Components of Naturally Occurring Petroleum Fluids

(CH-1)

By

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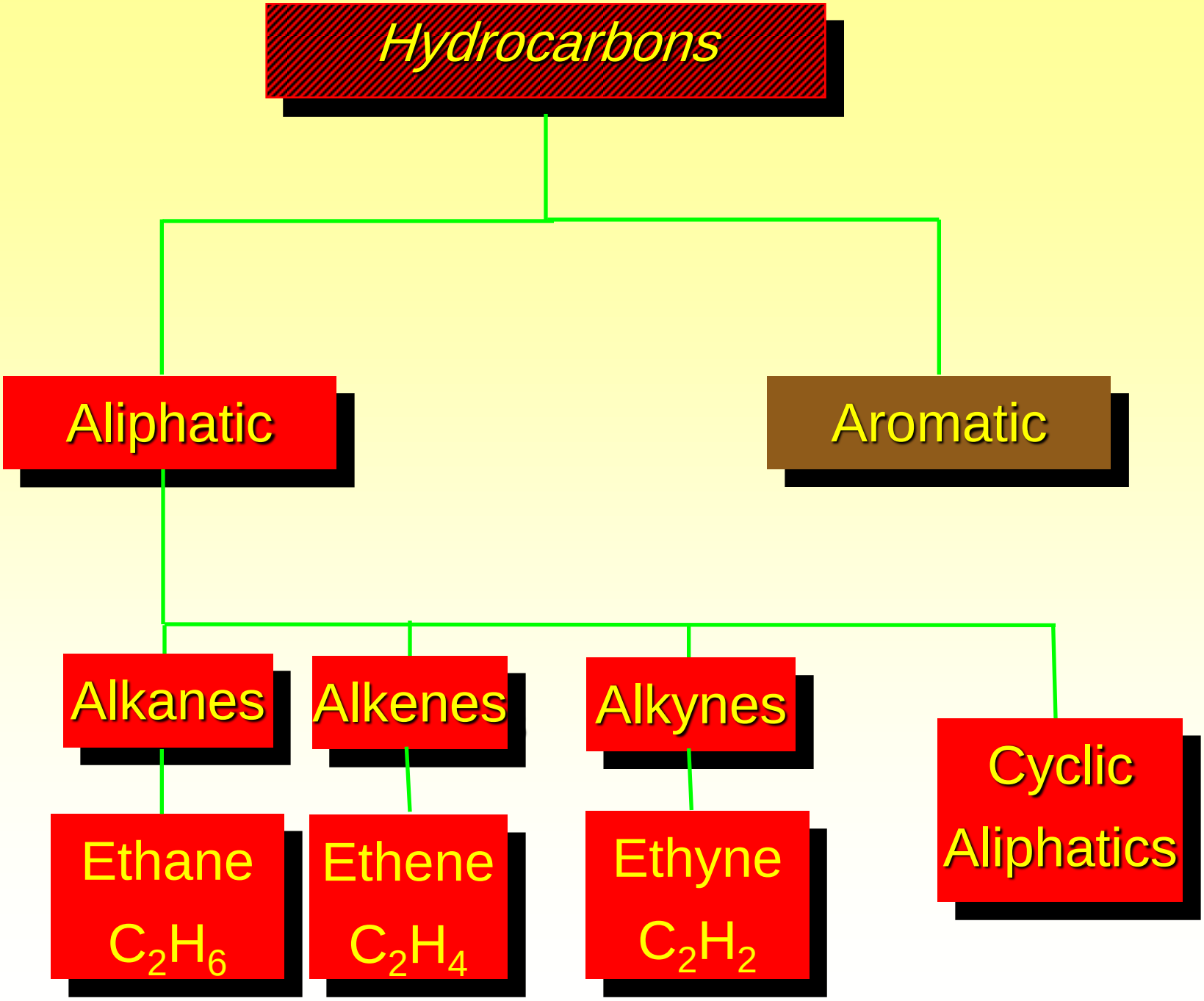
Hydrocarbons

Natural gas	
Hydrocarbon	
Methane	70–98%
Ethane	1–10%
Propane	trace–5%
Butanes	trace–2%
Pentanes	trace–1%
Hexanes	trace–½%
Heptanes +	trace–½%
Nonhydrocarbon	
Nitrogen	trace–15%
Carbon dioxide*	trace–5%
Hydrogen sulfide*	trace–3%
Helium	up to 5%, usually trace or none

*Occasionally natural gases are found which are predominately carbon dioxide or hydrogen sulfide.

