MTW3 9-12

Monday, September 12, 2022 3:17 PM

Today:
- π-bond, π-neg, Molecular Orbital Theory (MOT)
- Resonance and Orbitals required.
  ↳ localized vs. delocalized lone pairs (LP)

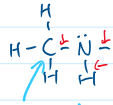
Last week:
- VSEPR and molecular Geometry
- Orbitals: Atomic, Hybridized, Phasing
- Bonding:
  σ-bond from Hybrid. orb. overlap
  π-bond from two 2p AO. overlap

more on π bonds:

(πe⊖: lone pairs, π-bonds)

★ If you can delocalize πe⊖ through 2p orbitals → DO IT!!

e.g:



what Hybridization state is the N atom?
- already 3 σ-bonds, can't be sp.

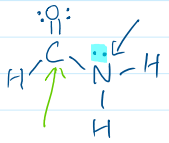
① If N is sp^2 hybridized:
↳ 3σ bonds use 3x (sp^2) hybridized orbitals
↳ 1 L.P. in 2p orbital
↳ 90° between N-H bonds and L.P.

② If N is sp^3 hybridized:
↳ 3σ bonds use 3x (sp^3) hybridized orbitals
↳ 1 L.P. in sp^3 orbital
↳ 109.5° between N-H bond and L.P.

Fact: sp^3 hybridized
NO 2p orbital

can't delocalize N-atom L.P. since C-atom does not have a 2p

So we put N lone pair as far apart as possible from other groups
↳ sp^3



If sp^2 hybridized, L.P. is in a 2p orbital
↳ can be delocalized because there is a 2p orbital on the C-atom.

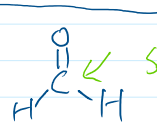
Fact: sp^2-hybridized
↳ has 2p orbital because that's needed for C=O

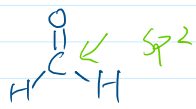
σ-, π-Bonds, Lone pairs (L.P.)

σ Bonds → single bonds → overlap of hybridized orbital

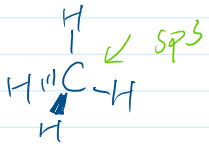
π-Bonds → double bond → overlap of unhybridized 2p atomic orbitals

Lone pairs → can exist in hybridized (sp, sp^2, sp^3) or unhybridized (2p) orbitals

Atomic Hybridization	# and types of orbitals
H−C≡C−H (C: sp)	2 sp hybridized orb. 2 2p atomic orb.] could make 2 π-bonds
 (C: sp^2)	3 sp^2 hybridized orb.



3 sp^2 hybridized orb.
1 2p atomic orb.] could make 1 π-bond

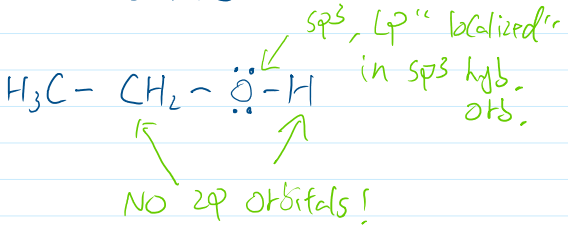


4 sp^3 hybridized orb.

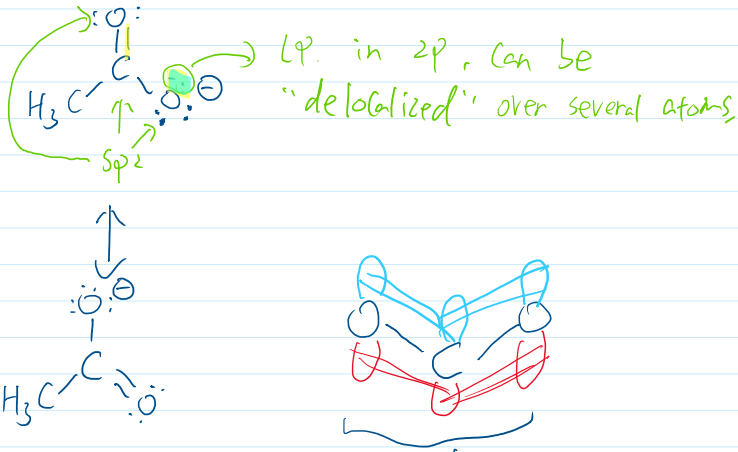
* Can't delocalize π e⊖s or charges in hybrid orbs.
* Need 2p orbital to delocalize π e⊖s and charges.

