REC 2 – CH. 2

MOLECULAR REPRESENTATIONS & RESONANCE

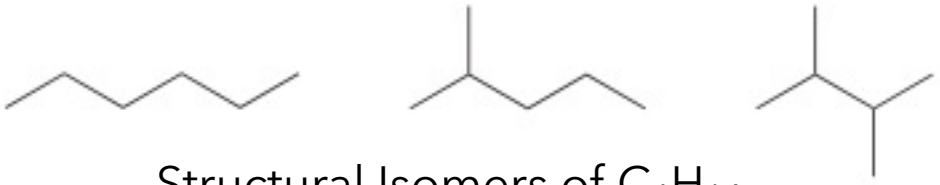
Answer Key at End of Presentation

Bond-Line Structures

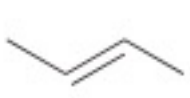
Bond-line structures simplify the Lewis structure by <u>not</u> explicitly drawing carbons or hydrogens, and only drawing *heteroatoms* (i.e. atoms other than C or H). While we never draw the H's that bonded to carbon, we always draw the H's that are bonded to heteroatoms.

The "zigzag" format is used to represent sp^2/sp^3 hybridization states, where bonds have either a 109° or 120° angle.

Double and triple bonds are represented with two and three lines, respectively.



Structural Isomers of C_6H_{14}

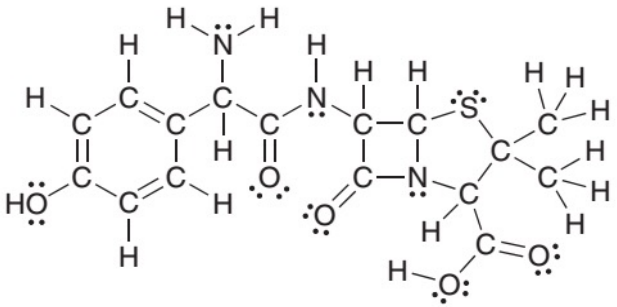


C_4H_8



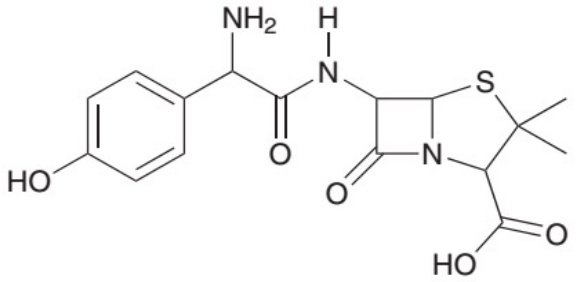
C_4H_6

Note: Triple bonds are **linear** (***sp* hybridized**), so we do not draw a "zigzag".



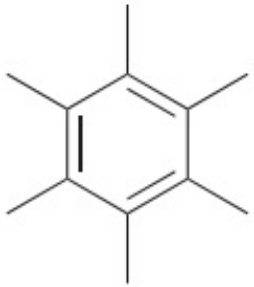
Amoxicillin

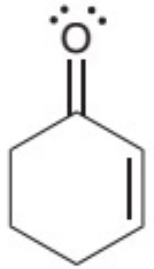
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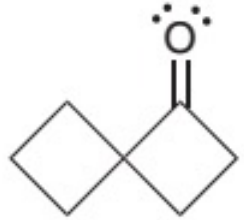


Q1a. Draw in the hydrogens and write the molecular formula for the following:

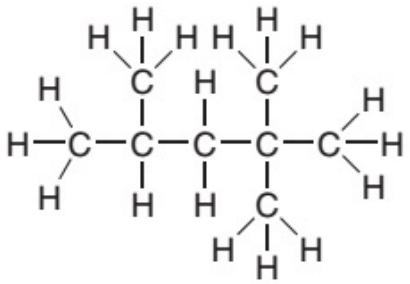








Q1b. Draw the bond-line structure for the following:



