



Components of Naturally Occurring Petroleum Fluids

(CH-1)

By

Dr. Mohammed A. Khamis

26-1-2016

Hydrocarbons

Natural gas

Hydrocarbon

Methane	70–98%
Ethane	1–10%
Propane	trace–5%
Butanes	trace–2%
Pentanes	trace–1%
Hexanes	trace– $\frac{1}{2}$ %
Heptanes +	trace– $\frac{1}{2}$ %

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	$\frac{1}{2}$ –7%
Pentanes	trace–3%
Hexanes	trace–2%
Heptanes +	none– $1\frac{1}{2}$ %

Nonhydrocarbon

Nitrogen	trace–up to 10%
Carbon dioxide	trace–4%
Hydrogen sulfide	none–trace–6%
Helium	none

Hydrocarbons

```
graph TD; A[Hydrocarbons] --> B[Aliphatic]; A --> C[Aromatic]; B --> D[Alkanes]; B --> E[Alkenes]; B --> F[Alkynes]; B --> G[Cyclic Aliphatics]; D --> H["Ethane<br/>C2H6"]; E --> I["Ethene<br/>C2H4"]; F --> J["Ethyne<br/>C2H2"];
```

Aliphatic

Aromatic

Alkanes

Alkenes

Alkynes

Cyclic
Aliphatics

Ethane

C_2H_6

Ethene

C_2H_4

Ethyne

C_2H_2

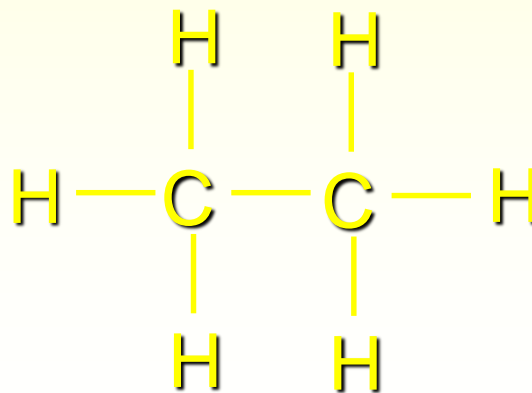
Hydrocarbons

```
graph TD; A[Hydrocarbons] --> B[Aliphatic]; B --> C[Alkanes]
```

Aliphatic

Alkanes

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



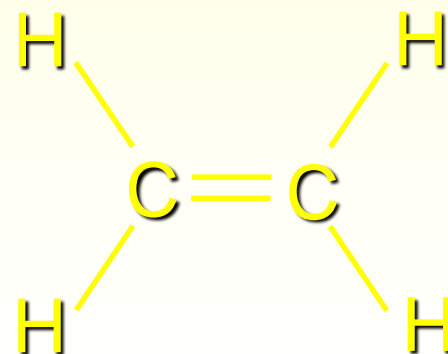
Hydrocarbons

```
graph TD; A[Hydrocarbons] --> B[Aliphatic]; A --> C[Aromatic]; B --> D[Alkenes]; B --> E[Alkynes]; B --> F[Alkanes]; B --> G[Alkynes];
```

Aliphatic

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

Alkenes



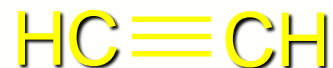
Hydrocarbons

```
graph TD; A[Hydrocarbons] --> B[Aliphatic]; A --> C[Alkynes]; B --> D[Alkynes]; C --- E[Alkynes are hydrocarbons that contain a carbon-carbon triple bond.]; D --- F[HC≡CH];
```

