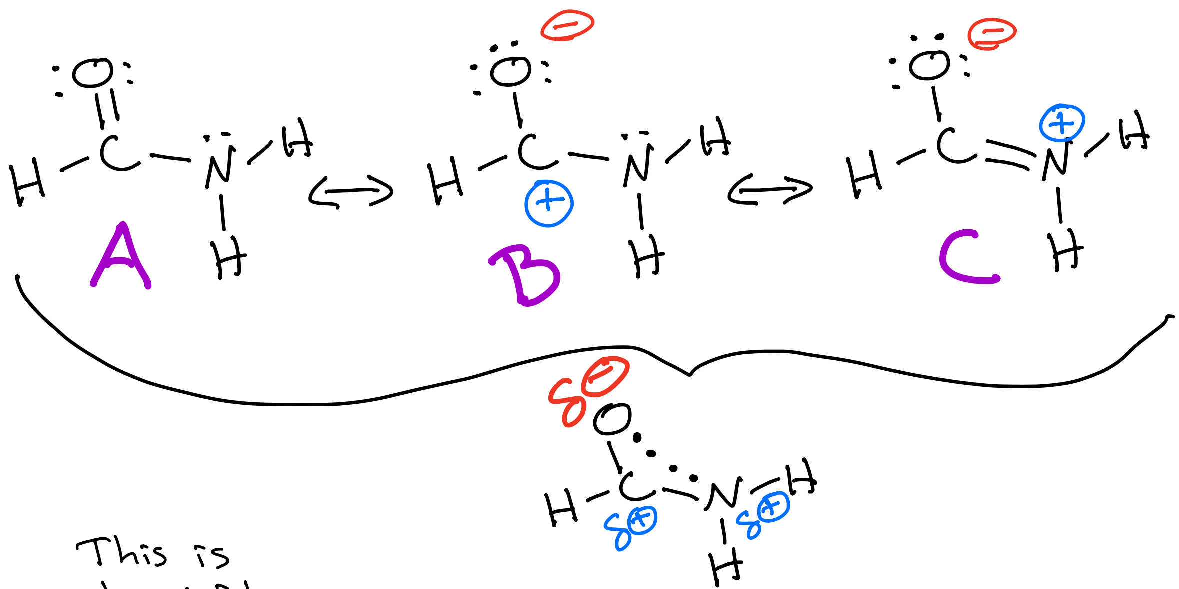
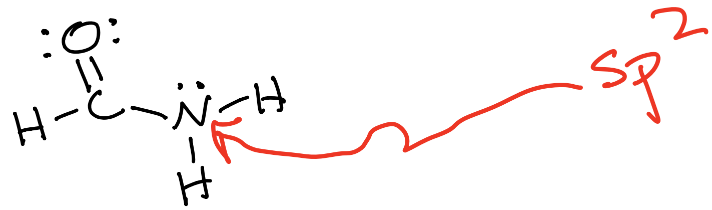
Amide contributing structures revisited



This is how it is drawn, but all 3 contributing structures must be considered ⟹

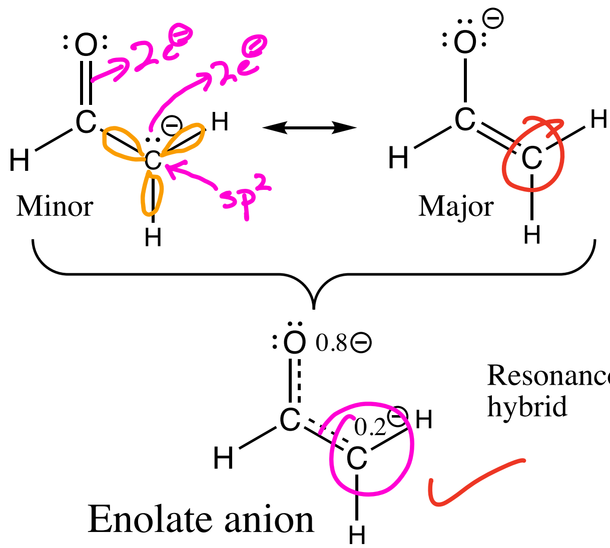


5. Delocalization of charge over a larger area is stabilizing. The majority of molecules you will encounter will be neutral, but some carry negative or positive charges because they contain an imbalance in their total number of electrons and protons. In general, charges are destabilizing (higher Gibbs free energy), increasing the reactivity of the molecules that possess them. Localized charges are the most destabilizing (highest Gibbs free energy). Delocalizing the charge over a larger area through interactions such as resonance, inductive effects, and hyperconjugation is stabilizing (lowering the Gibbs free energy). In addition, it is more stabilizing to have more negative charge on a more electronegative atom (e.g. O), and more positive charge on a less electronegative atom (e.g. C).