Gas from a well which also is producing petroleum liquid	
Hydrocarbon	
Methane	45–92%
Ethane	4–21%
Propane	1–15%
Butanes	½–7%
Pentanes	trace–3%
Hexanes	trace–2%
Heptanes +	none–1½%
Nonhydrocarbon	
Nitrogen	trace–up to 10%
Carbon dioxide	trace–4%
Hydrogen sulfide	none–trace–6%
Helium	none

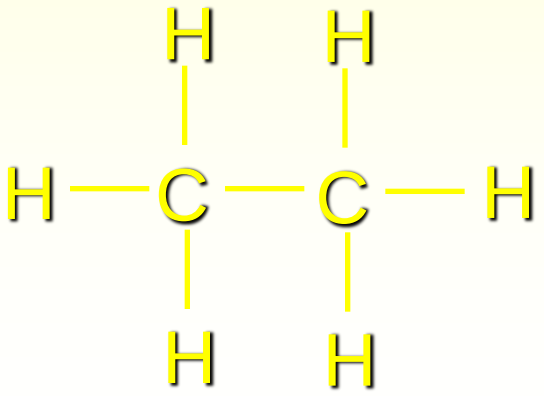

Hydrocarbons
Aliphatic
Aromatic
Alkanes
Alkenes
Alkynes
Cyclic Aliphatics
Ethane C_2H_6
Ethene C_2H_4
Ethyne C_2H_2

Hydrocarbons

Aliphatic

Alkanes

Alkanes are hydrocarbons in which all of the bonds are *single* bonds.

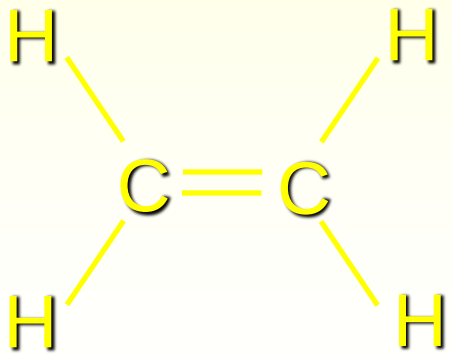


Hydrocarbons

Aliphatic

Alkenes

Alkenes are hydrocarbons that contain a carbon-carbon *double* bond.



Hydrocarbons

Aliphatic

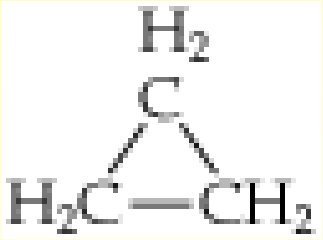
Alkynes are hydrocarbons that contain a carbon-carbon *triple* bond.