Aliphatic

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

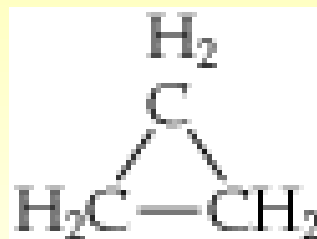
Alkynes



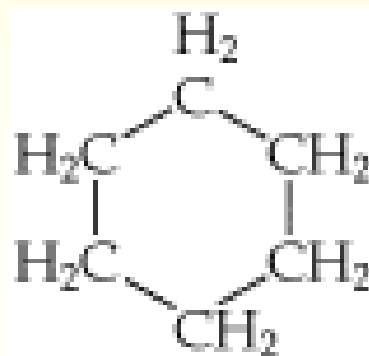
Cycloalkanes

- Carbon atoms that are joined in a ring or circle

- Simplest: Cyclopropane



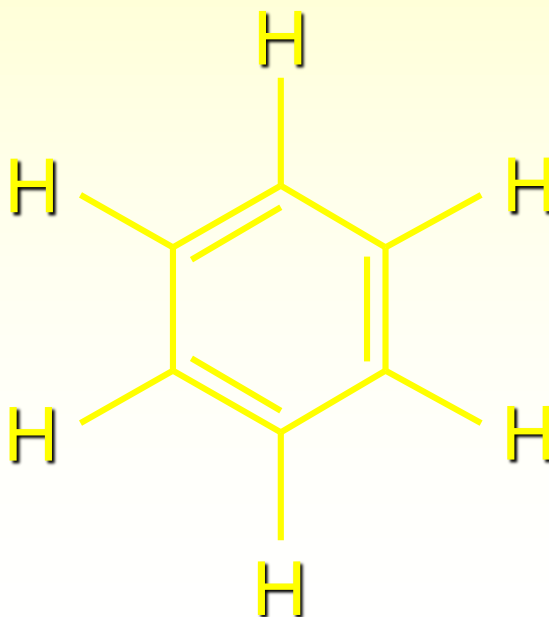
- Another: Cyclohexane



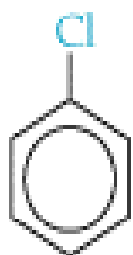
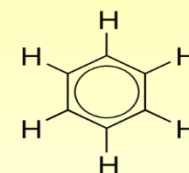
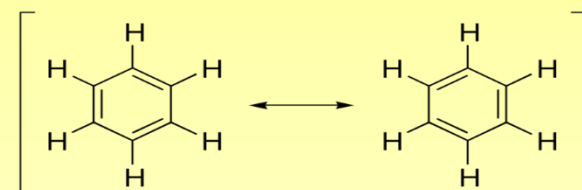
Hydrocarbons

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

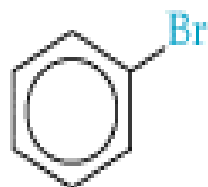
Aromatic



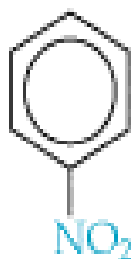
Aromatic



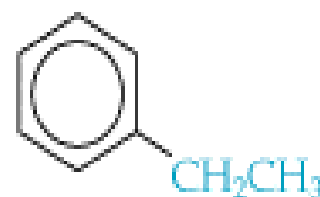
Chlorobenzene



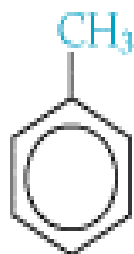
Bromobenzene



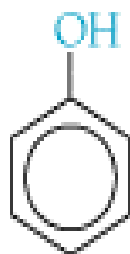
Nitrobenzene



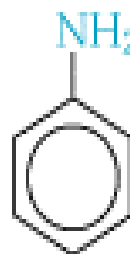
Ethylbenzene



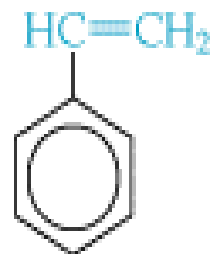
Toluene
(Methylbenzene)



Phenol
(Hydroxybenzene)



Aniline
(Aminobenzene)



Styrene
(Vinylbenzene)

General formula for an alkane



Examples:

Methane, CH_4

Ethane, C_2H_6

Propane, C_3H_8

The simplest alkanes

Methane (CH_4)