The reason "B" is important

7. Delocalization of pi electron density over a larger area is stabilizing. Pi electron density delocalization occurs through overlapping $2p$ orbitals, so to take part in pi electron density delocalization atoms must be $sp2$ or sp hybridized and reside in the same plane. Pi electron delocalization can involve even large numbers of such atoms. Pi electron density cannot delocalize onto or through $sp3$ hybridized atoms because an $sp3$ atom has no $2p$ orbital. Aromaticity is a special type of pi electron density delocalization involving rings and a specific number of pi electrons, and is the most stabilizing form of pi electron density delocalization.

The reason "C" is important



Contributing structures

Resonance hybrid

Enolate anion

Molecular Orbital Theory approach to bonding: Just add the individual orbital wave functions:

$$\Psi_{H1s} + \Psi_{H1s} + \Psi_{H1s} + \Psi_{C1s} + \Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py} + \Psi_{C2pz} + \Psi_{C1s} + \Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py} + \Psi_{C2pz} + \Psi_{O1s} + \Psi_{O2s} + \Psi_{O2px} + \Psi_{O2py} + \Psi_{O2pz}$$

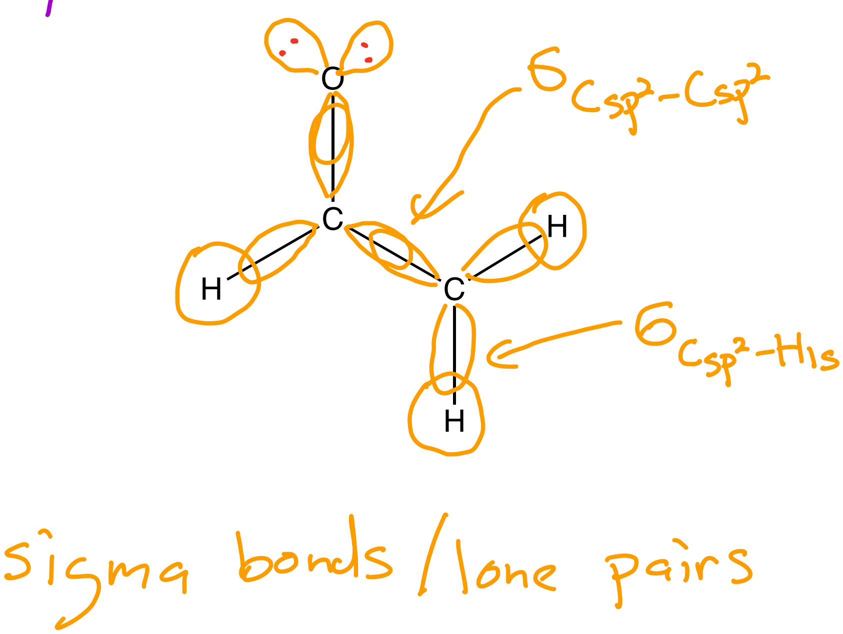
Valence Bond Theory approach to bonding: Hybridize the atomic orbitals on atoms first, then look for overlap with remaining orbital wave functions:

