

MTW 9.12.24

①

Topics: ① π -bond, π -way, molecular orbital theory (MOT)

② Resonance and orbitals required

↳ localized vs delocalized lone pairs (LPs)

σ , π -Bonds, Lone pairs (LPs)

σ bonds \rightarrow single bonds \rightarrow overlap of hybridized orbitals

π bonds \rightarrow double bonds \rightarrow overlap of unhybridized p atomic orbitals

Lone pairs \rightarrow can exist in hybridized or unhybridized orbitals.
sp, sp², sp³ p atomic orbital

(go back)

Atomic hybridization	# and type of orbitals
$\text{H}-\text{C}\equiv\text{C}-\text{H}$ \swarrow sp	2 sp hybridized orbitals 2 p atomic orbitals \Rightarrow could make 2 π bonds
$\begin{array}{c} \text{O} \\ \\ \text{H}-\text{C}-\text{H} \\ \swarrow \text{sp}^2 \end{array}$	3 sp ² hybridized orbitals 1 p atomic orbital \Rightarrow could make 1 π bond
$\begin{array}{c} \text{H} \\ \\ \text{H} \text{---} \text{C} \text{---} \text{H} \\ / \quad \backslash \\ \text{H} \quad \text{H} \\ \swarrow \text{sp}^3 \end{array}$	4 sp ³ hybridized orbitals

★ Need p orbital to delocalized πe^- s

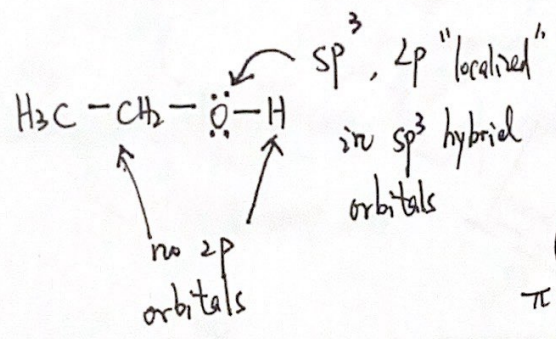
★ Can't delocalize πe^- s as charge in hybrid orbitals.

Localized

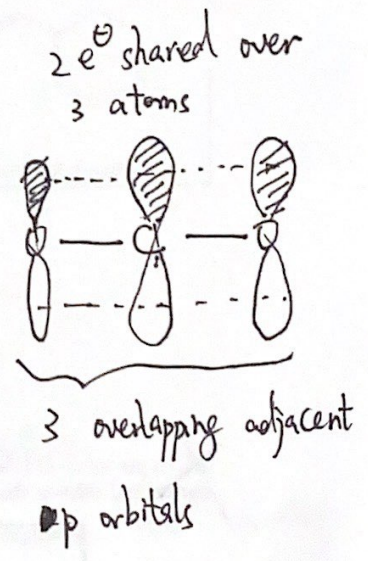
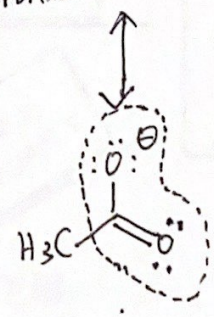
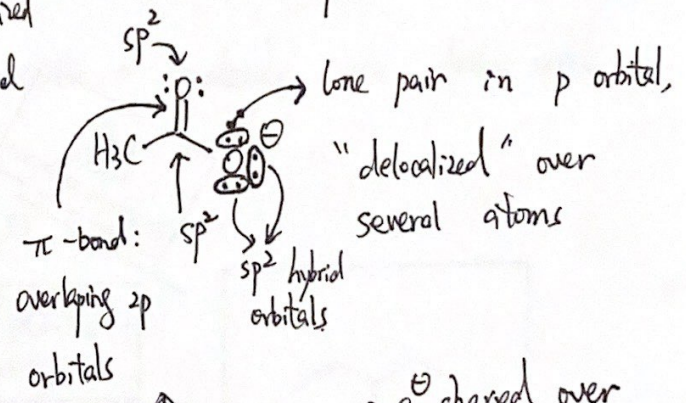
vs

delocalized e^- s :

↓
No resonance

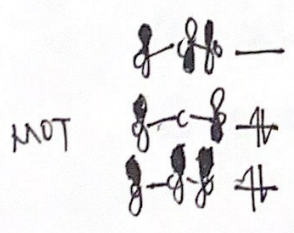


↓
Resonate L.p. (πe^- s, charge) over multiple atoms



How many e^- s are in p orbitals in H3C-C(=O)-O^-? "π way"

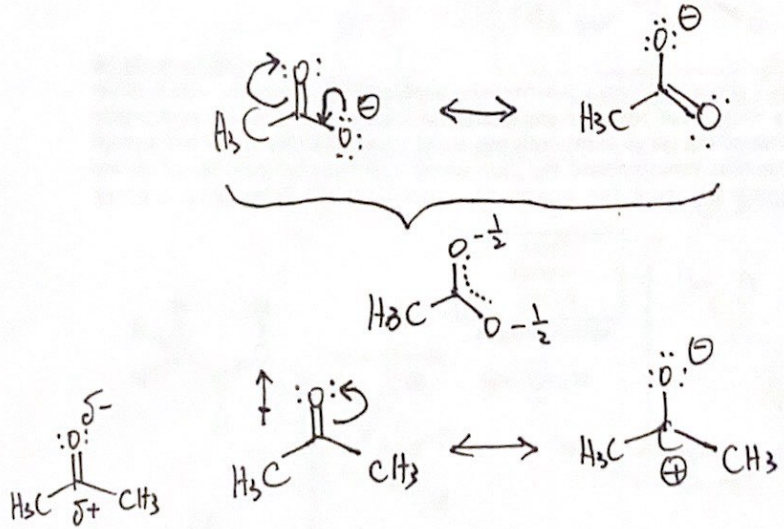
π -bond = 2 e^- s
 1 × lone pair on "O" = 2 e^- s } 4 e^- s in p orbitals
 III
 4 πe^- s



Resonance Contributing Structures.