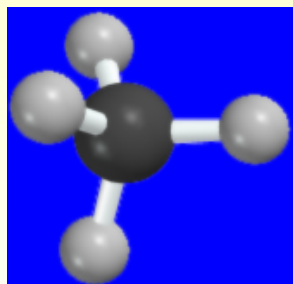
CH_4

Ethane (C_2H_6)

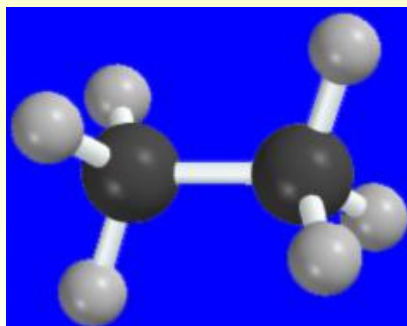
CH_3CH_3

Propane (C_3H_8)

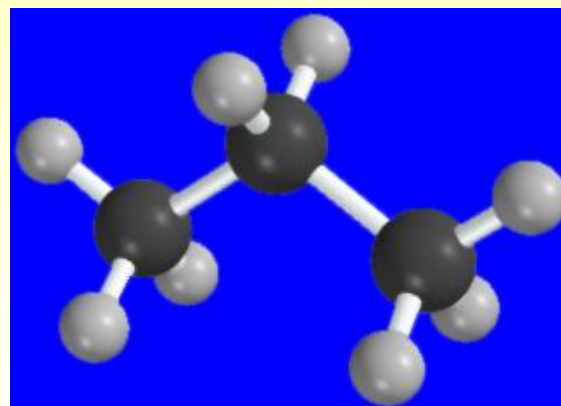
$\text{CH}_3\text{CH}_2\text{CH}_3$



bp -160°C



bp -89°C



bp -42°C

No **isomers** possible for **C1**, **C2**, **C₃** hydrocarbons

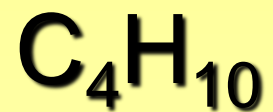
Isomers

Are molecules with the same molecular formula but different chemical structures

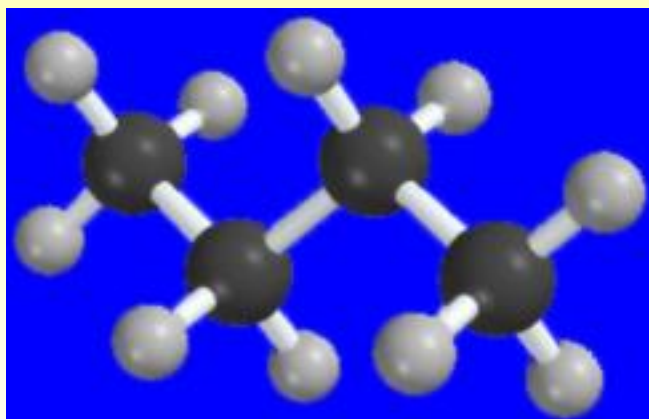
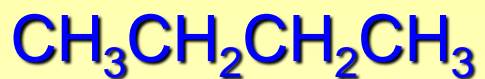
Isomeric Alkanes:
The Butanes



General formula for any butane

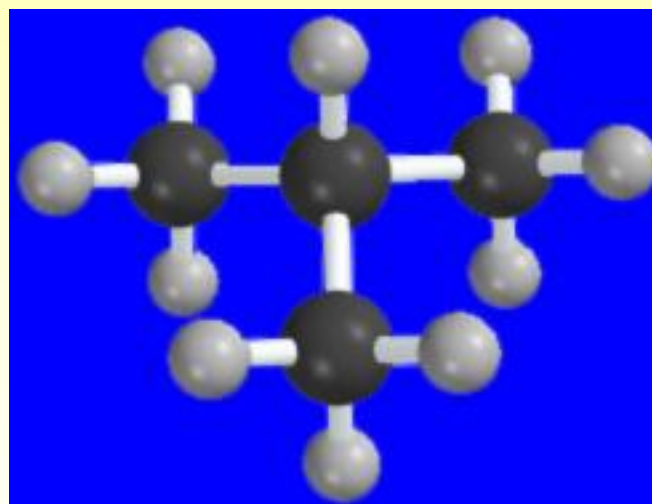
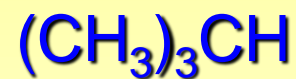