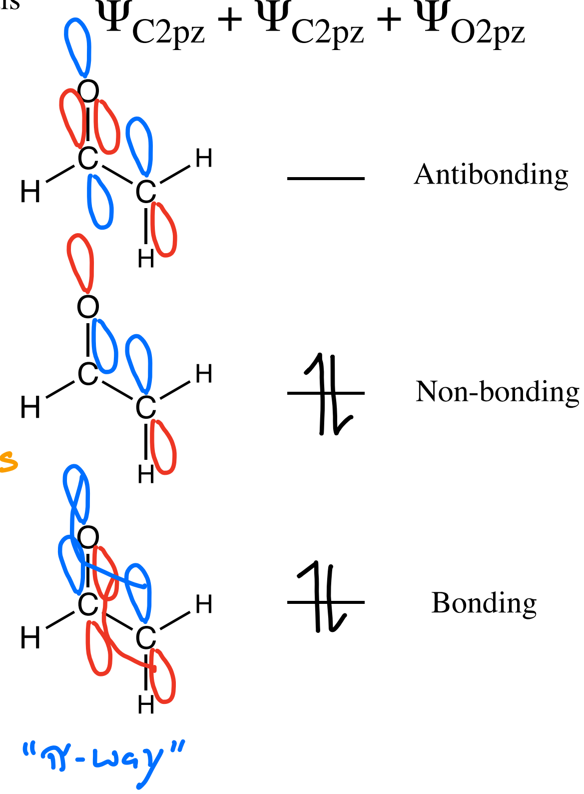
$$\Psi_{H1s} + \Psi_{H1s} + \Psi_{H1s} + \Psi_{C1s} + (\Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py}) + \Psi_{C2pz} + \Psi_{C1s} + (\Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py}) + \Psi_{C2pz} + \Psi_{O1s} + (\Psi_{O2s} + \Psi_{O2px} + \Psi_{O2py}) + \Psi_{O2pz}$$

Sigma (σ) bonding - overlap of hybridized orbitals

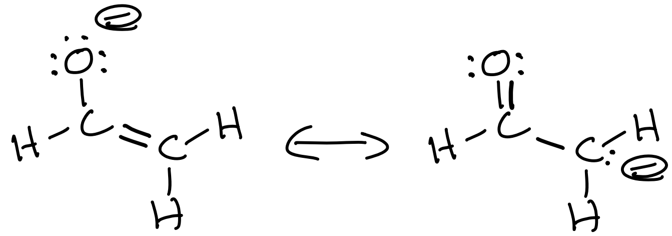
π-way bonding - overlap of 3 adjacent unhybridized 2p orbitals

