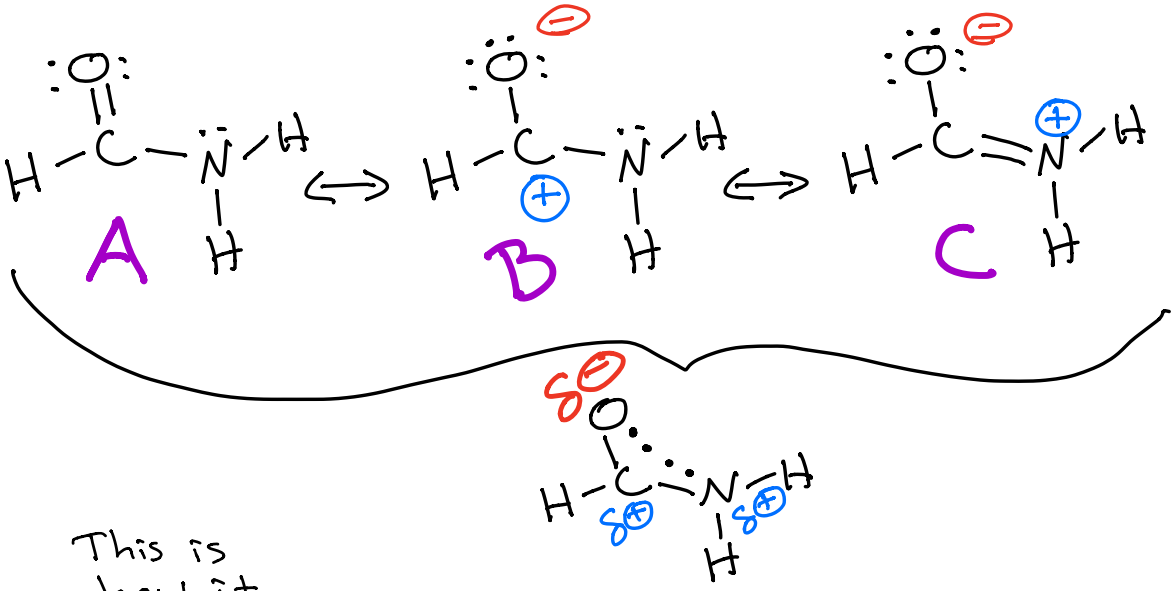
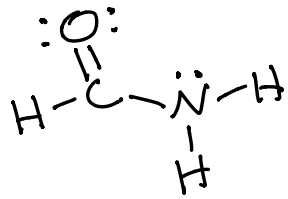
Amide contributing structures revisited



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).

7. Delocalization of pi electron density over a larger area is stabilizing. Pi electron density delocalization occurs through overlapping 2*p* 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 2*p* 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.

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)**	$-C(CH_3)_3$
Ethyl (Et)	$-CH_2CH_3$		
Propyl (Pr)	$-CH_2CH_2CH_3$	**Pentyl**	$-CH_2CH_2CH_2CH_2CH_3$
1-Methylethyl (isopropyl, iPr)	$-CH(CH_3)_2$	**3-Methylbutyl (isopentyl)**	$-CH_2CH_2CH(CH_3)_2$
Butyl (Bu)	$-CH_2CH_2CH_2CH_3$	**2-Methylbutyl**	$-CH_2CH(CH_3)CH_2CH_3$
2-Methylpropyl (isobutyl, iBu)	$-CH_2CH(CH_3)_2$		
1-Methylpropyl (*sec*-butyl, *s*-Bu)	$-CH(CH_3)CH_2CH_3$	**2,2-Dimethylpropyl (neopentyl)**	$-CH_2C(CH_3)_3$

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 →

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

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

ADDITIONAL RULES

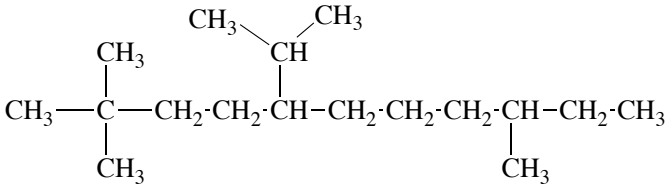
1) If a Molecule Contains Two of the Same Branching Alkyl Groups Use the Prefix di, if Three Use tri, if Four Use tetra, if Five Use penta, if Six Use hexa etc.
Ex. 2,3,4-trimethylhexane

