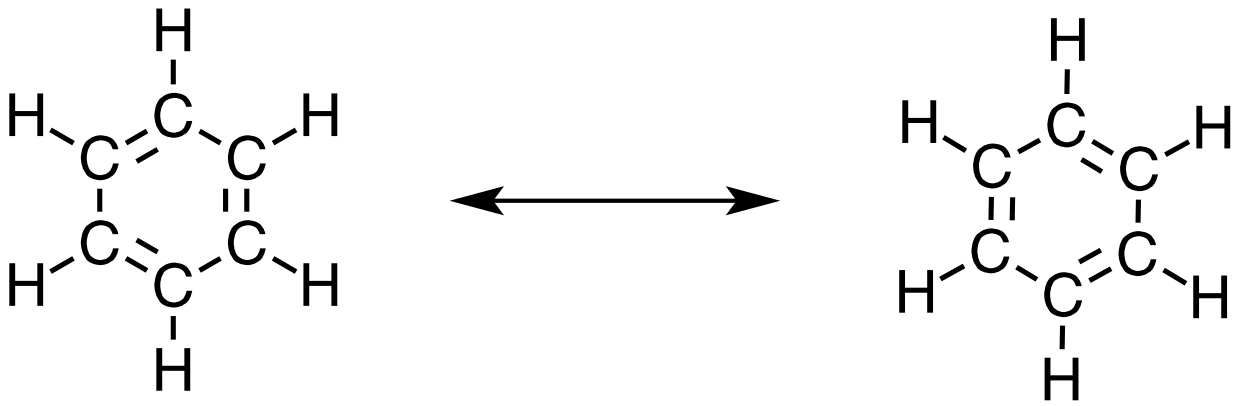
Explain the IR data.

In some cases, a Lewis structure (model) ≠ actual structure based on experimental data, e.g., x-ray structure.
If not, use two or more **Resonance Structures**.

RESONANCE STRUCTURES ARE *NOT* ISOMERS.

Each Resonance Structure has the **SAME** Connectivity.

Objective: Use **CURVED ARROWS** to go from one resonance structure to another. (See Klein, p. 68)



Resonance Structures:

CURVED ARROWS Show How Electrons Move
(which Electrons are Delocalized and which Atoms are Sharing Electrons)

CURVED ARROWS Show Bonds Breaking and Forming
1. Pi bond breaks to form pi bonds on adjacent bond
2. Pi bond breaks to form lone pair on atom
3. Lone pair on atom can form pi bond (reverse of #2)

Make sure structure rules are followed.
Check charge (use formal charge formula).
Usually, curved arrows (electron flow) goes from negative to positive.

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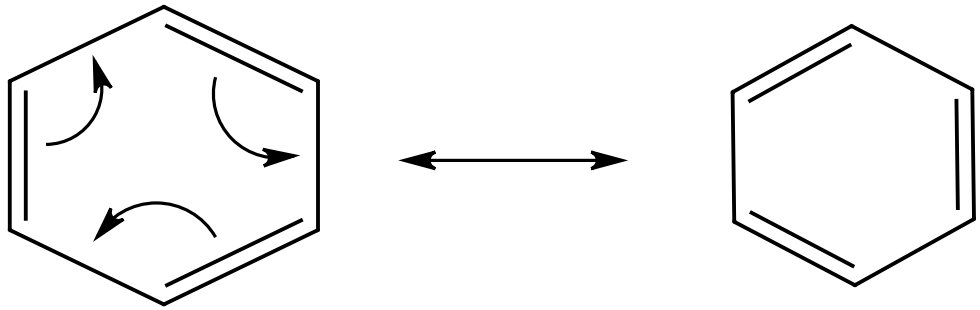


Structure ***Should*** Fit Experimental Data

The acetate ion, CH_3COO^-, has two C-O bonds of the same length.

a. Draw the Lewis structure of the acetate ion.