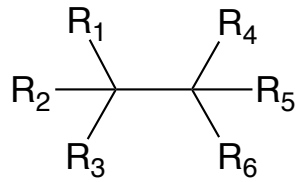
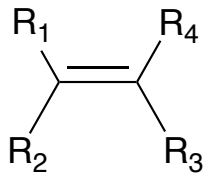
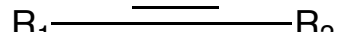
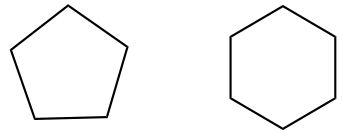
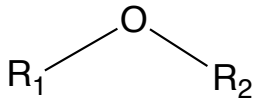
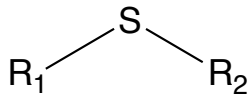
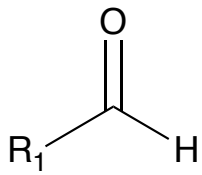
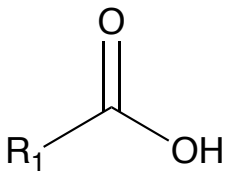
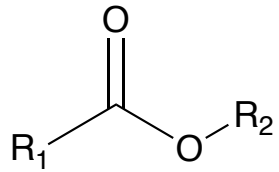
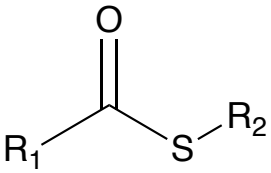
$CH_3CH_2CH_2OCH_3$

$(CH_3CH_2)_3COH$

Functional Groups, Pt. 1

Name the functional groups, identify the hybridization states and molecular geometry of the central atoms.

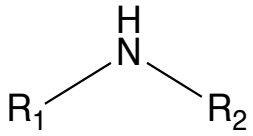
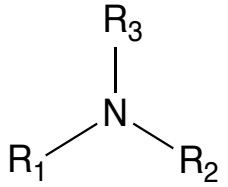
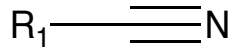
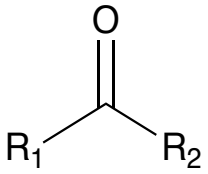
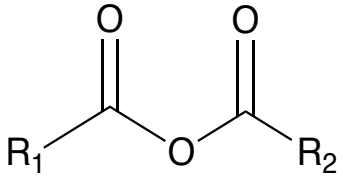
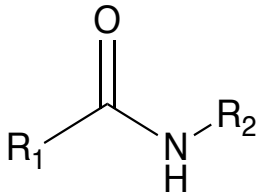
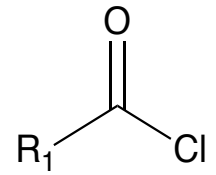
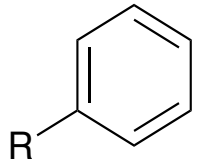
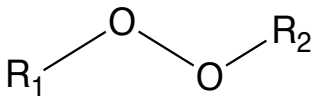
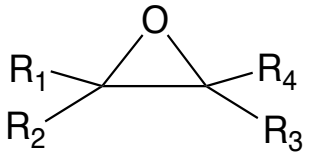
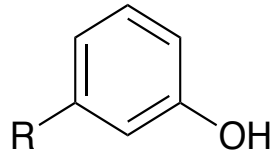
1.
2.
3.
4.
5.
6.
7.
8.
9.
10.
11.
12.

 1.	 2.	 3.	 4.
 5.	 6.	7.	 8.
 9.	 10.	 11.	 12.

