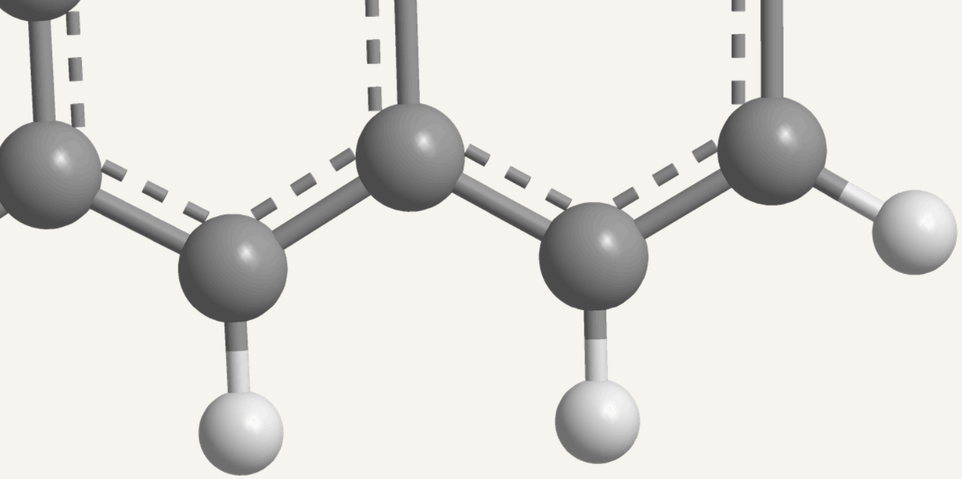
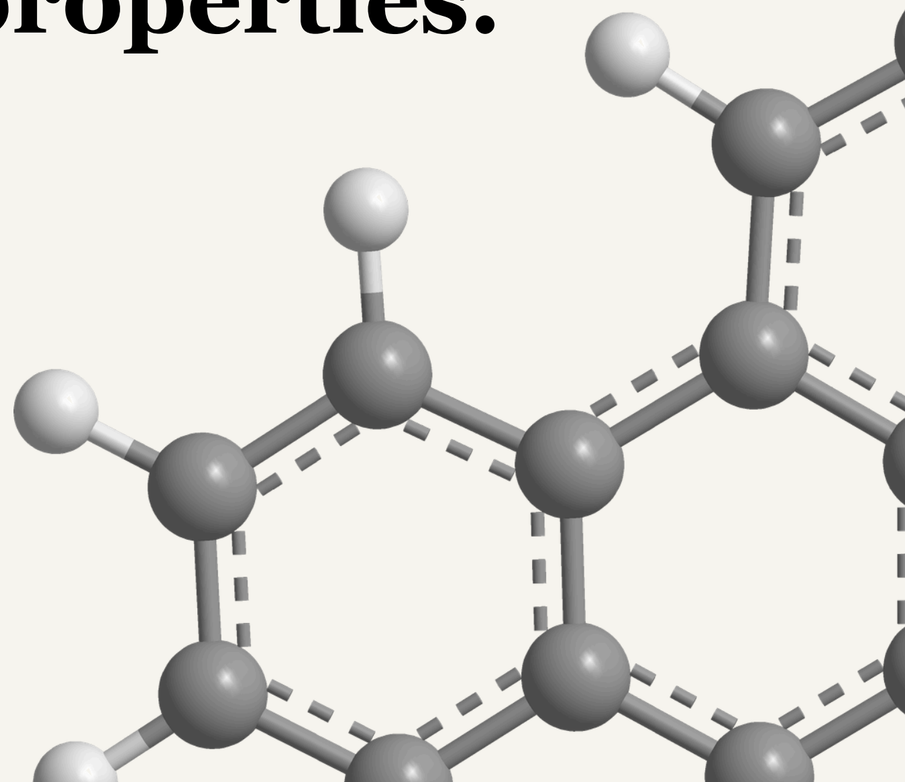


Lecture 6

Alkanes: isomerism, nomenclature, extraction and chemical properties.



