Hydrocarbons – Compounds that contain only Carbon and Hydrogen

Types of hydrocarbons:

Saturated:	Alkanes	only single, covalent C-C and C-H bonds, no rings
	Cycloalkanes	same, but contain rings
Unsaturated:	Alkenes	contain $\geq$ 1 C=C double bond
	Alkynes	contain $\geq$ 1 C≡C triple bond
	Aromatic	contain $\geq$ 1 benzene ring

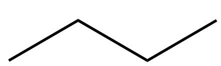
General formula for alkanes is: $\mathbf{C_nH_{2n+2}}$**, n = 1, 2, 3 ...**

All carbons in alkanes are sp^3 hybridized and tetrahedral (bond angles are 109.5°). The suffix "-ane" denotes an alkane. Be familiar with the variety of types of drawings of organic molecules. Know what atom is bonded to what atom. **Dashes/wedges**: recall that **dashed** bonds are going **into** the page, **wedged** bonds are coming **out** of the page, and **lines** are **in** the plane of the page. **Line drawings**: Each intersection or end of a line represents a carbon with the correct number of hydrogen atoms. Carbon always has four bonds in stable species. Hydrogens are often not drawn: be sure you know how many hydrogens are on each carbon: draw them in each time if it helps you. Be familiar with the following nomenclature:

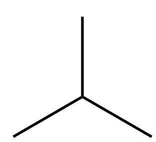
n = 1 methane	n = 5 pentane	n = 8 octane
n = 2 ethane	n = 6 hexane	n = 9 nonane
n = 3 propane	n = 7 heptane	n = 10 decane
n = 4 butane		

Interlude: What do we have to know? Will this be on the exam? Anything could appear on an exam. But you should focus on what you really need to know. Know the drawings and nomenclature (don't bother with index cards, most nomenclature comes just be doing homework). Don't worry about the case studies, etc. Use my emphasis, problem sets, and past exams as guides.

n-butane



boiling point: 0 °C
density: 0.622 g/mL



i-butane
iso-butane
methylpropane
2-methylpropane

boiling point: –12 °C
density: 0.604 g/mL

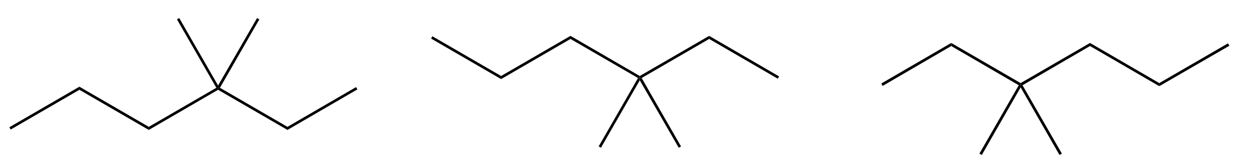
Note that when we get to C_4H_{10} (above) we have isomers. There are several types of isomers. These are constitutional isomers as defined below. They can be distinguished by name as we will go into below. Briefly, the "straight-chained" isomer (left) is called *n*-butane, where the "*n*" stands for "normal" meaning straight-chained. The other isomer (right) is branched at the middle carbon. In this case, the branches are equal, so the common prefix iso (equal; think isosceles triangle). There are a variety of ways to name molecules. Several are given above. Below we will focus on one systematic process for naming (IUPAC). Note the different physical properties of these isomers.

Constitutional (structural) isomers: Molecules with the same formulae but with the atoms arranged in a different order, *i.e.*, their connectivity differs. Constitutional isomers have different chemical and physical properties. The number of isomers increases dramatically with the number of carbon atoms (recall general formula: C_nH_{2n+2}):

N	Total number of isomers
1	1
2	1
3	1
4	2
5	3
6	5
7	9
8	18
9	35
10	75
20	366,319
40	62,491,178,805,831

It is evident that some form of systematic nomenclature is required to handle all of these isomers.

Test: See how quickly you can tell that the compounds below are the same molecule:



There are a number of ways to determine whether or not these are identical: use models, visualize them (move them around in your head), or name them. Visualization is a large part of organic chemistry.

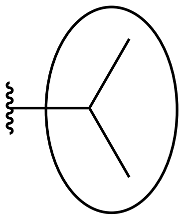
INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC)

IUPAC ALKANE NOMENCLATURE

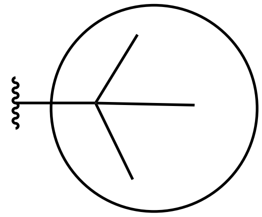
1. Find the longest continuous chain of carbon atoms. This chain determines the parent or base name of the alkane.
2. Number the chain beginning at the end of the chain nearest any branching, thus obtaining the use of lower numbers in the name.
3. Use these numbers to designate the location of the substituent (alkyl) groups whose names are obtained by changing the "-ane" suffix to "-yl".
4. If an alkyl group appears more than once, use the prefixes di, tri, tetra, penta, hexa, (2, 3, 4, 5, 6, respectively) for each type of alkyl group.
5. List the groups in any order, but be sure numbering is correct (IUPAC alphabetizes, but we won't bother with that rule).
6. Numbers are separated from letters by "-"; numbers are separated from numbers by ",".