$$\Psi_{C2pz} + \Psi_{C2pz} + \Psi_{O2pz}$$

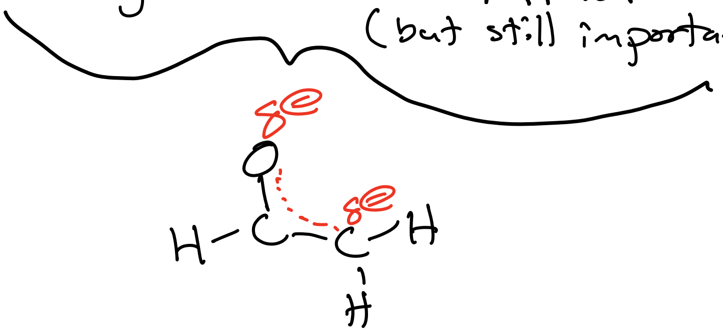


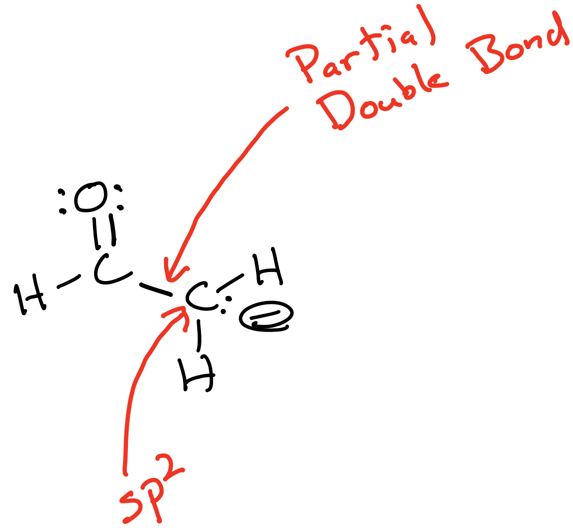


Enolate ion contributing structures

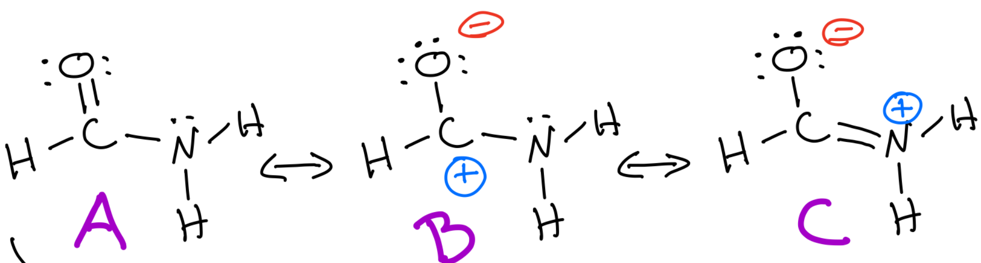


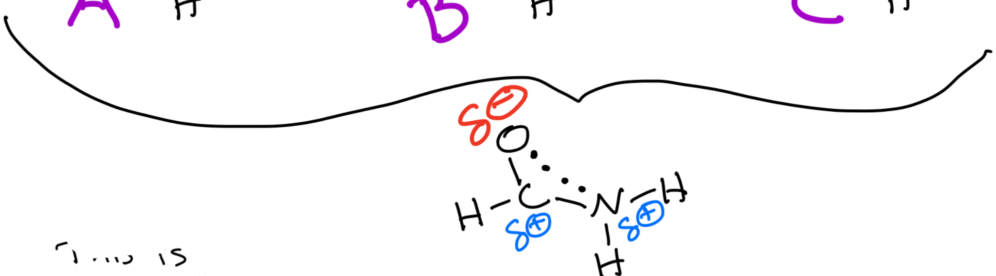
Major　　　　Minor (but still important)

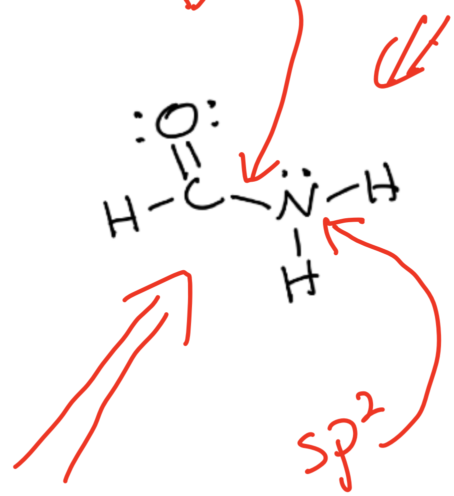




Amide contributing structures







The partial double bond of the C–N bond does not rotate at room temperature so this adds considerable rigidity to protein chains → enables precise 3-dimensional folding and LIFE AS WE KNOW IT!!!

Look at the POTD for today!

<u>Organic Chemistry</u> is the study of carbon-containing molecules.

This class has two points.

The first point of the class is to understand the organic chemistry of living systems. We will teach you how to think about and understand the most amazing things on the planet!!

> Water is essential for life, you will learn why water has such special properties. 8/27/25
>
> You will learn the secret structural reason proteins, the most important molecular machines in our bodies, can support the chemistry of life. 9/10/25
>
> You will learn why when you take Advil for pain, exactly half of what you take works, and the other half does nothing.
>
> You will learn how toothpaste works.
>
> You will learn how a single chlorofluorocarbon refrigerant molecule released into the atmosphere can destroy many, many ozone molecules, leading to an enlargement of the ozone hole.
>
> You will learn how medicines like Benadryl, Seldane, and Lipitor work.
>
> You will learn how Naloxone is an antidote for an opioid overdose.
>
> You will learn why Magic Johnson is still alive, decades after contracting HIV.
>
> You will learn how MRI scans work.

The second point of organic chemistry is the synthesis of complex molecules from simpler ones by making and breaking specific bonds.

> You will learn how to understand movies of reaction mechanisms like alkene hydration.
>
> You will learn reactions that once begun, will continue reacting such that each product molecule created starts a new reaction until all the starting material is used up.
>
> You will learn reactions that can make antifreeze from vodka.
>
> You will learn a reaction that can make nail polish remover from rubbing alcohol.
>
> You will learn how to look at a molecule and accurately predict which atoms will react to make new bonds, and which bonds will break during reactions.
>
> You will learn how to analyze a complex molecule's structure so that you can predict ways to make it via multiple reactions starting with less complex starting molecules.

Survival skill in OChem

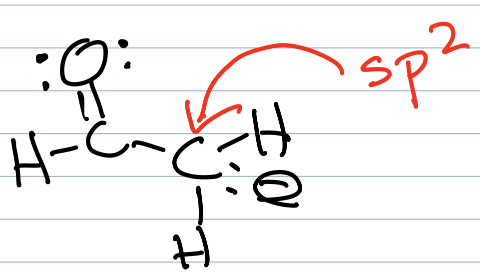
↳ Identify hybridization state of atoms in molecules