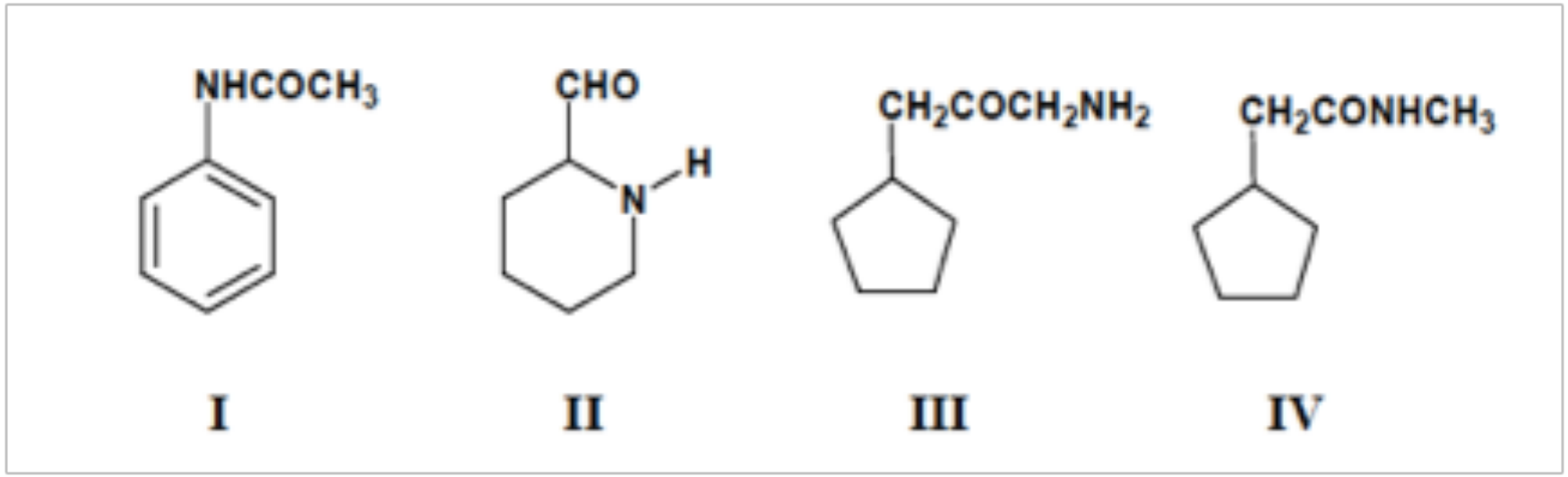
Functional Groups, Pt. 2

Name the functional groups, identify the hybridization states and molecular geometry of the central atoms.

13.
14.
15.
16.
17.
18.
19.
20.
21.
22.
23.
24.

 13.	 14.	 15.	 16.
 17.	 18.	 19.	 20.
 21.	 22.	 23.	 24.

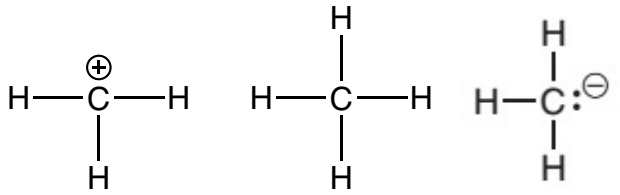
Q2. Draw the compressed substituents and label the functional groups. Which are amides?



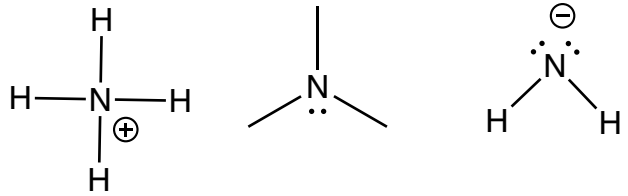
Formal Charge & Identifying Lone Pairs (LPs)

Remember: **FC** = valence – dots – lines

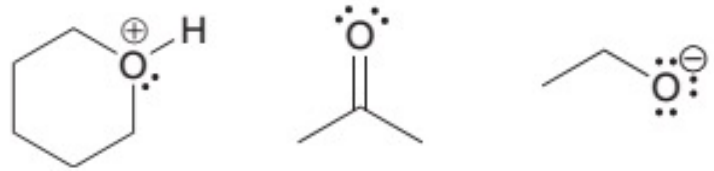
C – prefers 4 bonds



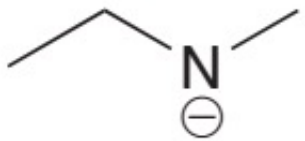
N – prefers 3 bonds, 1 LPs

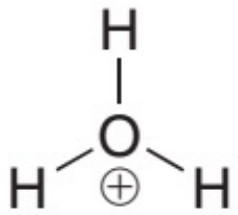


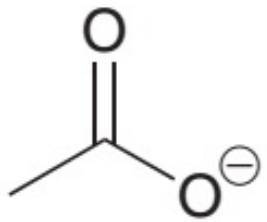
O – prefers 2 bonds, 2 LPs

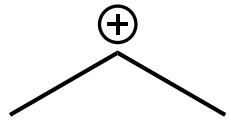


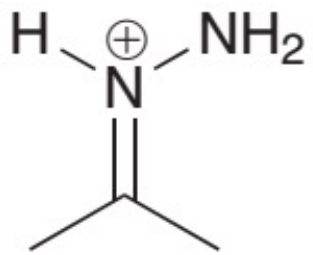
Let's Practice. Draw the lone pairs (if necessary) on the following compounds:









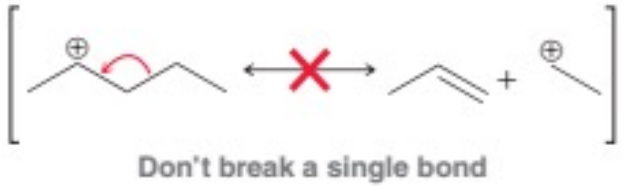


Arrow Drawing: Resonance

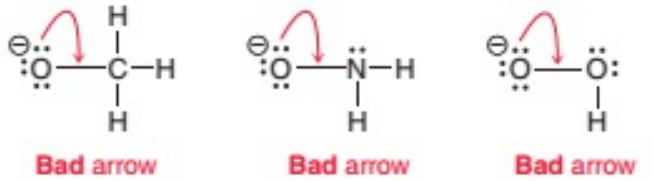


Rules

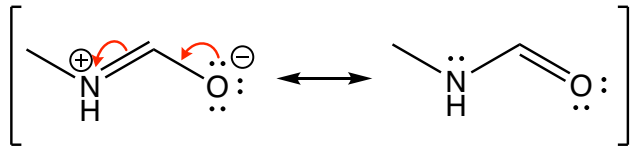
1. Do *not* break single bonds



2. Do *not* exceed octet (*for Row 2*)

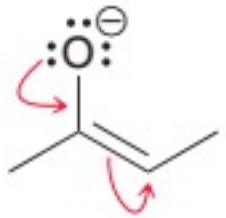
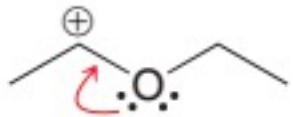
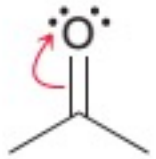


3. Conserve Charge



Both molecules are **net neutral**.

Patterns:

Allylic lone pair	Allylic carbocation	Lone pair adjacent to C+	π bond between two atoms of differing electronegativity	Conjugated π bonds enclosed in a ring
				
Two curved arrows	One curved arrow	One curved arrow	One curved arrow	Three curved arrows

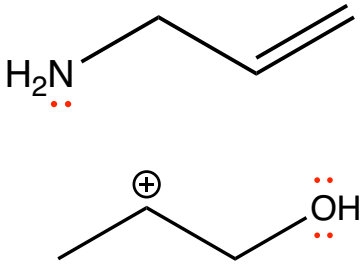
Resonance

Electrons can be *localized* or *delocalized*.

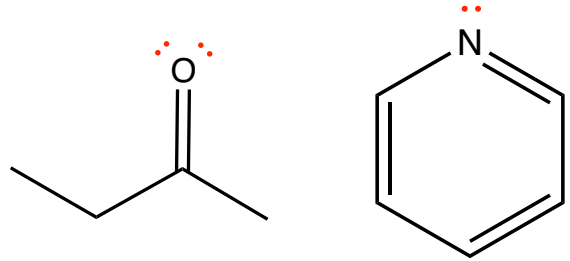
- **Localized** electrons do not move throughout the molecule.

  Note: When an atom possesses both a π bond and a lone pair, the lone pair is localized.

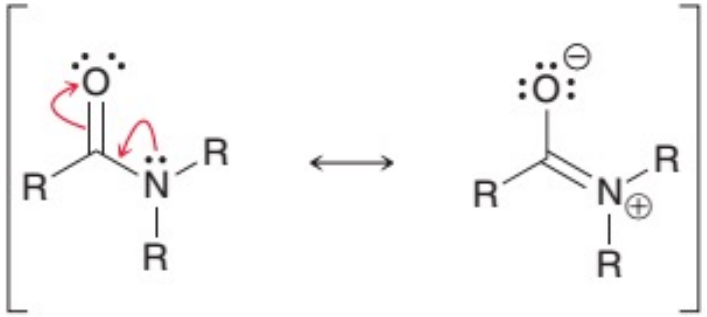
These lone pairs are localized because they are separated from other p orbitals by a sp^3 carbon.



These lone pairs are localized because their atom's p orbital is already occupied in a π bond!



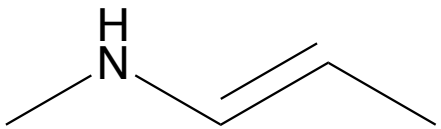
- **Delocalized** electrons can move throughout the molecule to other atoms and are in *resonance*.



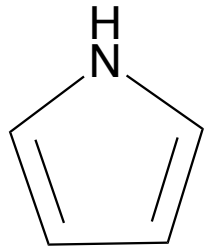
*This spread of negatively-charged electrons **stabilizes** the molecule!*

Q3. Draw the lone pairs on the structures below. Is the lone pair delocalized or localized?