Localized vs. Delocalized e⊖s :

↓ No Resonance



↘ resonance (resonate LP) over multiple atoms



3 overlapping adjacent 2p orbitals
↓
"π-way"

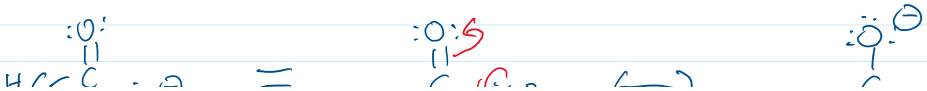
How many e⊖s are in the "π-way"?

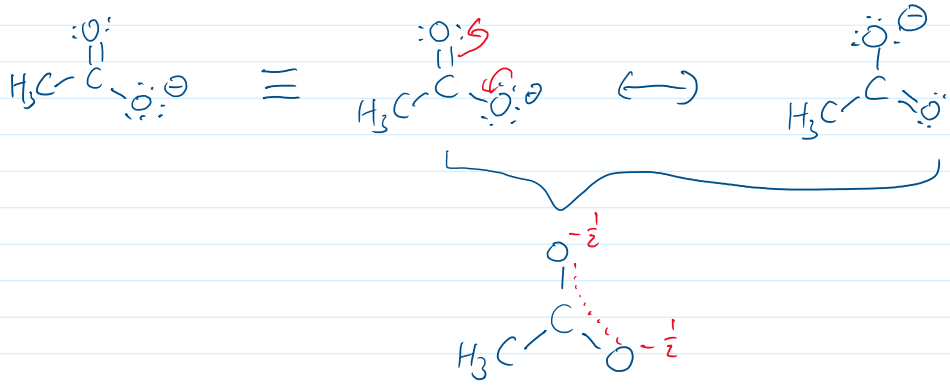
1 π-bond = 2 e⊖
1 LP = 2 e⊖
} 4 e⊖s in the π-way

Resonance Contributing Structures

Recall: Lewis Dot structures are diagrams that show bonding between atoms:
↳ No insight into: Geometry and e⊖ distribution

Resonance: different ways to represent a molecule we draw without line / dots





Each of these are "Resonance contributing structures"

↳ used when no single Lewis structure describes "true" bonding

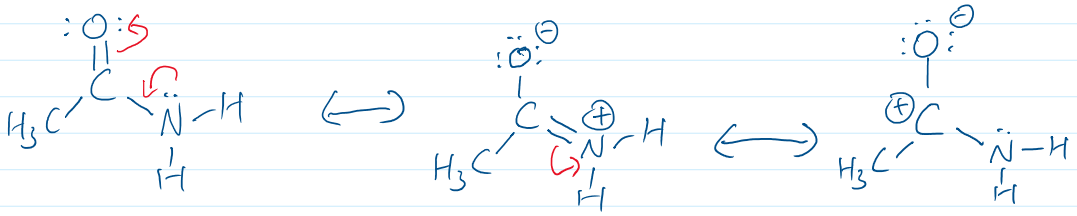
↳ Combined to make a hybrid structure that more accurately describe the e⊖s distribution and bonding.

Contributing structures should:

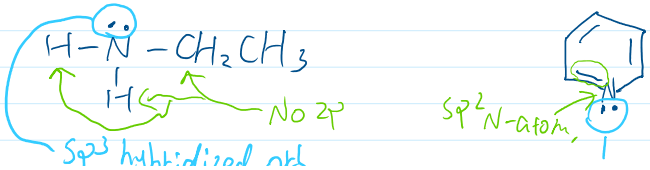
1. Be reasonable Lewis structures w/ all atoms surrounded by a filled valence
2. Maximize # of covalent bonds
3. Least # of unlike charges
4. ⊖ charges on the more E.N. atoms / ⊕ charges on the less E.N. atoms

Resonance: Interconverting π-bonds and LPs

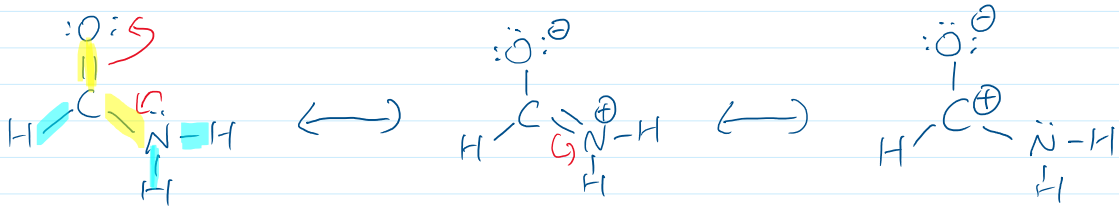
↳ is stabilizing!