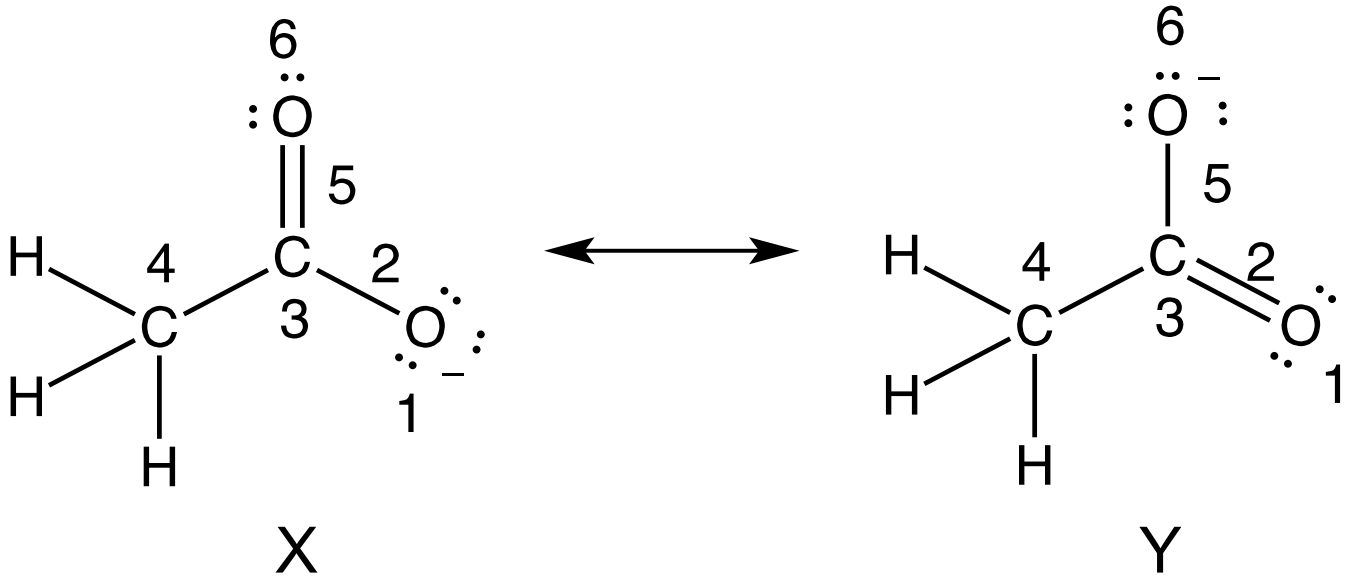
b. Does this structure fit the experimental data?

Objective: *Use Curved Arrows to Go from One Resonance Structure to Another*

The acetate ion, CH_3COO^-, has two C-O bonds of the same length.

Use numbers to represent curved arrows that transforms Resonance Structure X to Resonance Structure Y.

Report the arrow starting with smaller number first.



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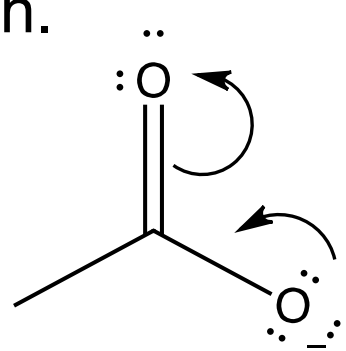
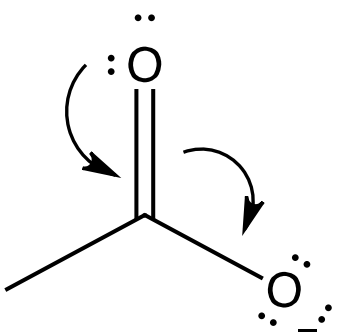
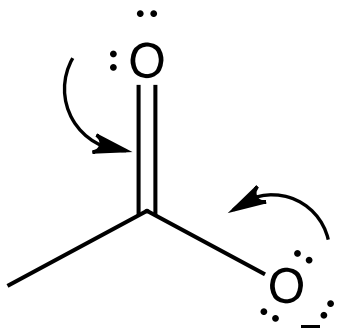


A



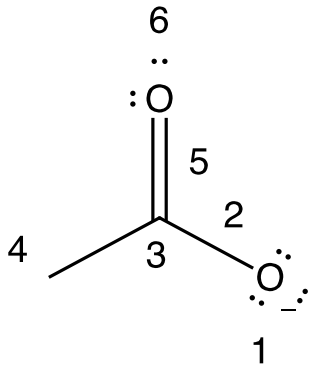
B



C

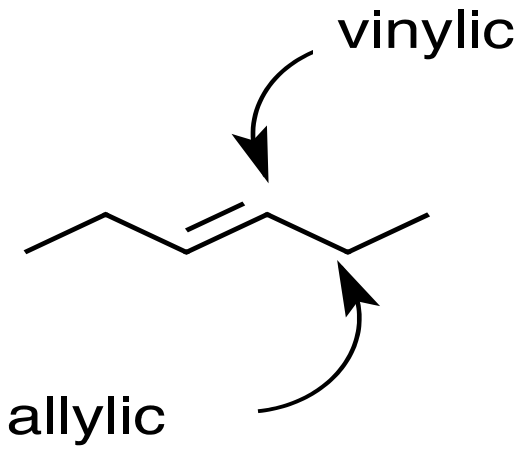
A works. Explain why B and C do not.