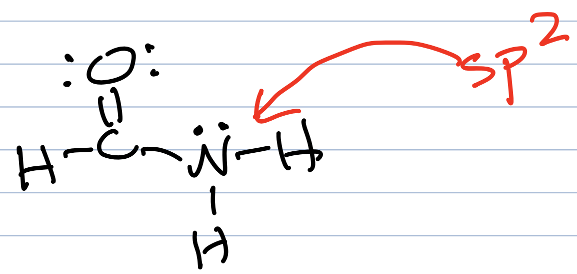
1) sp^3 → all sigma bonds and lone pairs

2) sp^2 → one pi bond and 3 sigma bonds / lone pairs

3) sp → two pi bonds and 2 sigma bonds / lone pairs

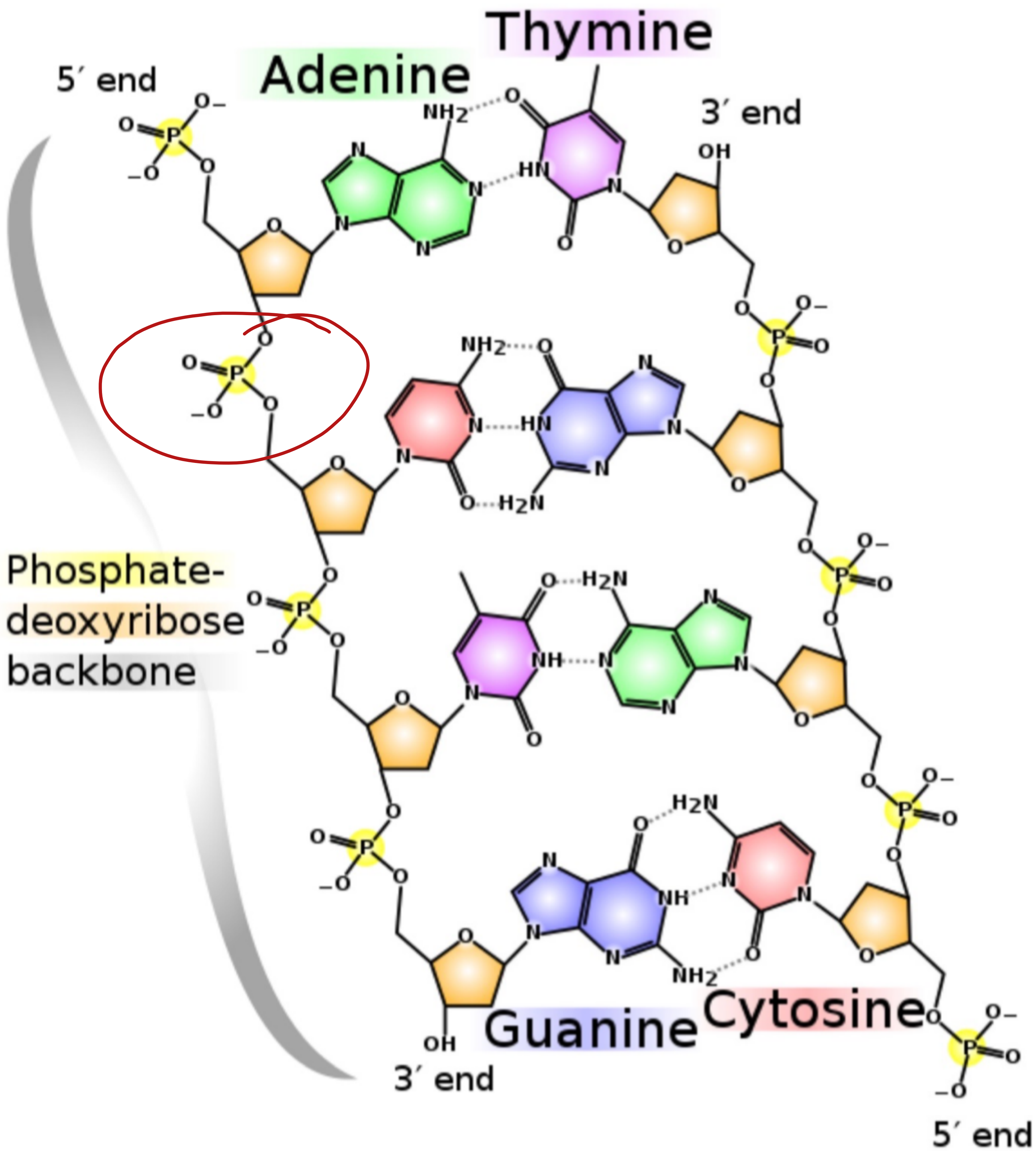
⇒ An atom counts as having a π bond if ANY significant contributing structure has a pi bond to the atom → part of a "π-way"