n-Butane



bp -0.4°C

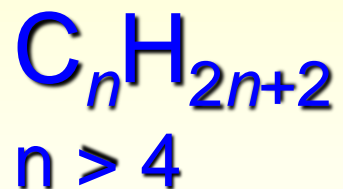
Isobutane



bp -10.2°C

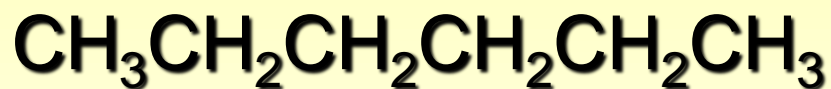
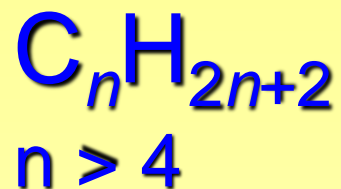
Higher *n*-Alkanes

Pentane (C₅H₁₂) and Beyond





n-Pentane

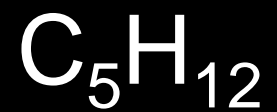


n-Hexane

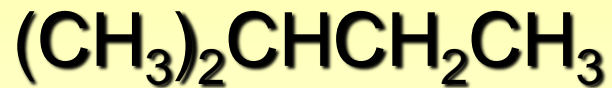
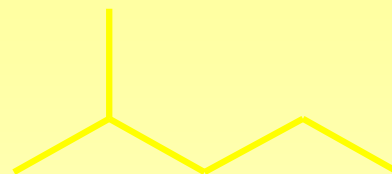


n-Heptane

The C₅H₁₂ Isomers



n-Pentane



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	$\text{C}_{10}\text{H}_{22}$	75
C_4H_{10}	2	$\text{C}_{15}\text{H}_{32}$	4,347
C_5H_{12}	3	$\text{C}_{20}\text{H}_{42}$	366,319
C_6H_{14}	5	$\text{C}_{40}\text{H}_{82}$	62,491,178,805,831
C_7H_{16}	9		