Alkynes

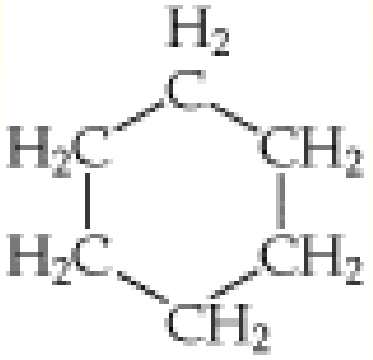
Cycloalkanes

- Carbon atoms that are joined in a ring or circle

- Simplest: Cyclopropane



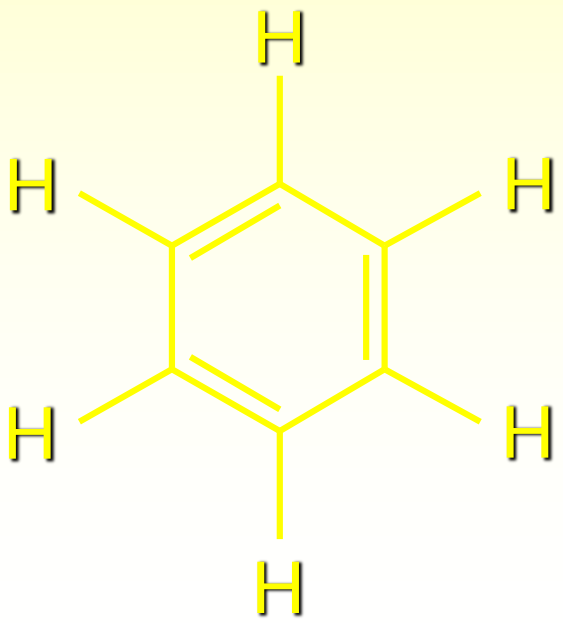
- Another: Cyclohexane



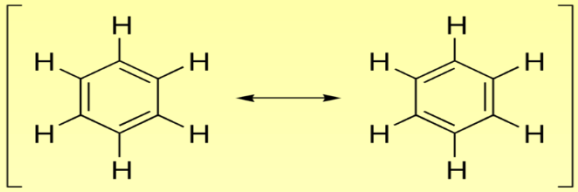
Hydrocarbons

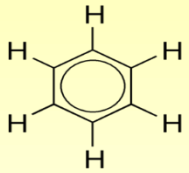
Aromatic

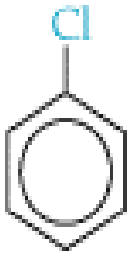
Is a hydrocarbon with alternating double and single bonds between carbon atoms forming rings.



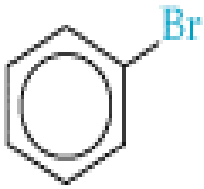
Aromatic



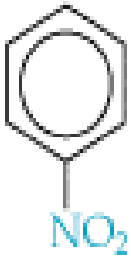




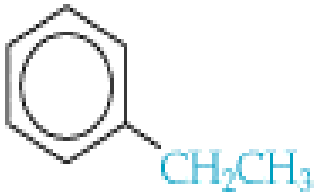
Chlorobenzene



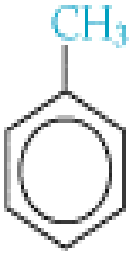
Bromobenzene



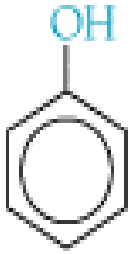
Nitrobenzene



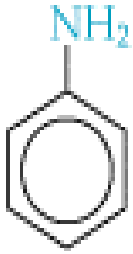
Ethylbenzene



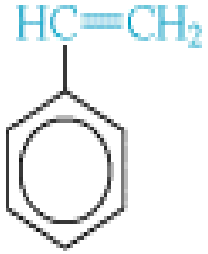
Toluene
(Methylbenzene)



Phenol
(Hydroxybenzene)



Aniline
(Aminobenzene)



Styrene
(Vinylbenzene)

General formula for an alkane

$$C_nH_{2n+2}$$

Examples:

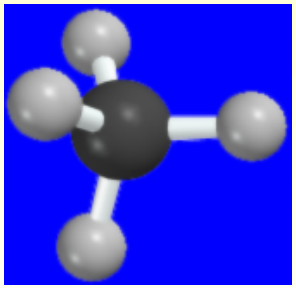
Methane, CH_4

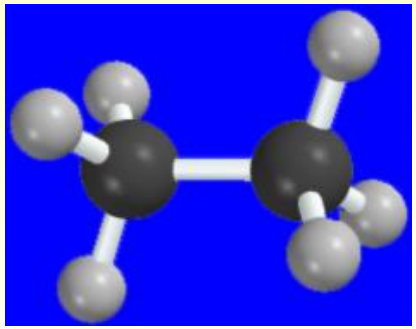
Ethane, C_2H_6

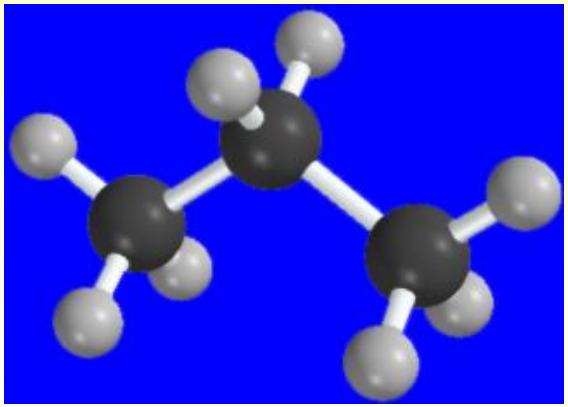
Propane, C_3H_8

The simplest alkanes

Methane (CH_4)	CH_4
Ethane (C_2H_6)	CH_3CH_3
Propane (C_3H_8)	$CH_3CH_2CH_3$







bp -160°C bp -89°C bp -42°C

No isomers possible for C1, C2, C_3 hydrocarbons

Isomers

Are molecules with the same molecular formula but different chemical structures

Isomeric Alkanes:

The Butanes

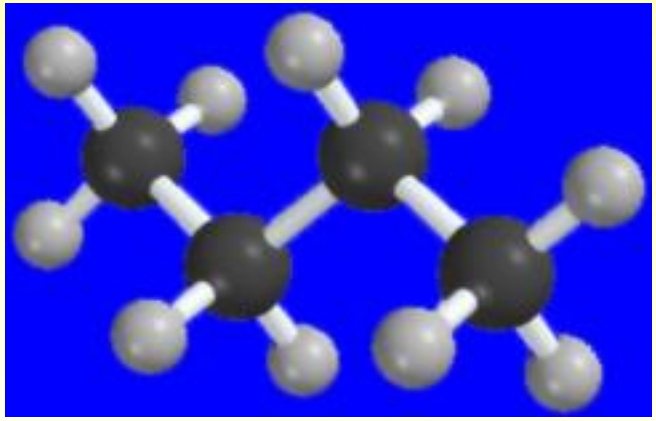
C_4H_{10}

General formula for any butane

C_4H_{10}

n-Butane

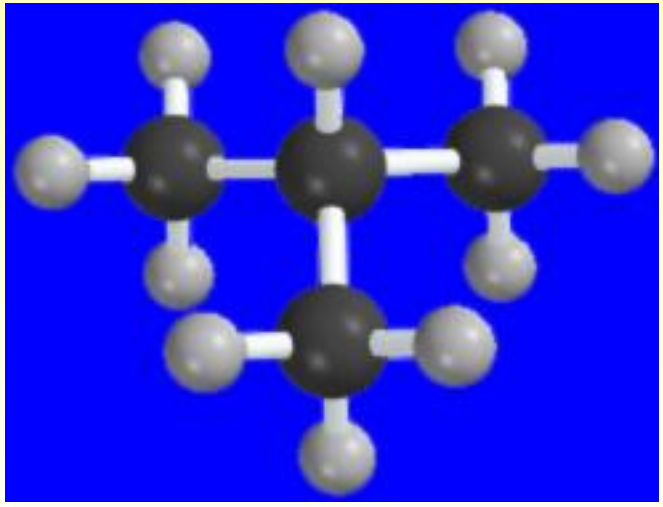
$CH_3CH_2CH_2CH_3$



bp -0.4°C

Isobutane

$(CH_3)_3CH$



bp -10.2°C

Higher *n*-Alkanes
Pentane (C_5H_{12}) and Beyond

C_nH_{2n+2}

$n > 4$

$CH_3CH_2CH_2CH_2CH_3$

n-Pentane

C_nH_{2n+2}

$n > 4$

$CH_3CH_2CH_2CH_2CH_2CH_3$

n-Hexane

$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

n-Heptane

The C_5H_{12} Isomers

C_5H_{12}

$CH_3CH_2CH_2CH_2CH_3$

n-Pentane

$(CH_3)_2CHCH_2CH_3$

Isopentane

How many isomers?

The number of isomeric alkanes increases as the number of carbons increase.

There is no simple way to predict how many isomers there are for a particular molecular formula.

Number of Constitutionally Isomeric Alkanes

CH_4	1
C_2H_6	1
C_3H_8	1
C_4H_{10}	2
C_5H_{12}	3
C_6H_{14}	5
C_7H_{16}	9

Number of Constitutionally Isomeric Alkanes

CH_4	1	C_8H_{18}	18
C_2H_6	1	C_9H_{20}	35
C_3H_8	1	$C_{10}H_{22}$	75
C_4H_{10}	2	$C_{15}H_{32}$	4,347
C_5H_{12}	3	$C_{20}H_{42}$	366,319
C_6H_{14}	5	$C_{40}H_{82}$	62,491,178,805,831
C_7H_{16}	9		