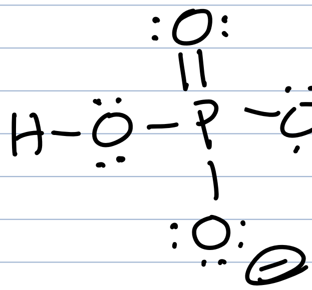


From Wikipedia 2020

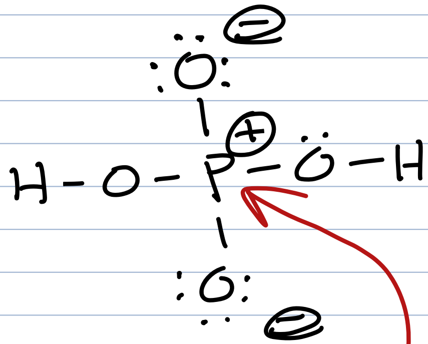
⇒ We messed up!



Chemical structure of DNA; hydrogen bonds shown as dotted lines



vs.

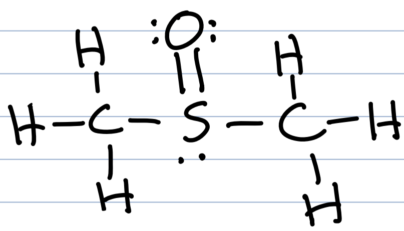


sp^3

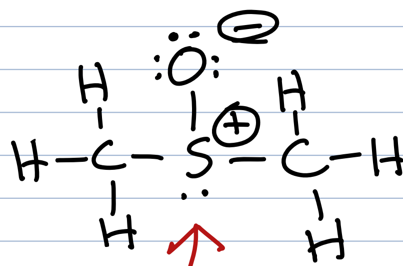
high level calculations have confirmed → the d orbitals are not involved

However ⇒ because traditions are hard to change we still write it the "old" way even though it is not accurate!

Here also!



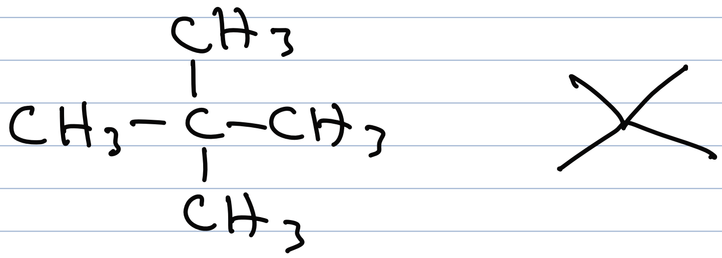
vs.