Normal alkyl groups:	CH_3-	methyl
	CH_3CH_2-	ethyl
	$CH_3CH_2CH_2$-	propyl
	$CH_3CH_2CH_2CH_2$-	butyl

Also know: **isopropyl** and ***t*-butyl** (= *tert*-butyl = tertiary-butyl). Tertiary means "of the third order," in this case, a carbon with three methyl groups attached to it. The circled portions below are isopropyl (left) and *t*-butyl (right). The squiggly line to the left in each drawing represents "the rest of the molecule."

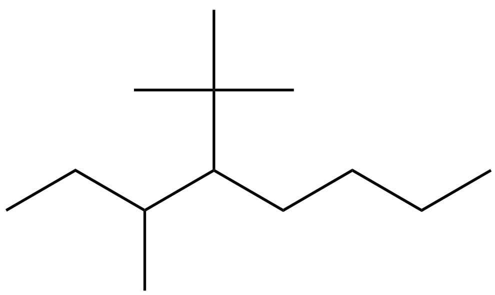


isopropyl

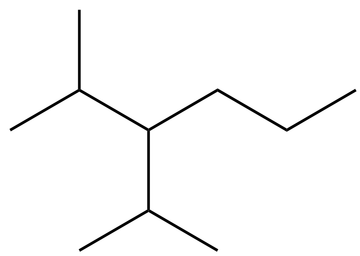


t-butyl

Examples:

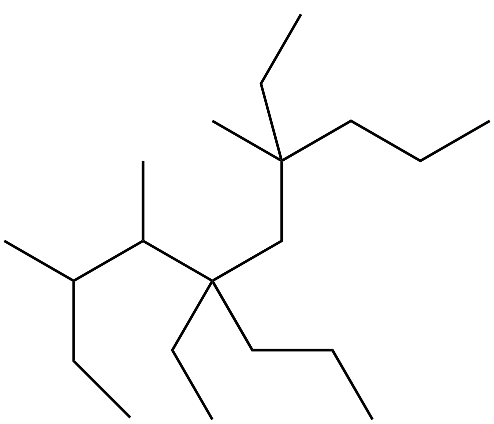


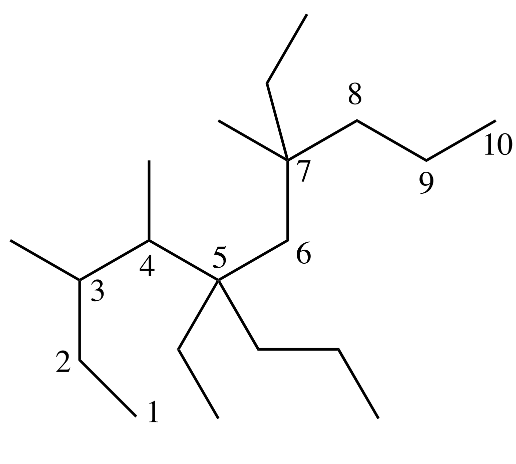
4-*t*-butyl-3-methyloctane



3-isoproply-2-methylhexane

Try naming the compound below without looking at the answer. This is as hard as we will go.

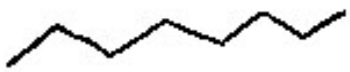




5,7-diethyl-3,4,7-trimethyl-5-propyldecane

For practice, draw and name the isomers below without looking at the answers. **Be sure not to draw any isomers twice.**

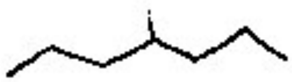
Draw and Name the 18 Constitutional Isomers of C_8H_{18}.



