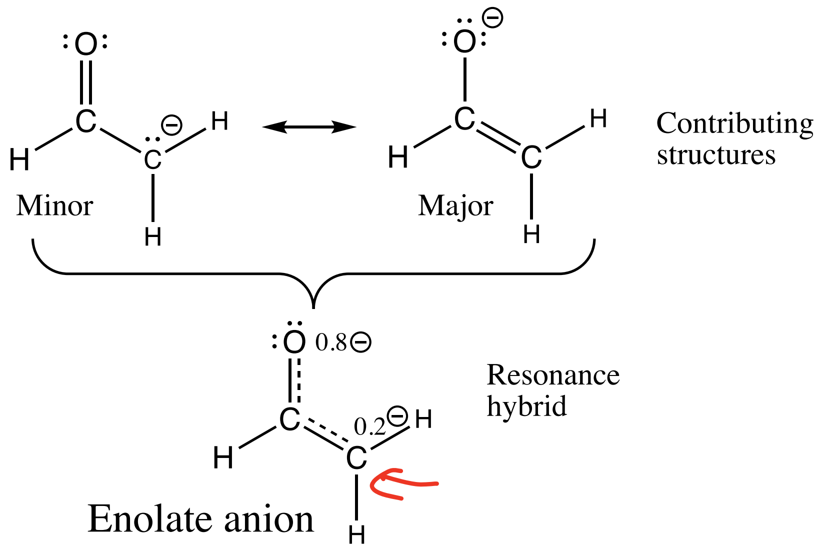


Molecular Orbital Theory approach to bonding: Just add the individual orbital wave functions:

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

Valence Bond Theory approach to bonding: Hybridize the atomic orbitals on atoms first, then look for overlap with remaining orbital wave functions: sp2

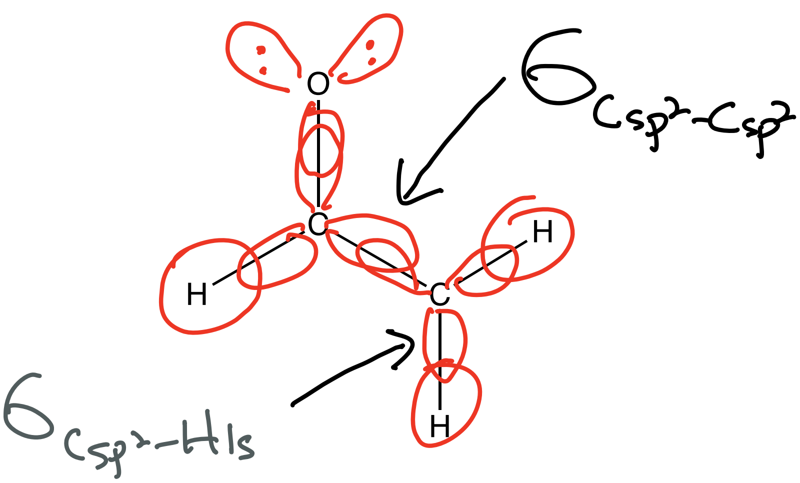
$$\Psi_{H1s} + \Psi_{H1s} + \Psi_{H1s} + \Psi_{C1s} + (\Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py}) + \Psi_{C2pz} + \Psi_{C1s} + (\Psi_{C2s} + \Psi_{C2px} + \Psi_{C2py}) + \Psi_{C2pz} + \Psi_{O1s} + (\Psi_{O2s} + \Psi_{O2px} + \Psi_{O2py}) + \Psi_{O2pz}$$