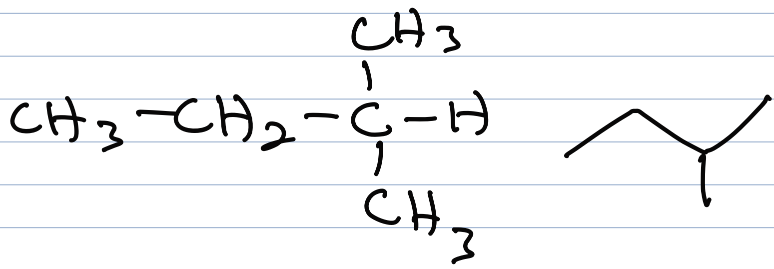
sp^3

⇓

again based on high level calculations

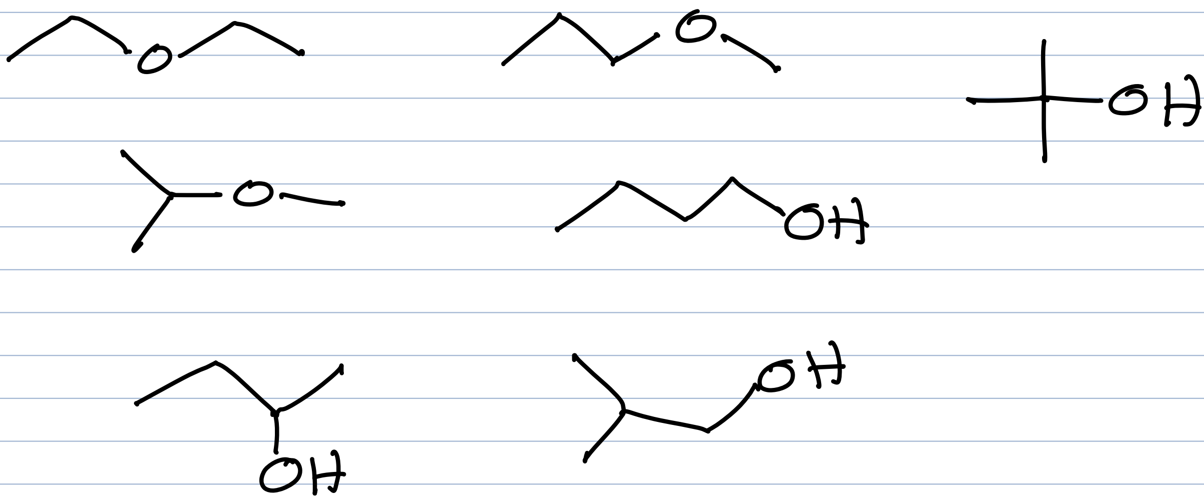


All of these are C_5H_{12}



Constitutional Isomers → same molecular formula, but the atoms are connected differently

$C_4H_{10}O$ → Constitutional Isomers



Nomenclature of molecules

2 systems → Common names → existed before systematic names

we will sometimes mention them but you will never see on an exam

IUPAC → systematic name process for structures

We will test you on this

→ Molecules are named as the longest chain, with groups branching off the main

You MUST → Memorize Table 2.1–2.3 in the book

Add "ane" to indicate it is an alkane

Table 2.1 Names, Molecular Formulas, and Condensed Structural Formulas for the First 20 Alkanes with Unbranched Chains

Name	Molecular Formula	Condensed Structural Formula	Name	Molecular Formula	Condensed Structural Formula
Methane	CH_4	CH_4	Undecane	$C_{11}H_{24}$	$CH_3(CH_2)_9CH_3$
Ethane	C_2H_6	CH_3CH_3	Dodecane	$C_{12}H_{26}$	$CH_3(CH_2)_{10}CH_3$
Propane	C_3H_8	$CH_3CH_2CH_3$	Tridecane	$C_{13}H_{28}$	$CH_3(CH_2)_{11}CH_3$
Butane	C_4H_{10}	$CH_3(CH_2)_2CH_3$	Tetradecane	$C_{14}H_{30}$	$CH_3(CH_2)_{12}CH_3$
Pentane	C_5H_{12}	$CH_3(CH_2)_3CH_3$	Pentadecane	$C_{15}H_{32}$	$CH_3(CH_2)_{13}CH_3$
Hexane	C_6H_{14}	$CH_3(CH_2)_4CH_3$	Hexadecane	$C_{16}H_{34}$	$CH_3(CH_2)_{14}CH_3$
Heptane	C_7H_{16}	$CH_3(CH_2)_5CH_3$	Heptadecane	$C_{17}H_{36}$	$CH_3(CH_2)_{15}CH_3$
Octane	C_8H_{18}	$CH_3(CH_2)_6CH_3$	Octadecane	$C_{18}H_{38}$	$CH_3(CH_2)_{16}CH_3$
Nonane	C_9H_{20}	$CH_3(CH_2)_7CH_3$	Nonadecane	$C_{19}H_{40}$	$CH_3(CH_2)_{17}CH_3$
Decane	$C_{10}H_{22}$	$CH_3(CH_2)_8CH_3$	Eicosane	$C_{20}H_{42}$	$CH_3(CH_2)_{18}CH_3$

Table 2.2 Prefixes Used in the IUPAC System to Show the Presence of 1 to 20 Carbon Atoms in an Unbranched Chain

Prefix	Number of Carbon Atoms	Prefix	Number of Carbon Atoms
meth-	1	undec-	11
eth-	2	dodec-	12
prop-	3	tridec-	13
but-	4	tetradec-	14
pent-	5	pentadec-	15
hex-	6	hexadec-	16
hept-	7	heptadec-	17
oct-	8	octadec-	18
non-	9	nonadec-	19
dec-	10	eicos-	20

Table 2.3 Names for Alkyl Groups with One to Five Carbons. Common Names and Their Abbreviations Are Given in Parentheses