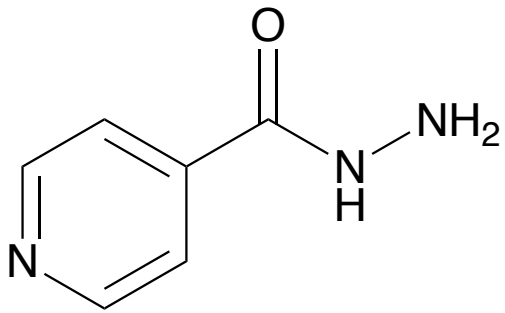
a)



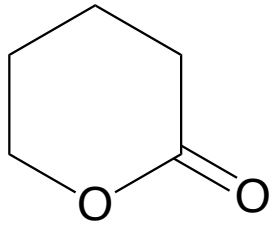
b)



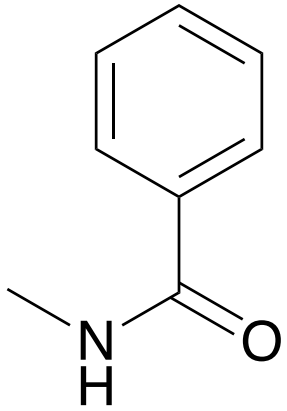
c)

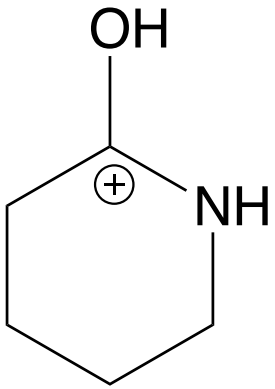


d)

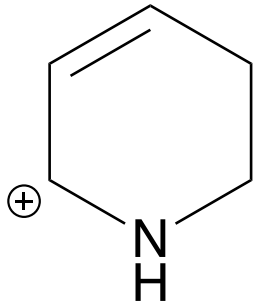


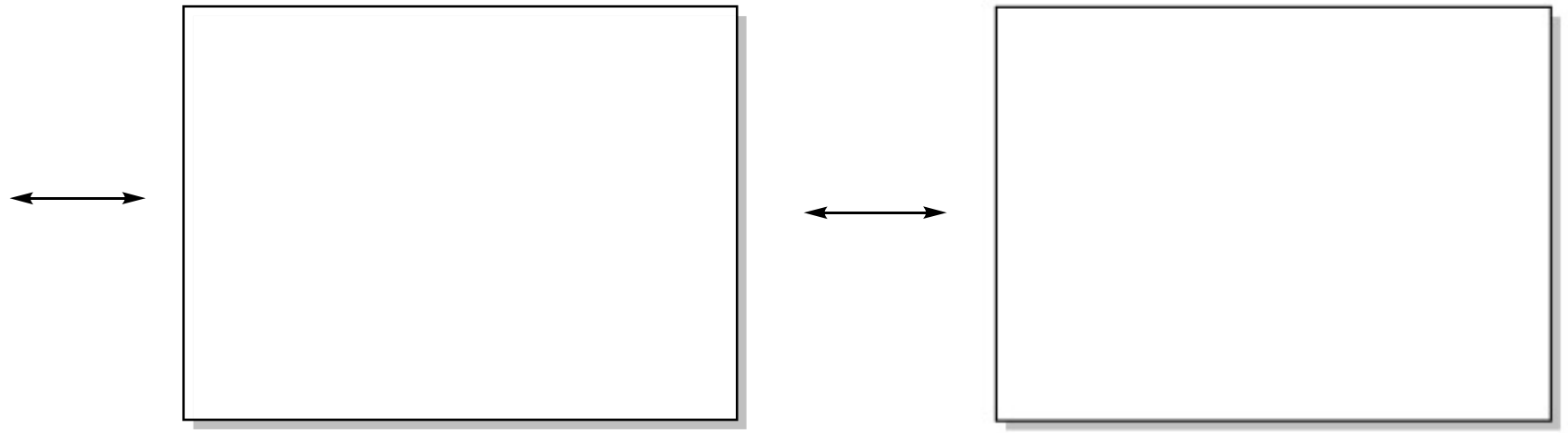
Q4. Draw curved arrows and the resonance forms(s) of the compounds shown below. Do not draw degenerate structures. Include all lone pairs.