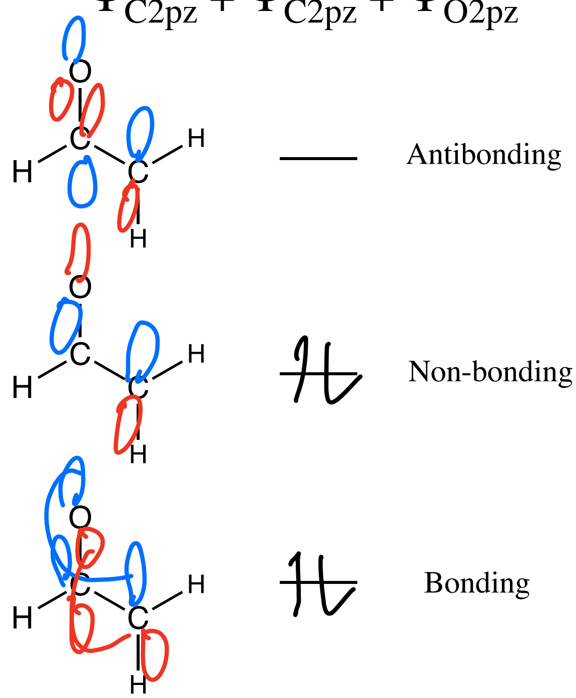
sp2 sp2

Sigma (σ) bonding - overlap of hybridized orbitals

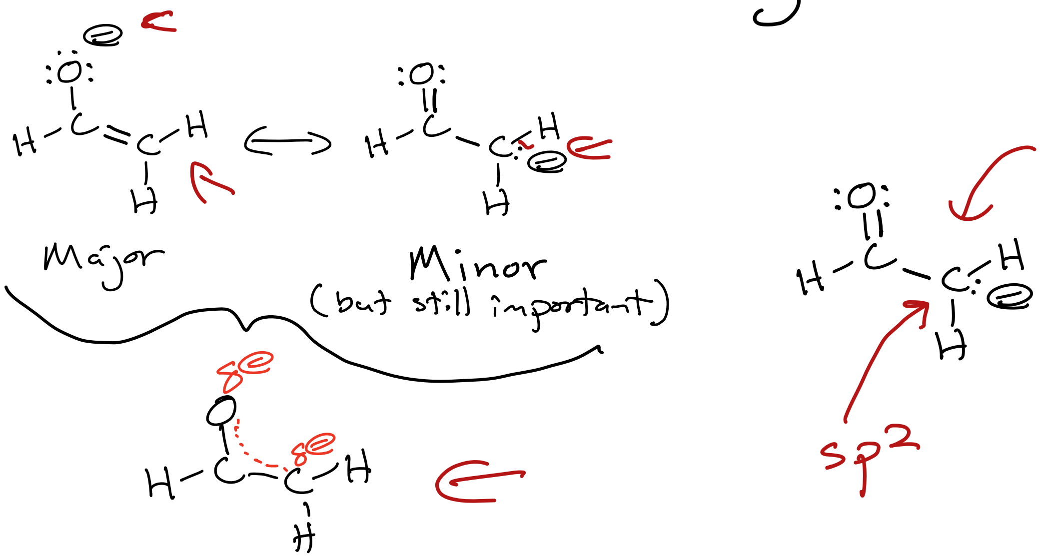
π-way bonding - overlap of 3 adjacent unhybridized 2p orbitals