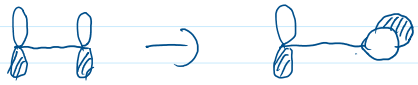
what type of orbitals is the LP in?



H−C≡N: ← sp hybridized orbital



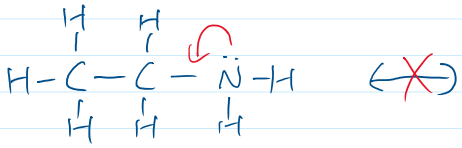
(partial) double bonds cannot rotate at room temperature

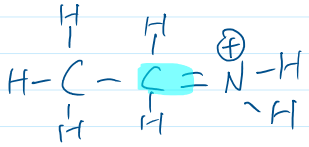


These bonds can rotate

Partial double bonds cannot rotate

Bad Resonance Structures

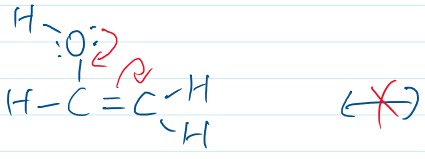


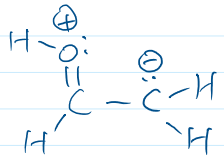


σ-bonds to C!

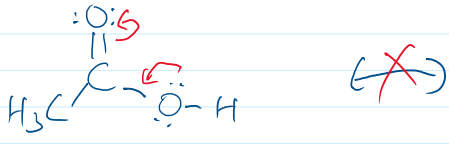
↓

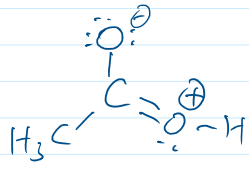
Never!



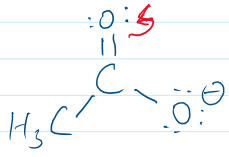


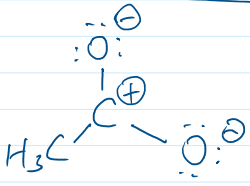
⊕ on the more E.N atom
⊖ on the less E.N C





⊕ and ⊖ on O atoms





Nomenclature

1) Practice

2) Memorize Table 2.1 – 2.3

#Cs =	1	2	3	4
	methyl	Ethyl	Propyl	Butyl
	me	Eat	Peanut	Butter

3) Learn rules (flow chart and class note)

4) practice

General Formula :

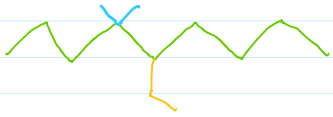
Alphasetize => But don't count "mono, di, tri, etc." "sec-, tert-"

(# – prefix substituent) parent chain name sufix → alk–(ane) → all C–H, no π bonds

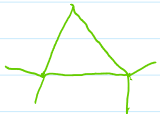
- # : Position of the substituent on the parent chain; separate multiple #s w/ a comma
- prefix : # of that type of group
- substituent : group
- parent chain name : length of the parent chain

separate multiple substituents w/ a dash

Structure A: 5- ethyl – 4,4- dimethyl nonane

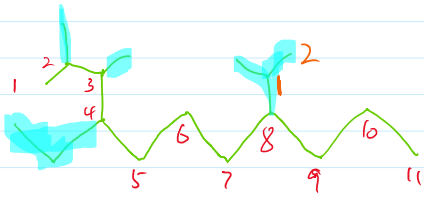


B:



1,1,2,2 – tetramethyl Cyclo propane

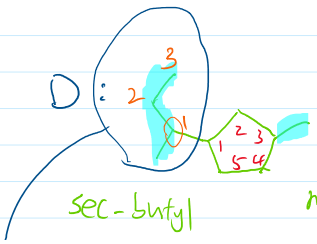
C:



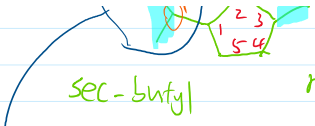
4- ethyl – 2,3- dimethyl – 8-(1-methylethyl) undecane

4 - ethyl - 8 - isopropyl - 2,3-dimethyl undecane

D:



1- sec-butyl – 3- methyl Cyclo pentane



sec-butyl methyl

1- sec-butyl - 3- methyl cyclopentane

For this substituent:

- the "parent chain": propyl (3 C-atoms)
- the numbering: "1" is for the C-atom directly attached to the parent chain

1- methyl propyl

If use Iupac name for the left substituent: ① numbering counterclockwise, with "methyl" as "1"

② : 1 - methyl - 3-(1-methyl propyl) cyclopentane