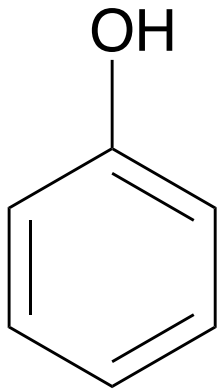


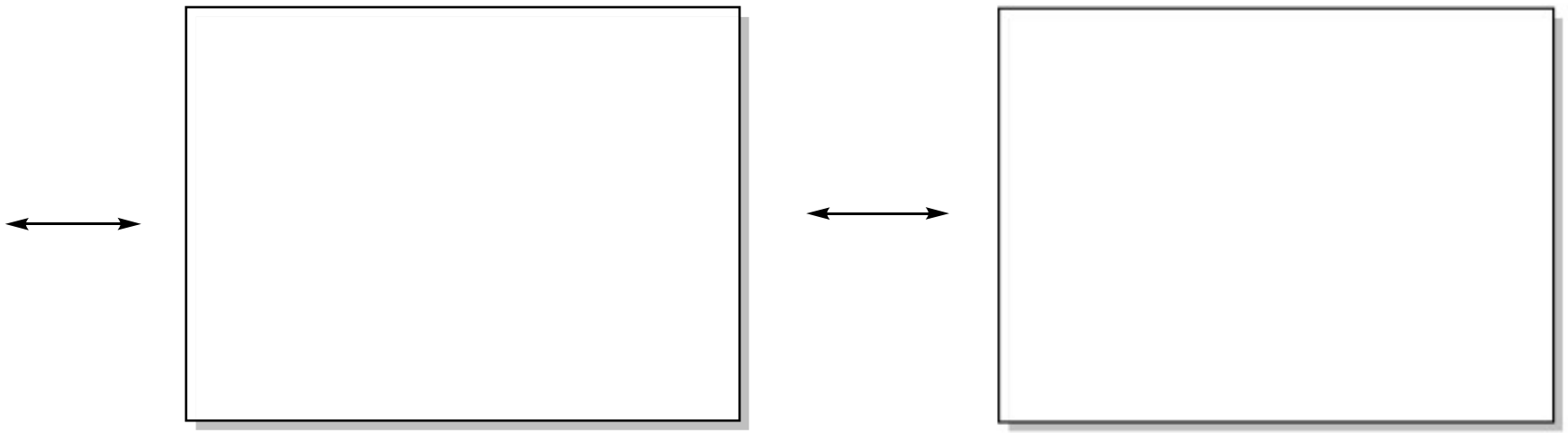


Q5. Draw curved arrows and the resonance forms(s) of the compounds shown below. Do not draw degenerate structures. Include all lone pairs.



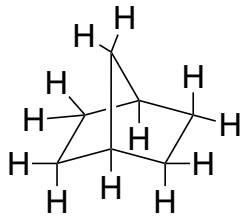




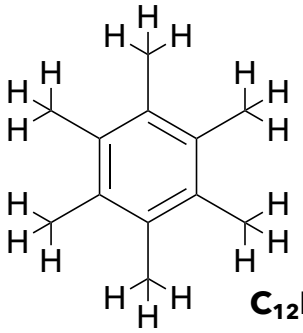


ANSWER KEY

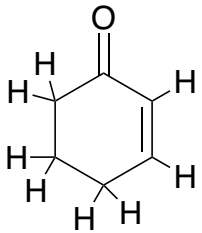
- **Q1a**:



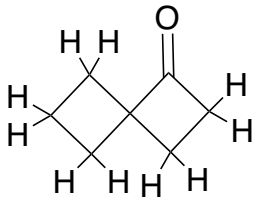
C_7H_{12}



$C_{12}H_{18}$

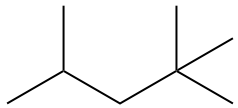


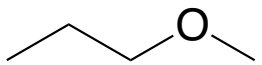
C_5H_8O

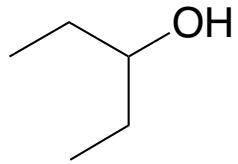


$C_7H_{10}O$

- **Q1b**:





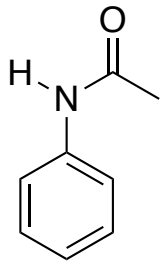


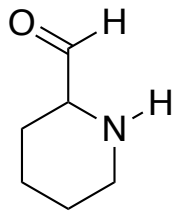
- **Functional Groups**

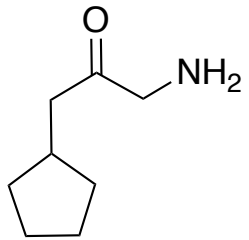
1. Alkane (sp^3)
2. Alkene
3. Alkyne
4. Cycloalkane
5. Alcohol
6. Ether
7. Thiol / Sulfyl Hydryl
8. Thioester / Sulfide
9. Aldehyde
10. Carboxylic Acid
11. Ester
12. Thioester
13. 1° Amine
14. 2° Amine
15. 3° Amine
16. Nitrile
17. Ketone
18. Anhydride
19. Amide (2°)
20. Acyl Halide
21. Phenyl / Benzyl / Aryl
22. Peroxy Acid
23. Epoxide
24. Phenol

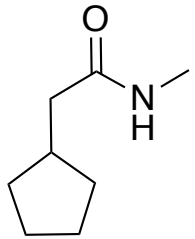
ANSWER KEY

- **Q2**:



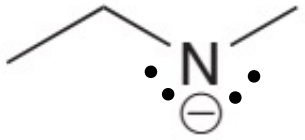


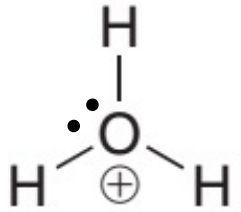


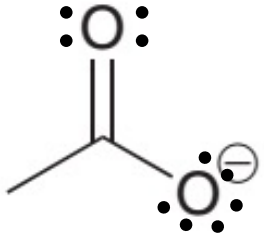


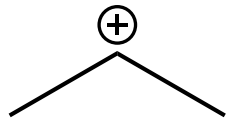
I and IV are both 2° amides.
II is an aldehyde with a 2° amine
III is a ketone with a 1° amine.

- **Slide 7**:

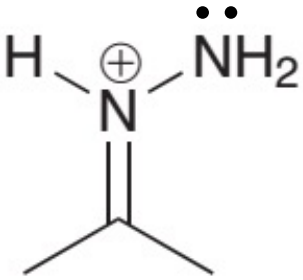






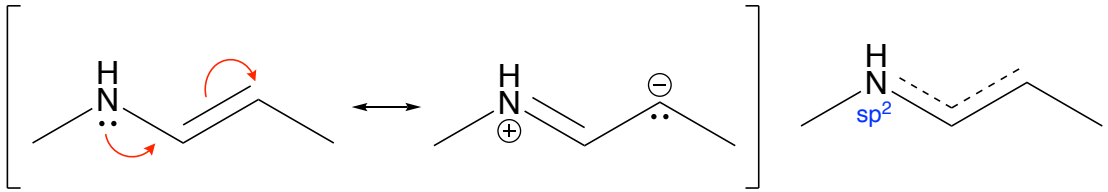


No lone pairs

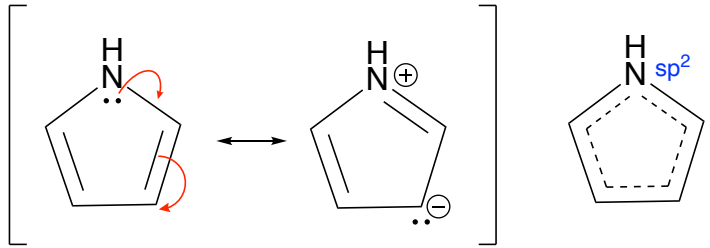


ANSWER KEY: Q3

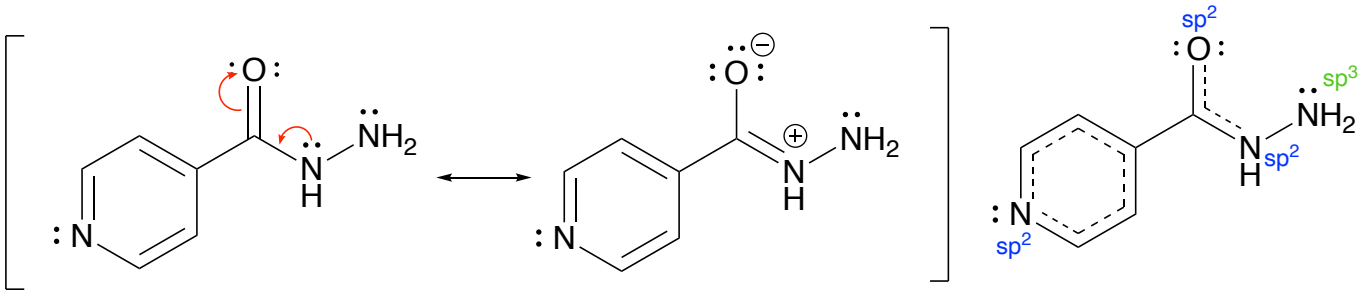
The answers for lone pair localized/delocalization refer to the starting molecular structure.



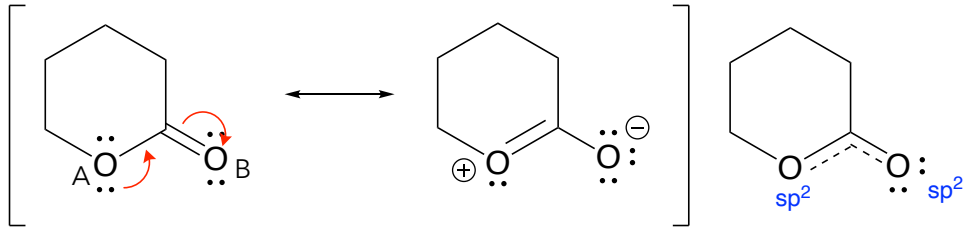
Nitrogen lone pair is *delocalized*.