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

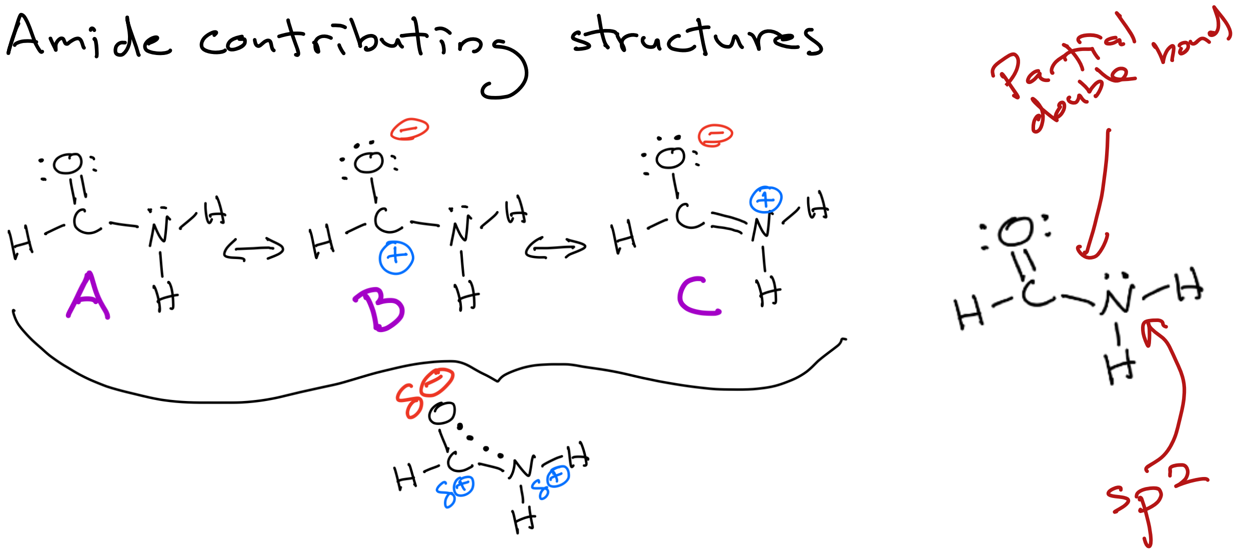




Enolate ion contributing structures



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!!!

<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. 8/25/2022

You will learn the secret structural reason proteins, the most important molecular machines in our bodies, can support the chemistry of life. 9/6/22

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.

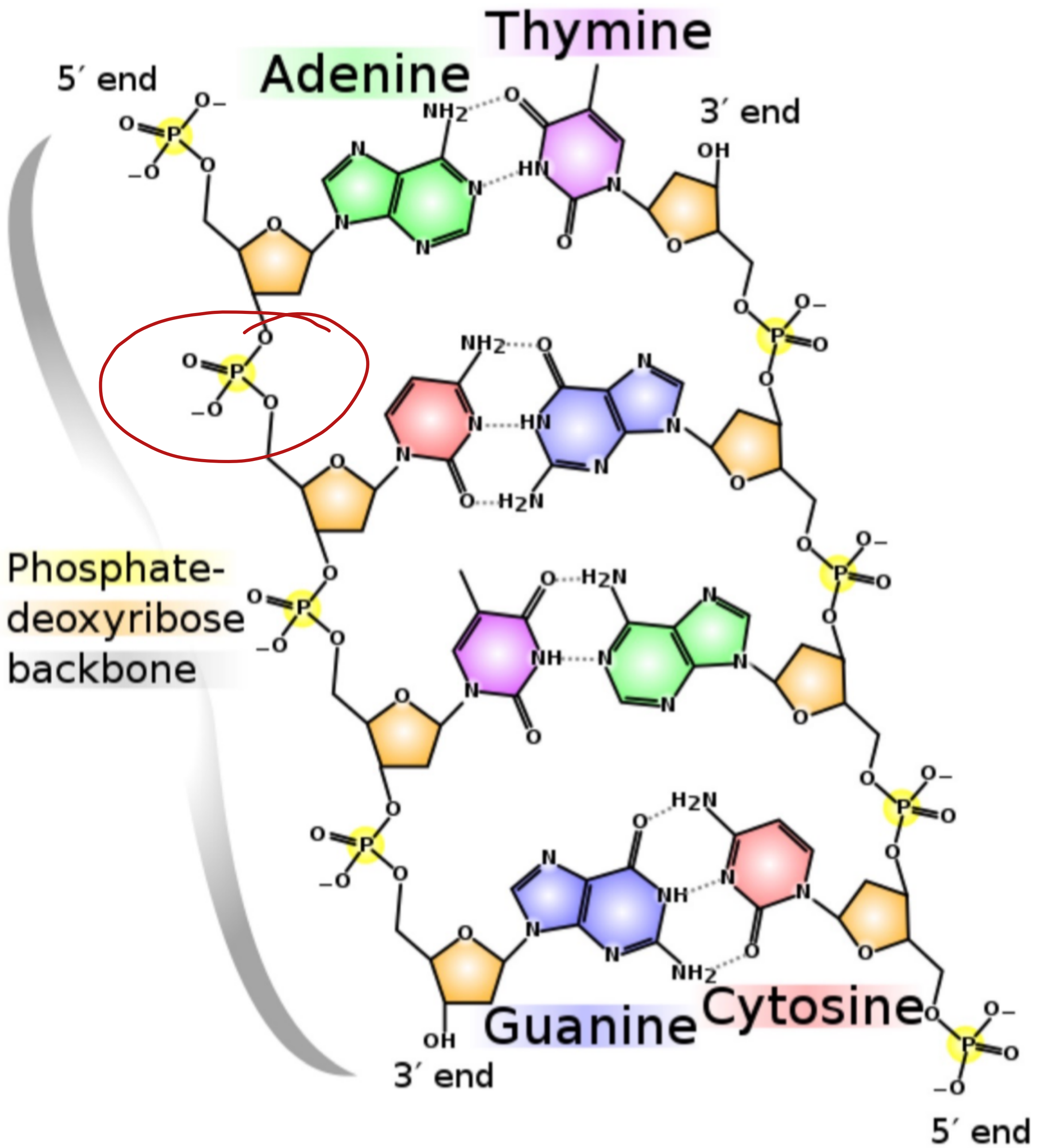
You will learn a reaction that can make nail polish remover from rubbing alcohol.