1256

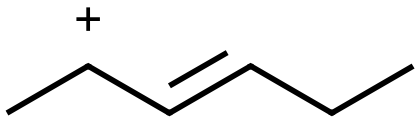


Structural Features (Patterns) that Suggest (w/o experimental data) Resonance Structures (Klein, p. 73):

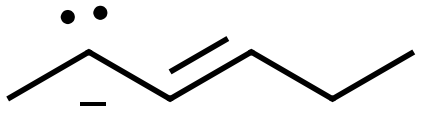
1. Identify the vinylic and allylic positions.



2. Experiments show delocalization in the allylic cation and allylic anion.



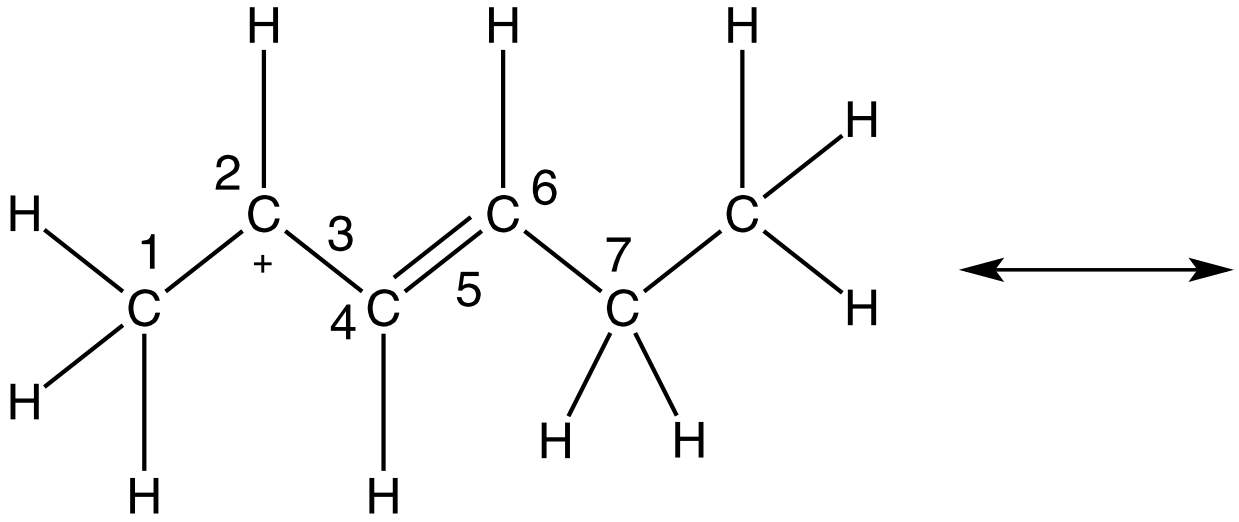
allylic (+) charge



allylic lone pair

Structural Features (Patterns) that Suggest (w/o experimental data) Resonance Structures (Klein, p. 73):

Use numbers to represent curved arrows that transforms the resonance structure shown to another resonance structure. Over how many atoms are e^- delocalized?



Allylic (+) charge
Why does C-2 have a (+) charge?
Hint: start arrow at pi bond.

Structural Features (Patterns) that Suggest (w/o experimental data) Resonance Structures (Klein, p. 73):