Physical Properties of Alkanes

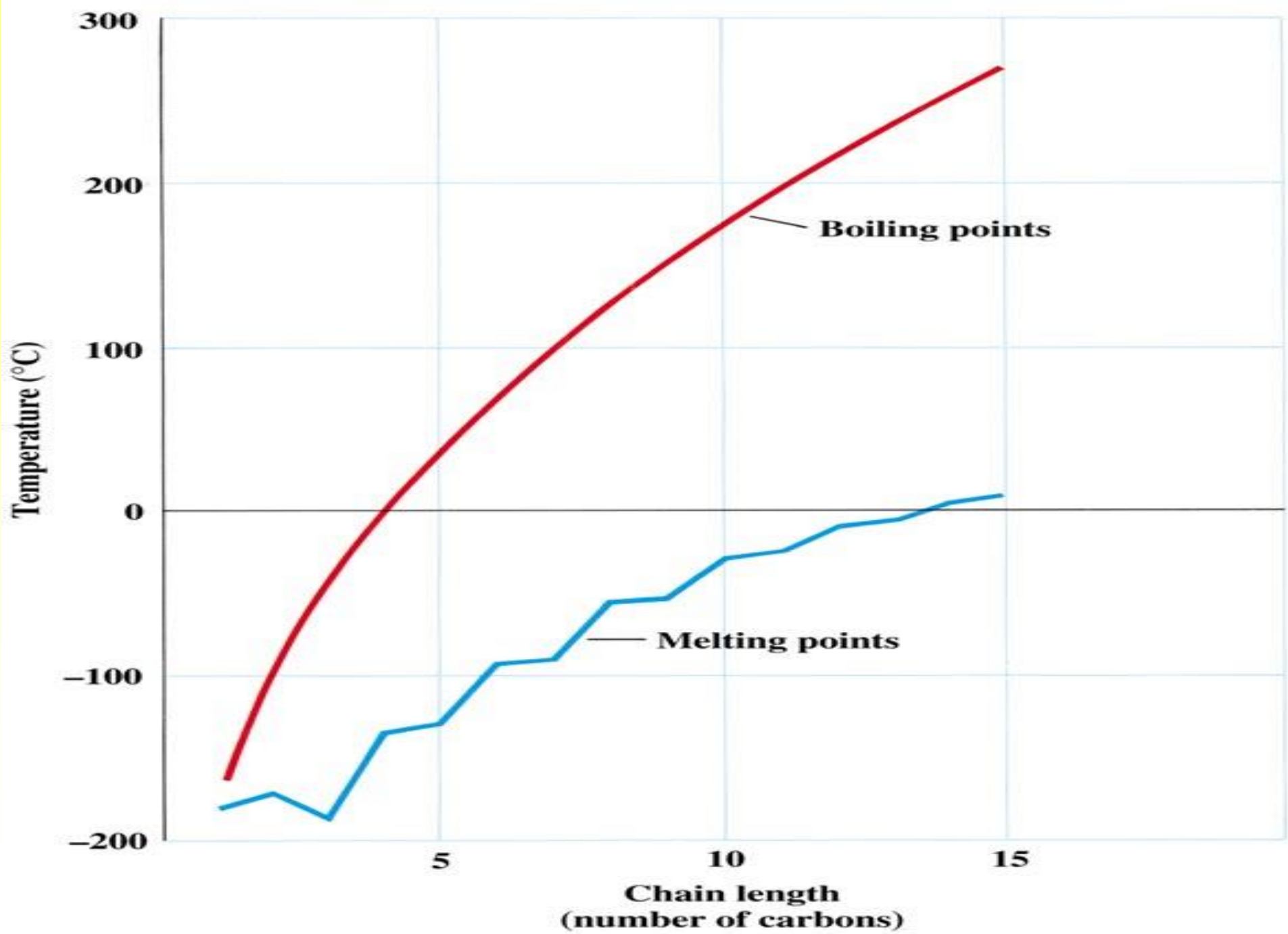
Boiling Points

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
bp 98°C



Octane
bp 125°C



Nonane
bp 150°C

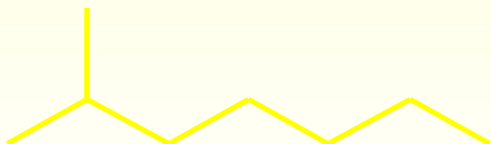
Boiling Points

Decrease with chain branching

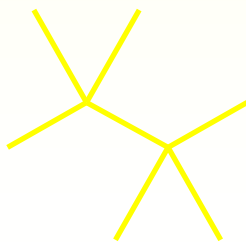
branched molecules are more compact with smaller surface area—fewer points of contact with other molecules



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

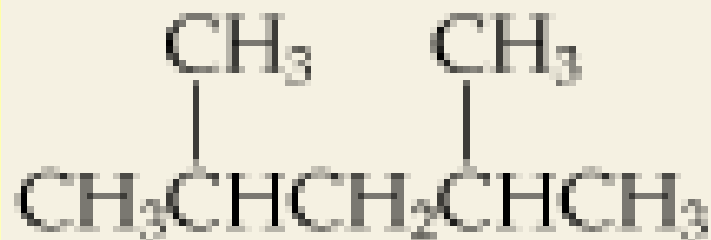
4. Use prefixes to indicate the amount of attached groups.
5. If there are more than two or more different substituents, list them in alphabetical order. If at equal points, lower alphabetical order given lowest number.
6. Prefixes not included in alphabetizing

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