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.

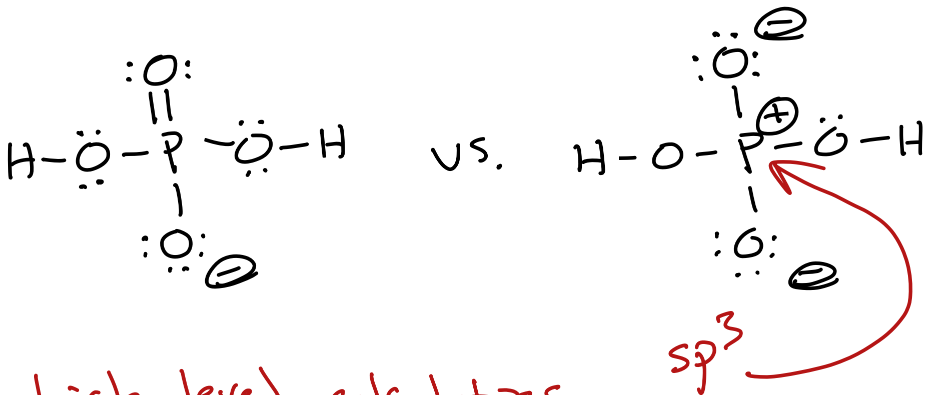
You will learn how to analyze a complex molecule's structure so that you can predict ways to make it via multiple reactions starting with less complex starting molecules.

ooPS → We messed up!

From Wikipedia 9/2020



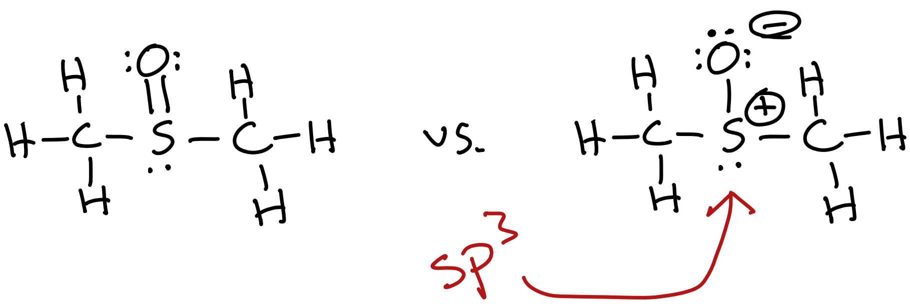
Chemical structure of DNA; hydrogen bonds shown as dotted lines



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

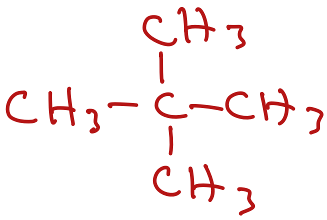
However → because traditions are hard to change we still write it the "old" way even though it is not accurate!

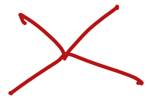
Here also!