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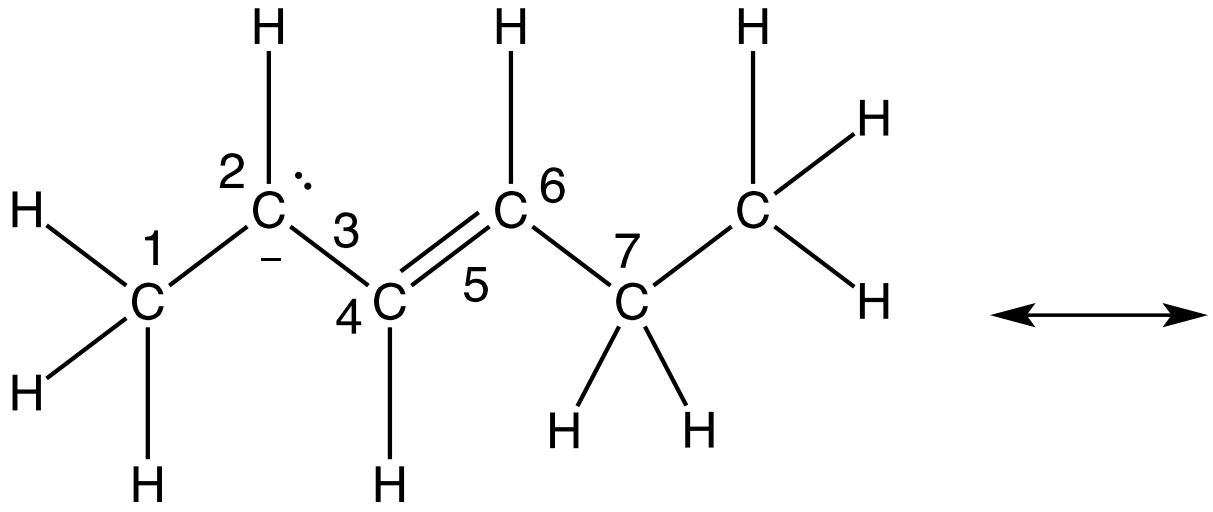
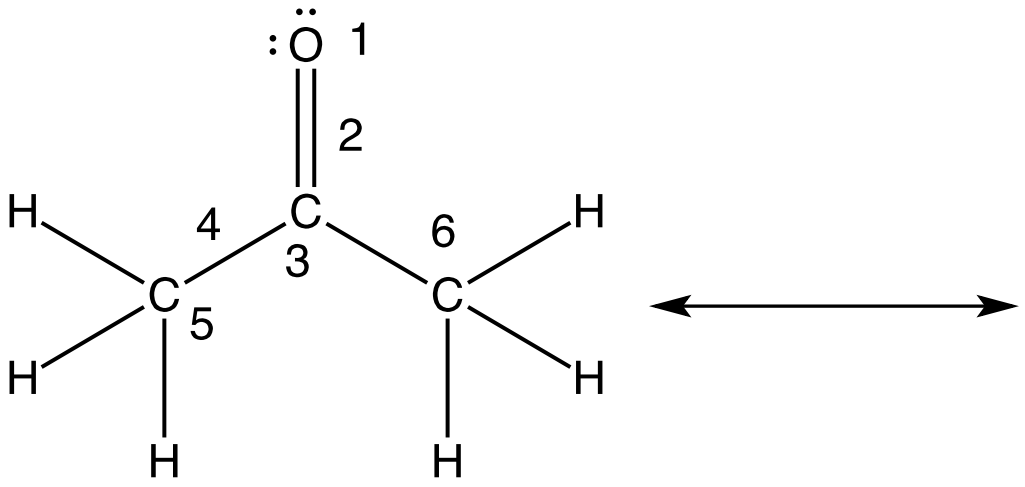


Allylic lone pair
Why does C-2 have a (-) charge?

More structural features that suggest resonance:

Use numbers to represent curved arrows that transforms the resonance structure shown to another resonance structure.
Report the arrow starting with smaller number first.
Over how many atoms are e^- delocalized?



pi bond between
two different atoms

lone pair adjacent to
a (+) charge

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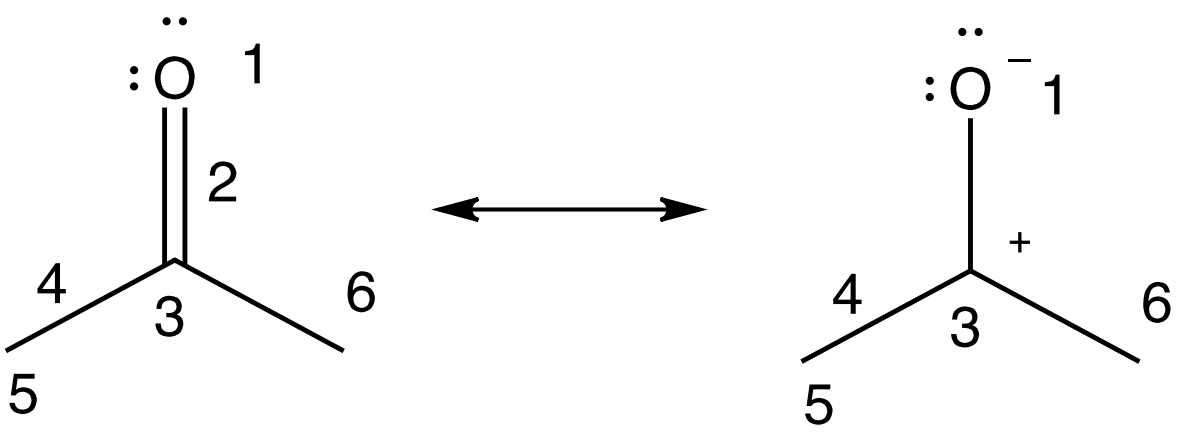