Physical Properties of Alkanes

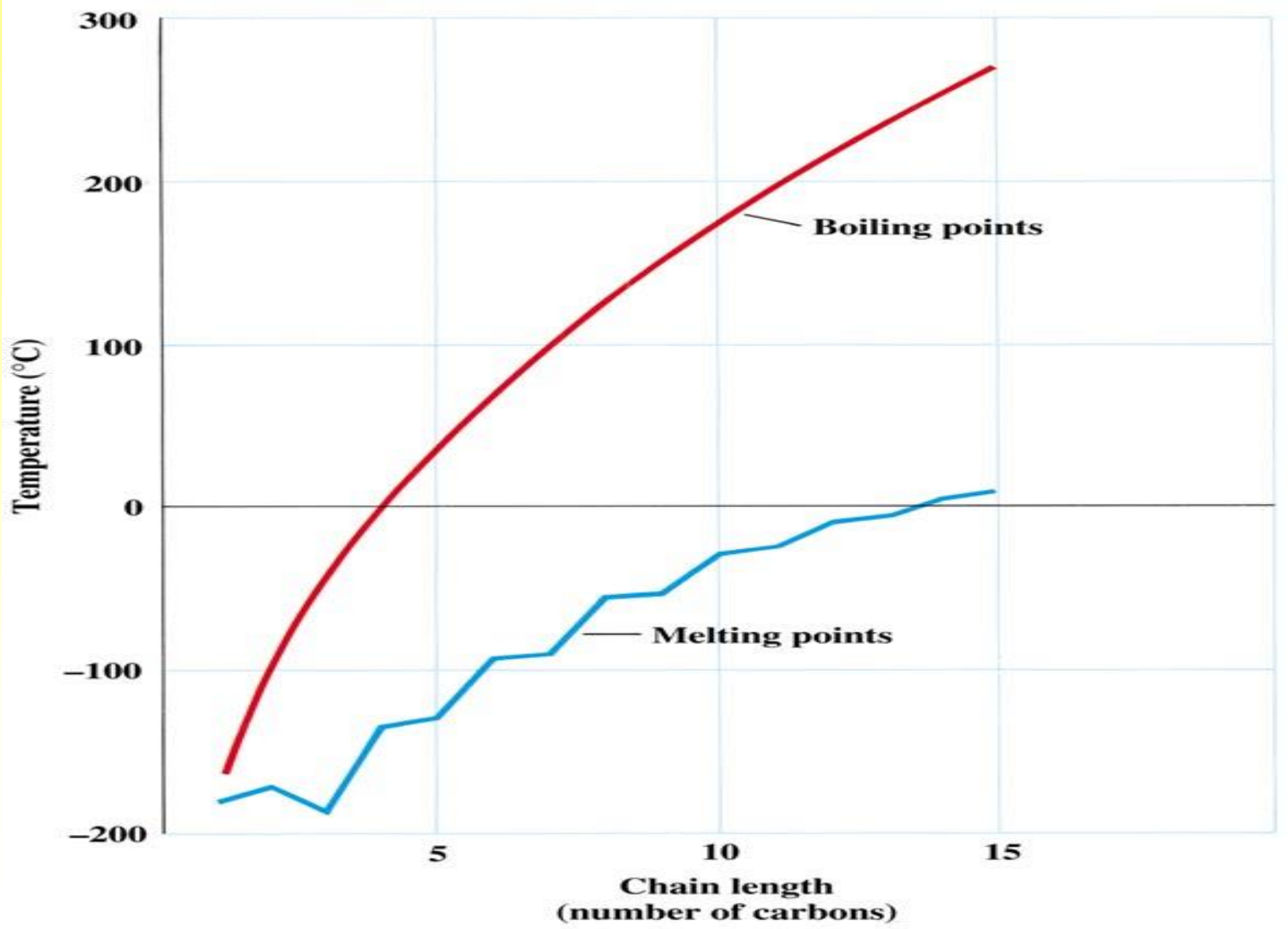
Boiling Points

Increase with increasing number of carbons?

more atoms, more electrons, ….

Decrease with chain branching?

branched molecules are more compact with smaller surface area—fewer points of contact with other molecules



Boiling Points

Increase with increasing number of carbons

more atoms, more electrons, …..