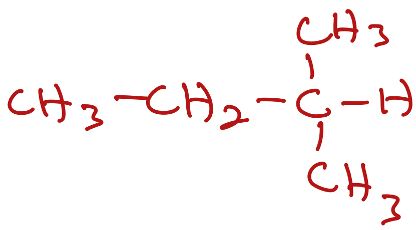
⇓

again based on high level calculations





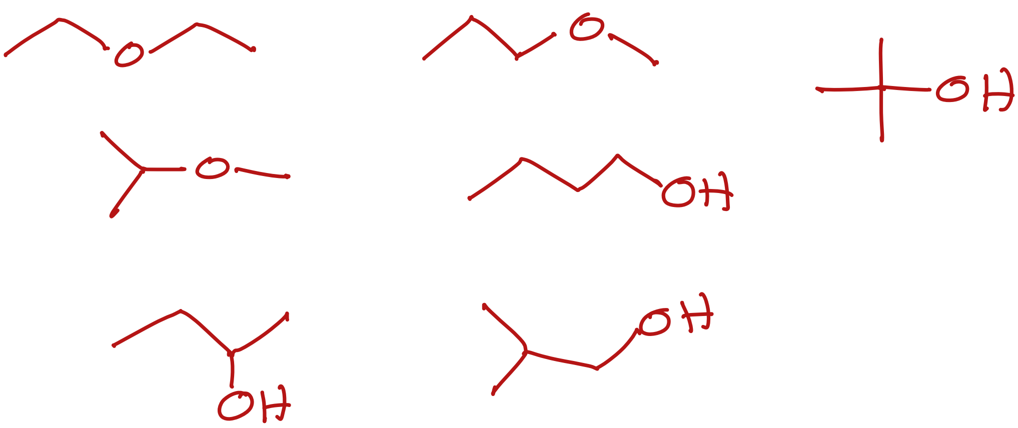
All of these are C_5H_{12}



$CH_3-CH_2-CH_2-CH_2-CH_3$

<u>Constitutional isomers</u> → same molecular formula, but the atoms are connected differently

$C_4H_{10}O$ → Constitutional Isomer



Nomenclature of molecules

2 systems → Common names → existed before systematic names

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

IUPAC → systematic name process for structures

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

We will test you on this

Step 1 → Memorize Tables 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)	$-C(CH_3)_2CH_3$ (drawn as $-CCH_3$ with CH_3 above and below)
Ethyl (Et)	$-CH_2CH_3$		
Propyl (Pr)	$-CH_2CH_2CH_3$	Pentyl	$-CH_2CH_2CH_2CH_2CH_3$
1-Methylethyl (isopropyl, iPr)	$-CHCH_3$ with CH_3 below the CH	3-Methylbutyl (isopentyl)	$-CH_2CH_2CHCH_3$ with CH_3 below the CH
Butyl (Bu)	$-CH_2CH_2CH_2CH_3$	2-Methylbutyl	$-CH_2CHCH_2CH_3$ with CH_3 below the CH
2-Methylpropyl (isobutyl, iBu)	$-CH_2CHCH_3$ with CH_3 below the CH	2,2-Dimethylpropyl (neopentyl)	$-CH_2CCH_3$ with CH_3 above and below the C
1-Methylpropyl (*sec*-butyl, *s*-Bu)	$-CHCH_2CH_3$ with CH_3 below the CH		

Step 2 → 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

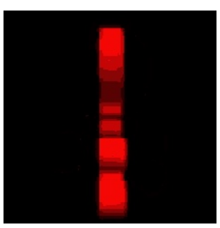
in the alphabet

Step 3 → 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 4 → Alphabetize substituents and list in alphabetical order

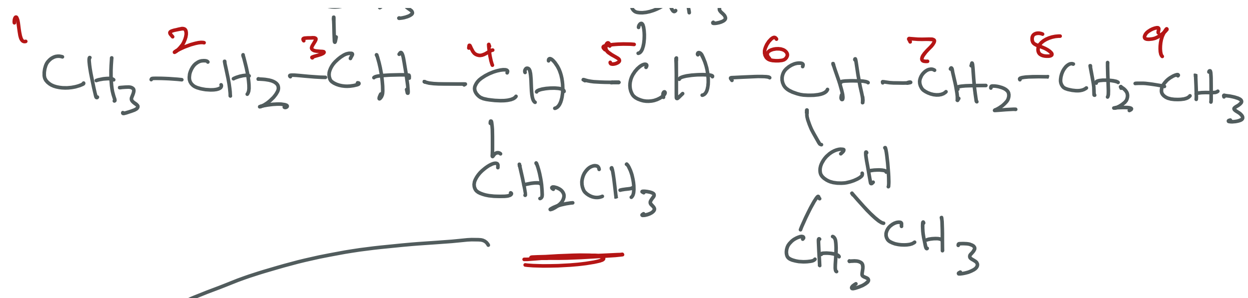


When more than one of the same substituent is present we use "di-, tri-, tetra-, penta- to indicate exactly how many