Recall: Lewis Dots structures are diagrams that show bonding btw atoms: no insight into geometry / e^- distribution

Resonance: different ways to represent a molecule, we draw with lines/letters/dots.



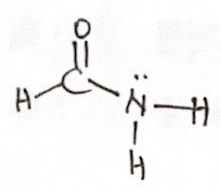
Resonance structures are "Resonance contributing structures", used when no single Lewis structures describes "true" bonding

Contributing structures should:

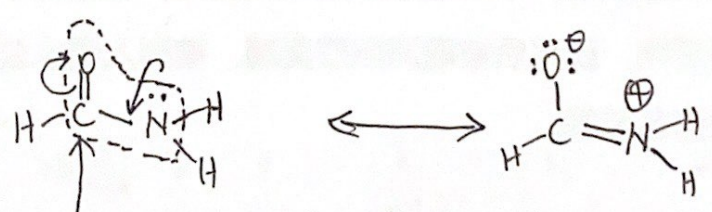
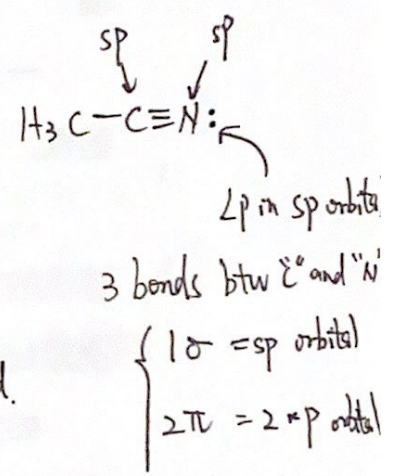
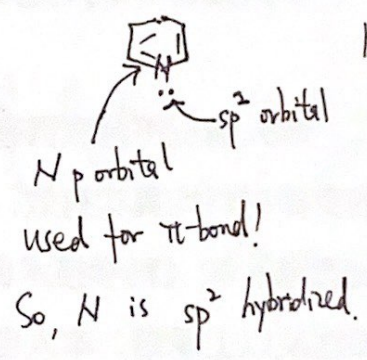
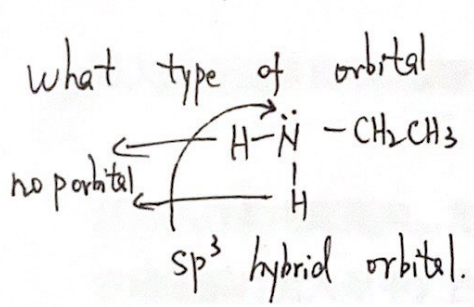
- ① Be reasonable Lewis structures with the correct charge
- ② maximize # of covalent bonds
- ③ least # of unlike charges
- ④ \ominus charge on more electron negative atoms / \oplus on ~~more~~ less electron negative atoms.

Resonance interconvert π -bonds and \angle ps. (mostly)

\hookrightarrow is stabilizing!



If you can delocalize π e^- s, lone pairs, do it!



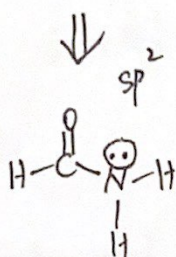
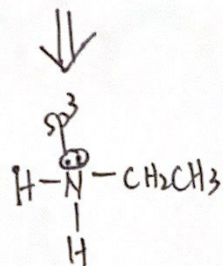
C has a " π " (double bond), it has a p orbital.

the \angle p of "N" want to delocalize in the " π -way"
multiple (≥ 3) adjacent p orbitals

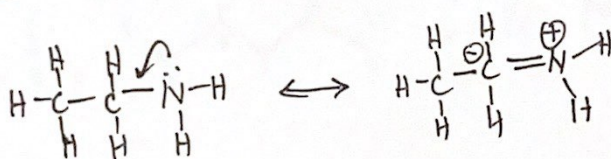
For this single Lewis structure,
VSEPR doesn't accurately predict N
 sp^2 hybridization.

Recall: ~~VSEPR~~ VSEPR will work only if we consider all relevant contributing structures.

Localized Vs delocalized lone pair



Bad Resonance structures



5 bonds to C!
10⁺ valence e⁻s
NEVER HAPPEN!

Nomenclature.

# Cs =	1	2	3	4
	Methyl	Ethyl	Propyl	Butyl
	"Me	"Et	"propyl	"butyl"

General Formula: $(\text{# - prefix substituent})$ parent name

Alphabetize \Rightarrow but don't count "mono, di, tri," etc.

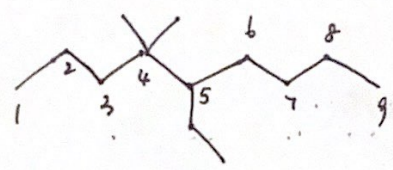
↑ position of the substituent on the parent chain

↑ # of that type of group

↑ group

↑ length of the parent chain

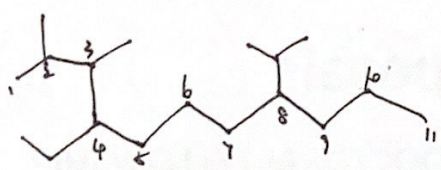
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5-ethyl-4,4-dimethyl-nonane



1,1,2,2-tetramethyl cyclo propane



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