Heptane	Octane	Nonane
bp 98°C	bp 125°C	bp 150°C

Boiling Points

Decrease with chain branching

branched molecules are more compact with smaller surface area—fewer points of contact with other molecules

Octane: bp 125°C

2-Methylheptane: bp 118°C

2,2,3,3-Tetramethylbutane: bp 107°C

IUPAC Nomenclature

IUPAC Rules

International Union of Pure and Applied Chemistry

1. Name the longest chain in the parent compound. End in –ane. (Root name)
   - Number each carbon

2. Note the alkyl groups attached.

3. Number the carbon that the group is attached to.
   - Must use the lowest number possible.

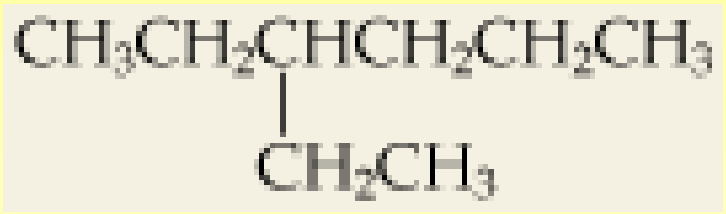
IUPAC Rules

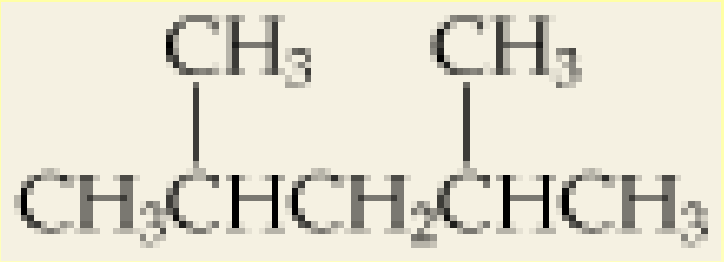
4. Use prefixes to indicate the amount of attached groups.

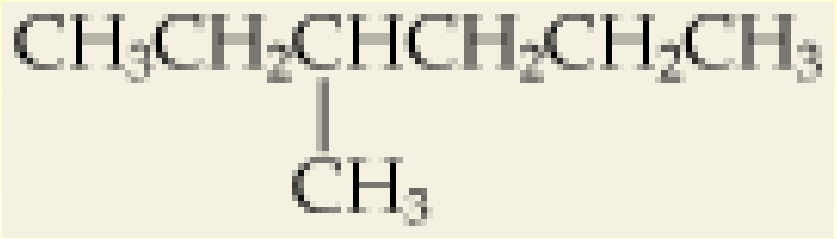
5. If there are more than two or more different substituents, list them in alphabetical order. If at equal points, lower alphabetical order given lowest number.

6. Prefixes not included in alphabetizing

Name each of the following

A. 

B. 

C. 

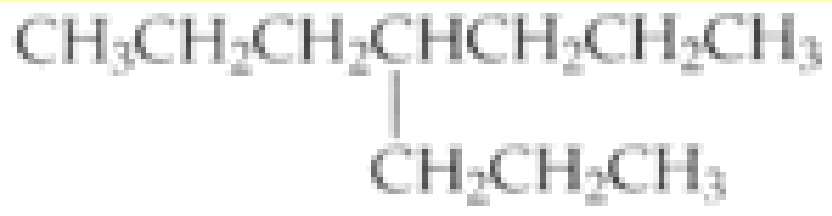
Answers

A. 3-ethylhexane
B. 2,4-dimethylpentane
C. 3-methylhexane

Draw the structural formulas for each of the following

1. 4-propylheptane
2. 3-ethyl-2-methylpentane

Answers

- 1 
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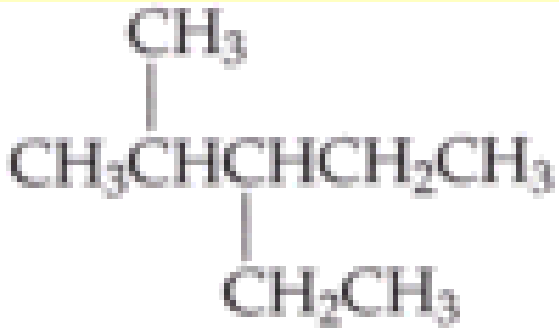
CH2CH2CH3
- 2 
CH3
CH3CHCHCH2CH3
CH2CH3

Q