Name	Condensed Structural Formula	Name	Condensed Structural Formula
Methyl (Me)	$-CH_3$	1,1-Dimethylethyl (*tert*-butyl, *t*-Bu)	$-\overset{\substack{CH_3\\ \mid}}{\underset{\substack{\mid\\ CH_3}}{C}}CH_3$
Ethyl (Et)	$-CH_2CH_3$		
Propyl (Pr)	$-CH_2CH_2CH_3$	Pentyl	$-CH_2CH_2CH_2CH_2CH_3$
1-Methylethyl (isopropyl, iPr)	$-\underset{\substack{\mid\\ CH_3}}{C}HCH_3$	3-Methylbutyl (isopentyl)	$-CH_2CH_2\underset{\substack{\mid\\ CH_3}}{C}HCH_3$
Butyl (Bu)	$-CH_2CH_2CH_2CH_3$	2-Methylbutyl	$-CH_2\underset{\substack{\mid\\ CH_3}}{C}HCH_2CH_3$
2-Methylpropyl (isobutyl, iBu)	$-CH_2\underset{\substack{\mid\\ CH_3}}{C}HCH_3$	2,2-Dimethylpropyl (neopentyl)	$-CH_2\overset{\substack{CH_3\\ \mid}}{\underset{\substack{\mid\\ CH_3}}{C}}CH_3$
1-Methylpropyl (*sec*-butyl, *s*-Bu)	$-\underset{\substack{\mid\\ CH_3}}{C}HCH_2CH_3$		

Step 1 → Identify the parent chain then number it.

longest continuos chain of carbon atoms

→ Number the chain so that the first group (substituent) has the lower number *

* if there is a "tie" on numbers use the lower number for the the substituent that comes first in the alphabetization

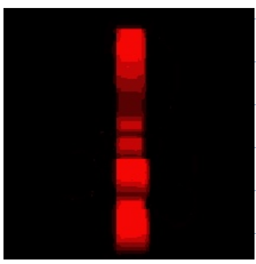
Step 2 → Name the substituents →
changing "ane" to "yl"
see Table 2.3

⟹ You can always use the common names in Table 2.3

ex. isopropyl or
1-methylethyl are
both OK

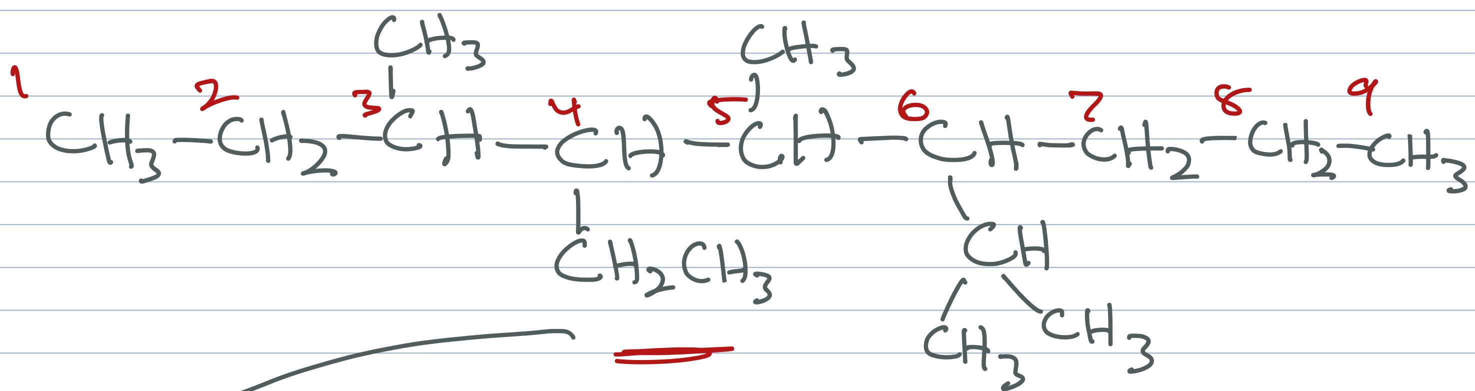
Step 3 → Number the substituents and list in alphabetical order

When more than one of the same substituents is present we use "di-", "tri-", "tetra-", "penta-" to indicate exactly how many are there



→ do not consider "di-, tri-, tetra-" etc. when alphabetizing

Putting it all together:



nonane → 9 carbons in the parent chain

dimethyl 3,5

ethyl 4

isopropyl 6

4-ethyl-6-isopropyl-3,5-dimethylnonane