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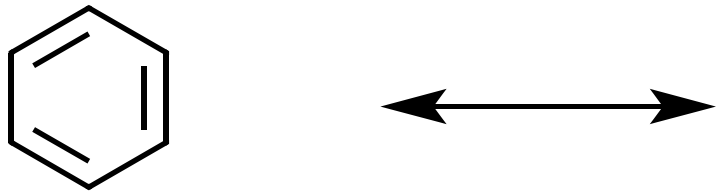
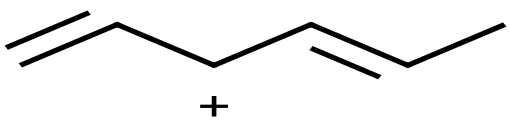
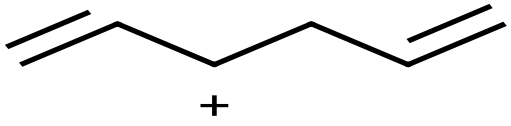


conjugated pi bonds
in a ring

Draw resonance structures of each ion.
Which ion is more stable, A or B?



A



B

Resonance Stabilization: More Resonance Structures ==> More Delocalized (spread out) ==> More Stable

How To Use Formal Charge To Predict The Major/Minor Resonance Contributor

Formal Charge on atom = (# of valence electrons) - (# of lines) - (# of dots)

0 or Lowest Formal Charge --> most stable structure

A resonance structure in which C, N, O fits octet rule is more stable than a structure in which atom(s) lack an octet.

Negative FC on the more electronegative atoms is preferred.

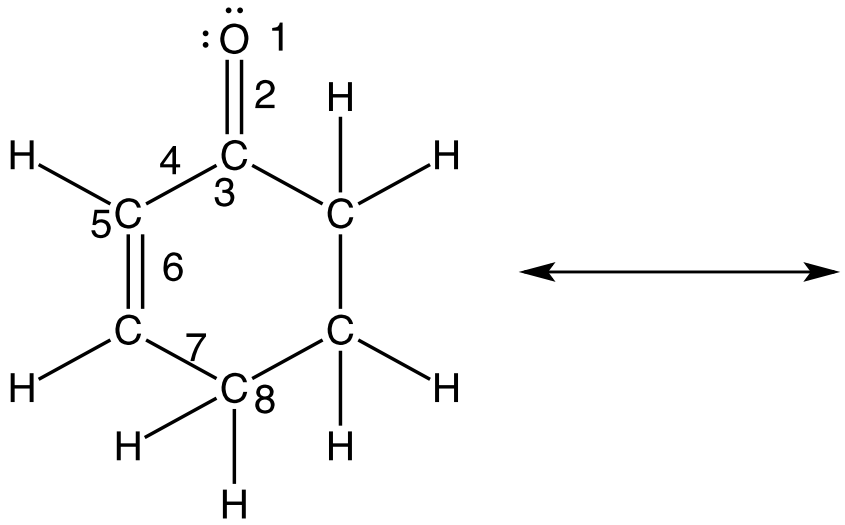
Resonance Structures may Not be Equivalent

Use Formal Charge rules to determine the Major (more stable) and Minor (less stable) Contributor

Use numbers to represent curved arrows that transforms the resonance structure shown to another resonance structure. Report the arrow starting with smaller number first.

Are the resonance structures equivalent?

If not, which structure is the preferred structure (major contributor)? Which structure is less stable?