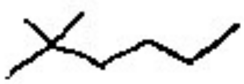
n-octane

2-methylheptane

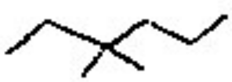
3-methylheptane



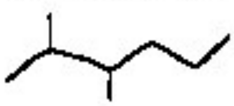
4-methylheptane



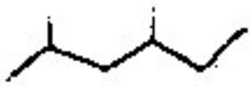
2,2-dimethylhexane



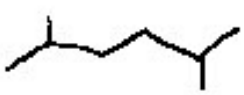
3,3-dimethylhexane



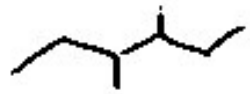
2,3-dimethylhexane



2,4-dimethylhexane



2,5-dimethylhexane



3,4-dimethylhexane

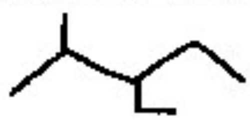
3-ethylhexane

2,2,3-trimethylpentane

2,2,4-trimethylpentane

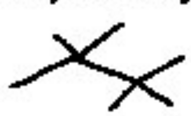
2,3,3-trimethylpentane

2,3,4-trimethylpentane



3-ethyl-2-methylpentane

3-ethyl-3-methylpentane



2,2,3,3-tetramethylbutane

Physical Properties of Hydrocarbons. Hydrocarbons are nonpolar. In general, nonpolar substances are insoluble in H_2O and soluble in nonpolar solvents such as alkanes, CCl_4, benzene, *etc*. "Like dissolves like." e.g., oil and vinegar are immiscible (form separate layers); oil-based paint needs turpentine to wash off, etc. All alkanes, alkenes, alkynes and aromatics are less dense than water—thus, they float on water's surface (think oil/vinegar; oil tanker spills). NaCl will not dissolve in gasoline (alkanes). Generally, boiling point and melting points go up with the molecular weights of compounds due to an increase in the surface area, which allows for more intermolecular interactions. The intermolecular interactions between hydrocarbons are much weaker than between water molecules. This also results in lower density for hydrocarbons compared to water. Finally, hydrocarbons burn easily because the balanced equation upon oxidation yields CO_2 and H_2O, which are highly stable.

$$2C_nH_{2n+2} + (3n+1)O_2 \longrightarrow 2nCO_2 + (2n+2)H_2O + \text{heat}$$

Major Sources of Carbon Compounds

Animal materials – Fats and oils
Vegetable matter – oils, sucrose, starch, cellulose, lignin, carbohydrates
Coal
Natural gas (methane, ethane)
Petroleum
Tar sands, shale
Metal carbonates – limestone ($CaCO_3$)

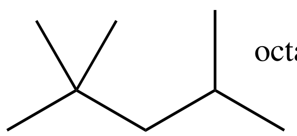
Well over 90% of organic chemical (petrochemical industry) manufacture is based on natural gas and petroleum. Previously it was coal. What is the source of natural gas and petroleum? Prehistoric plant and animal life, predominantly marine microorganisms (plankton) that settled to the bottom of oceans and under pressure was converted over hundreds of thousands of years to a complex hydrocarbon mixture. NONRENEWABLE! The compositions of natural gas and petroleum vary depending on their sources. Natural gas is ~ 80% CH_4 with lesser amounts of higher alkanes. Petroleum is a complex mixture of hydrocarbons up to ~ C_{50}. There > 500 separate compounds, including alkanes, cycloalkanes, alkenes and aromatics.

bp range	No. of carbons	Uses
< 20°	C_1-C_4	Natural gas propane (bottled in steel cylinders; BBQ) butane: lighters heating fuels--much still "flared"
20-70	C_5-C_6	Petroleum ether -- paint thinner, solvents
40-200	C_6-C_{12}	"Straight run" gasoline--low octane rating--not suitable for auto fuel
200-275	C_{12}-C_{15}	Kerosene, jet fuel
250-350	C_{15}-C_{18}	Fuel oil, diesel fuel, cracking stock
	C_{18}-C_{10}	Lubricants, mineral oil (baby oil, cold cream, sun-tan oil, hair oil), vaseline, cracking stock
> 300	C_{21}-C_{40}	Wax (wax paper, candles), grease
	> C_{40}	Asphalt, tar

The structure of a molecule determines, in part, its physical properties. Constitutional isomers have different physical properties even though their molecular formulae are identical.

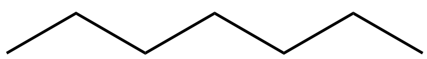
Examples #1. Gasoline octane rating: The best situation for internal-combustion engine is smooth, even burning with burning proceeding out from spark plug at 25-250 ft/sec. Sometimes combustion occurs too rapidly—the result is internal explosion (1000 ft/sec), shock wave, knocking, (pre-ignition). Branched alkanes are better (burn more slowly) than straight-chained.

Octane number of test fuel = % isooctane in a mixture with *n*-heptane that gives the same performance as the fuel being tested.



octane rating assigned: 100

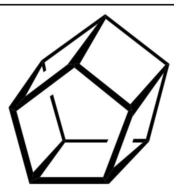
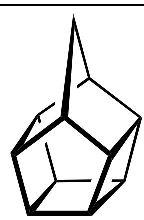
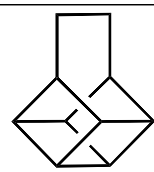
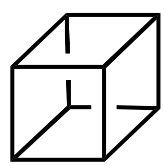
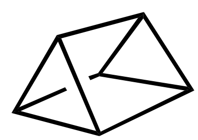
isooctane
2,2,4-trimethylpentane



octane rating assigned: 0

n-heptane

Some funny organic compound names:

 **Housane**	 **Churchane**	 **Basketane**	 **Cubane**	 **Prismane**