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

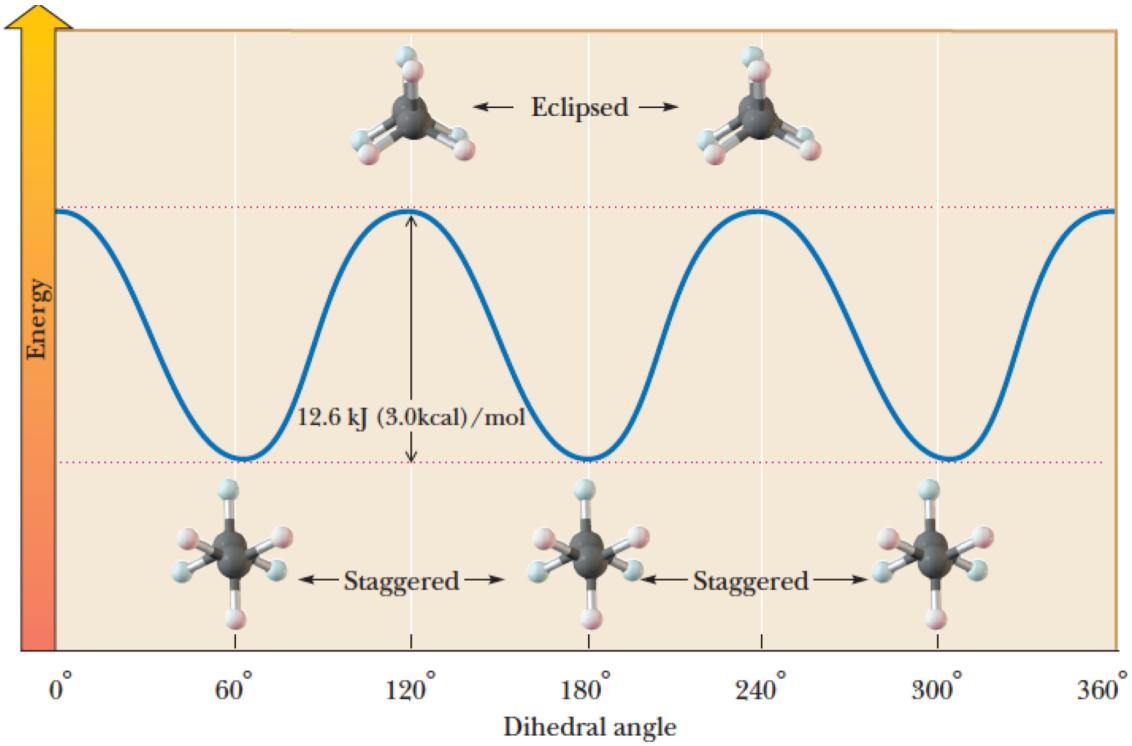
3) If More Than One Branch, List Them in Alphabetical Order, NOT Numerical Order.
Ex. 5-ethyl-3,4-diisopropyl-7-methyldecane

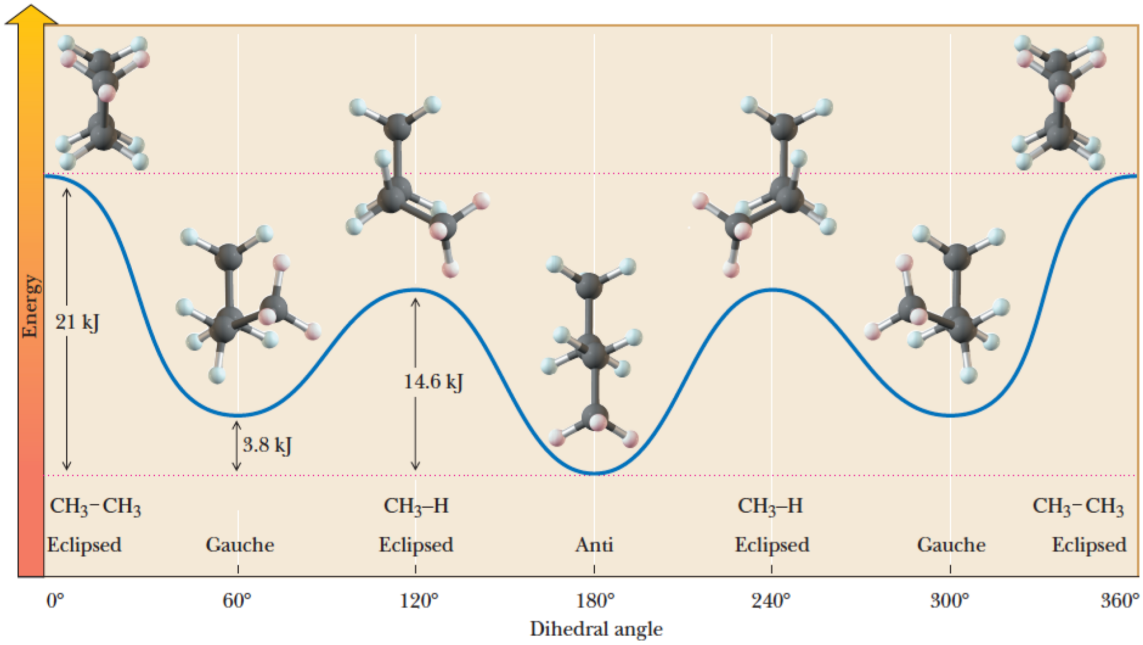
4) DO NOT Include the Italicized Prefixes *n*-, *sec*-, and *tert*- OR the Mulitplying Prefixes di, tri, tetra, etc. When Alphabetizing Simple Substitutents. All Other Prefixes (iso, neo, etc.) are Included When Alphabetizing Simple Substituents. No Need to Argue, I Did Not Invent TheseRules!
Ex. 5-*tert*-butyl-2-methyldecane

Big Old Hairy Example:



5-Isopropyl-2,2,9-trimethylundecane


Eclipsed
Energy
12.6 kJ (3.0kcal)/mol
Staggered
Staggered
0°
60°
120°
180°
240°
300°
360°
Dihedral angle


Energy
21 kJ
3.8 kJ
14.6 kJ
CH3–CH3
Eclipsed
Gauche
CH3–H
Eclipsed
Anti
CH3–H
Eclipsed
Gauche
CH3–CH3
Eclipsed
0°
60°
120°
180°
240°
300°
360°
Dihedral angle