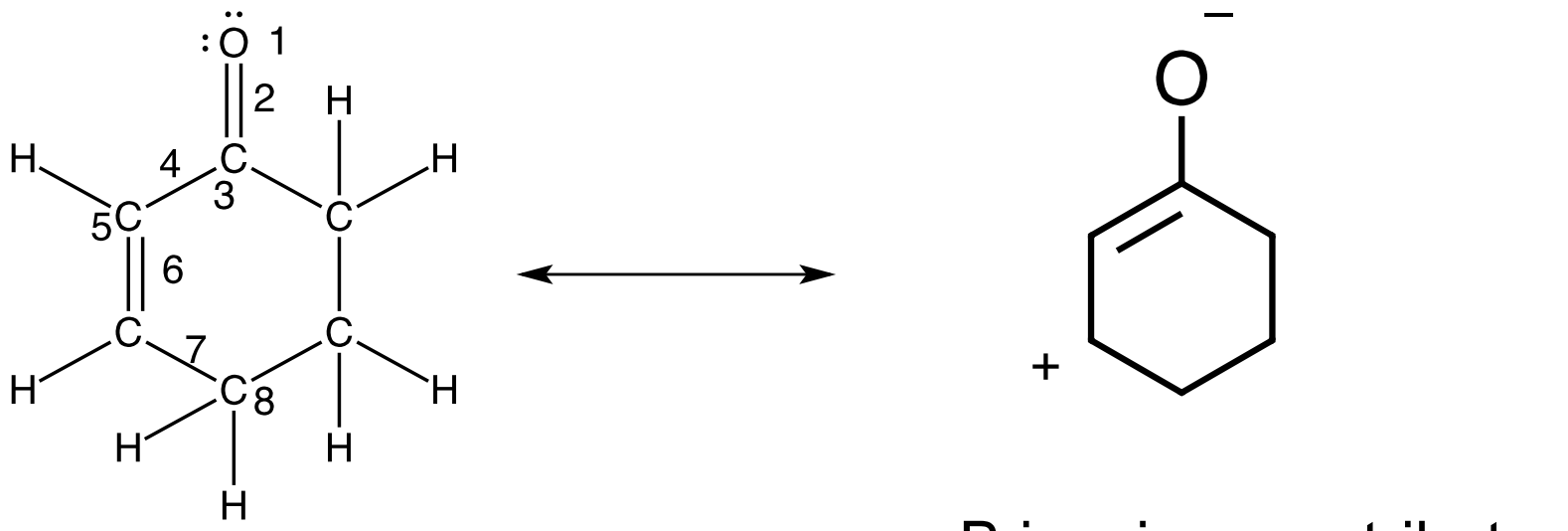


A B

Resonance Structures may Not be Equivalent

Use Formal Charge rules to determine the Major (more stable) and Minor (less stable) Contributor

Are the resonance structures equivalent?
If not, which structure is the preferred structure (major contributor)? Which structure is less stable?



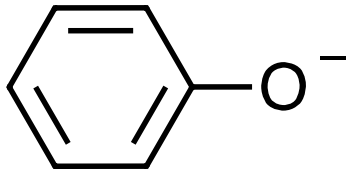
A is major contributor because _____

B is minor contributor (less stable) because _____

Objectives: 1. Draw resonance structures
2. Determine major resonance contributor

Draw resonance structures for the following compounds.
For each compound, are the resonance structures equivalent?
If not, which structure is the preferred structure (major contributor)? Which structure is less stable?

a. CH_3-C^+H-CH=CH_2

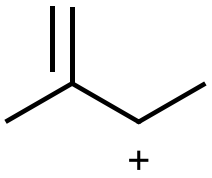
b. $C_6H_5O^-$ (phenoxide anion) 

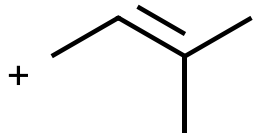
c. CH_3-O-CH_2^+

Objective: ID same structure, resonance structures, and isomers

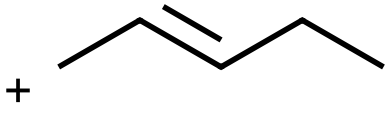
Consider each set of structures. Are the two structures the same, resonance structures, or isomers?

a.

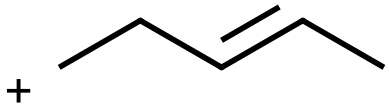




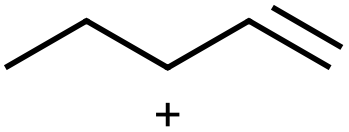
b.



(i)



(ii)



(iii)

Klein, 2.56 Are the two structures resonance structures or constitutional isomers?