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

Putting it all together:

CH_3 CH_3



nonane → 9 carbons in the parent chain

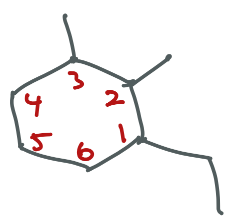
dimethyl 3,5

ethyl 4

isopropyl 6

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

Cyclic Structures



1-ethyl-2,3-dimethylcyclohexane

When there are more atoms in the ring compared to any of the substituents → the parent chain is the ring → add "cyclo" to the parent chain name

Number the ring to give the lowest

overall numbers (1,2,3 not 4,5,6).

If there is a tie the first substituent by alphabet gets the lower number

IUPAC PROCEDURE FOR NAMING ALKANES

Before you begin you must:
1) Memorize alkane chain names (Table 2.1)
2) Memorize substituent names (Tables 2.2 and 2.3)
[I apologize on behalf of all chemists for the crazy names you have to memorize. I wish I knew an easier way, but I do not]

START HERE

Locate Longest Continuous Carbon Chain and Count Number of Carbon Atoms. Find the Alkane Name that Corresponds to the Chain (ex. heptane, dodecane, etc.) and Write this Down Leaving Room in Front of the Name for More Writing. If There are Alkane Branches Continue, if Not You are Done. Go Have a Party.

↓

Number the Main Chain Such that the First Substituent Will Be Branching Off from the Lowest Numbered Carbon (this is not as hard as it sounds since there are only two choices on which way to number, choose the origin as being closest to the first branch point). If There are Substituents in Equivalent Positions from Either End, the Lower Number Goes to the One that Comes First in Alphabetical Order.

↓

Does Branch have Branching ?

No Branching On Branch Itself →

1) Count the Number of Carbon Atoms in The Chain
2) Find the Name Corresponding to that Chain Length
3) Change the Suffix from ane to yl. This is Name of the Branch .

Yes, Branch Has Branches Of Its Own →

1) Does Entire Branch Group Have a Trivial Name? (isopropyl, isobutyl, neopentyl etc.)

Yes →

Write Number of Main Chain Carbon at Branch Point then a Dash (-) Followed by Name of Branch All Preceding Original Main Chain Name as One Word

No →

Use Same Rules as for the Rest of Alkane: Pick Longest Continuous Chain, Name Branches Including Numbers But Use Parentheses Around Branch Name
Ex. 6-(2,3-dimethylbutyl)dodecane

ADDITIONAL RULES

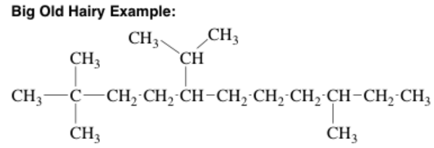
1) If a Molecule Contains Two of the Same Branching Alkyl Groups Use the Prefix di, if Three Use tri, if Four Use tetra, if Five Use penta, if Six Use hexa etc.
Ex. 2,3,4-trimethylhexane

2) If Structure Contains a Ring That Has More Carbon Atoms Than Any Other Open Chain, the Main Chain is the Ring and is Named by Adding cyclo to the Name of the Alkane with the Same Number of Carbon Atoms as the Ring. The Rest is the Same as for Normal Alkane Except You Need to Keep the Total Numbers as Small as Possible When Numbering.
Ex. 1,2-dimethylcyclohexane

3) If More Than One Branch, List Them in Alphabetical Order, NOT Numerical Order.
Ex. 5-ethyl-3,4-diisopropyl-7-methyldecane

4) DO NOT Include the Italicized Prefixes *n-*, *sec-*, and *tert-* OR the Mulitplying Prefixes di, tri, tetra, etc. When Alphabetizing Simple Substitutents. All Other Prefixes (iso, neo, etc.) are Included When Alphabetizing Simple Substituents. No Need to Argue, I Did Not Invent TheseRules!
Ex. 5-*tert*-butyl-2-methyldecane

Big Old Hairy Example:



5-Isopropyl-2,2,9-trimethylundecane