Nitrogen lone pair is *delocalized*.

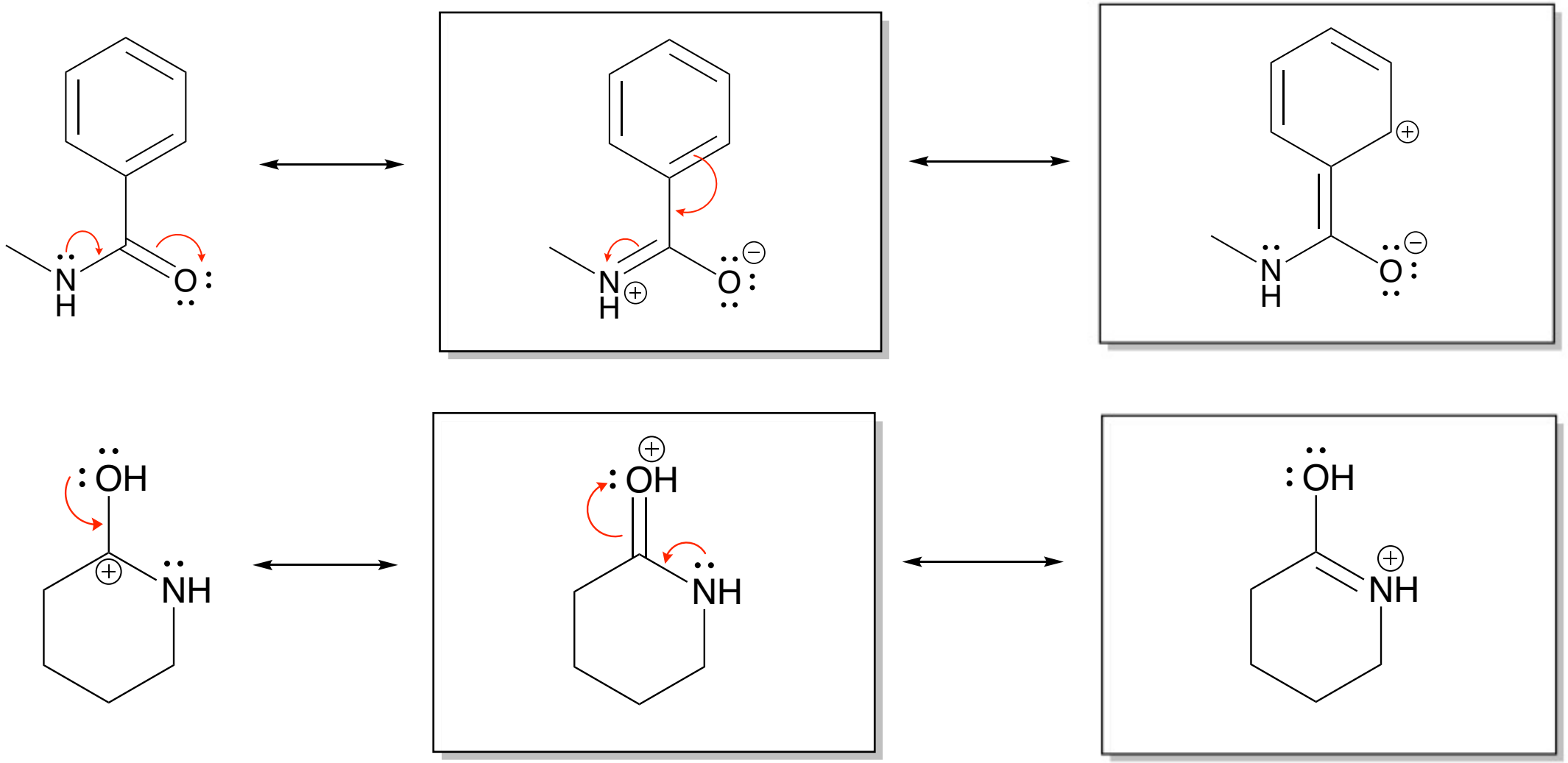


Amide N lone pair is *delocalized*.
1° Amine N lone pair is *localized*.
Pyridine N lone pair is *localized*.



O_A has 1 *delocalized* lone pair.
O_B has 2 *localized* lone pairs.

ANSWER KEY: Q4



ANSWER KEY: Q5