Lecture: PhD, acc. professor: Kudaibergenova B.M

Aim and objectives

Aim: study structure, isomerism, nomenclature, preparation and chemical properties of alkanes and their importance in chemistry and industry

1. Define alkanes and their general formula
2. Structure and classification
3. Structural isomerism
4. IUPAC nomenclature
5. Physical properties
6. Preparation methods
7. Main chemical reactions
8. Industrial applications

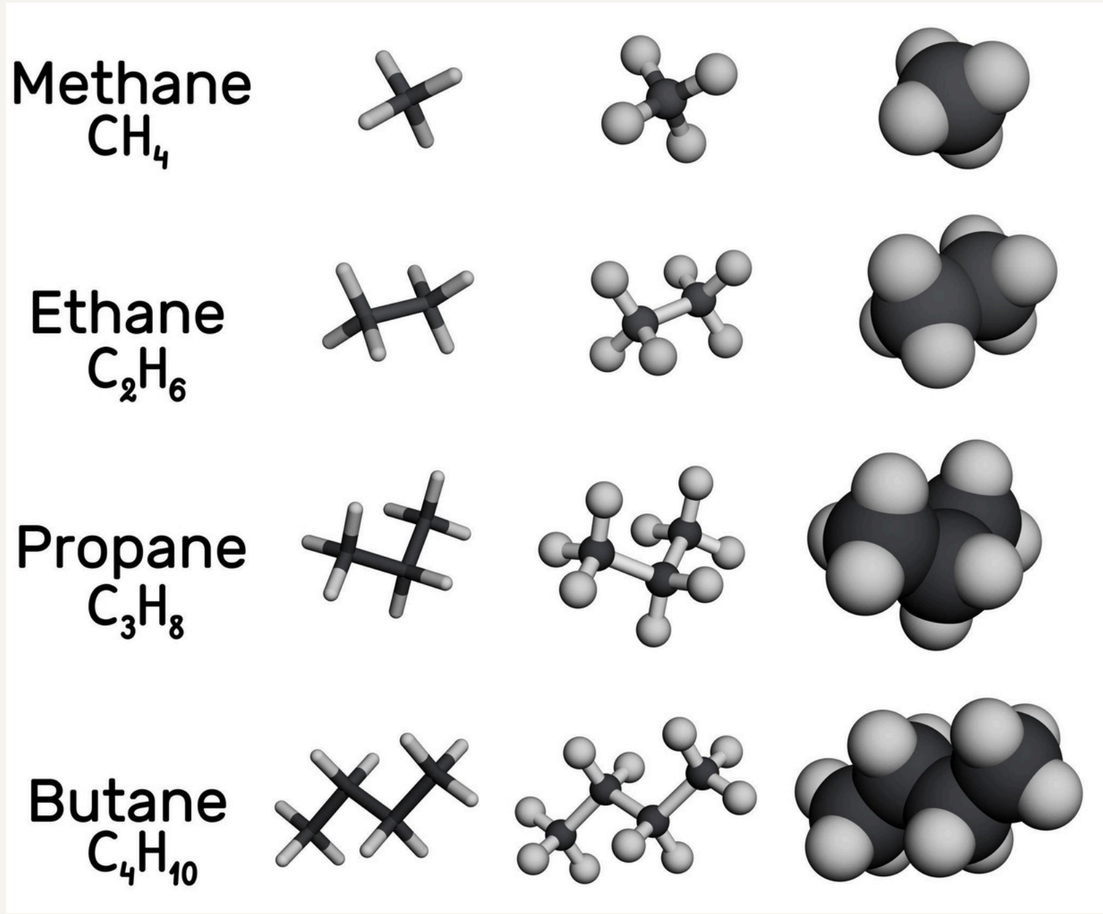
What are alkanes?

Alkanes are a class of saturated hydrocarbons composed exclusively of carbon and hydrogen atoms. They contain only single covalent bonds between carbon atoms and between carbon and hydrogen atoms. Because they do not contain carbon–carbon double or triple bonds, alkanes are classified as saturated organic compounds.

$$C_nH_{2n+2}$$

General formula

- **Saturated acyclic hydrocarbons**
- **Only C–C and C–H single bonds**
- **sp^3 carbon, bond angle ≈ 109.5°**
- **Relatively unreactive**



Homologous series

Each member differs from the previous by $–CH_2–$

A homologous series is a group of organic compounds that have the same general formula, similar chemical properties, and a gradual change in physical properties.Alkanes form a homologous series in which each successive compound differs from the previous one by a methylene group ($–CH_2–$).

C atoms	**Alkane**	**Formula**
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}

Structure and bonding

The molecular structure of alkanes is determined by the bonding properties of carbon atoms. Each carbon atom forms four sigma bonds through sp^3 hybrid orbitals.

Important structural properties:

1. Sigma bonds

All bonds in alkanes are sigma (σ) bonds. Sigma bonds are formed through direct orbital overlap along the line connecting two nuclei.

2. Tetrahedral geometry

The four bonds around an sp^3-hybridized carbon atom are arranged approximately 109.5° apart.

3. Carbon–carbon single bonds

The C–C bond in alkanes is formed by the overlap of two sp^3 orbitals.

4. Carbon–hydrogen bonds

The C–H bond is formed by the overlap of a carbon sp^3 orbital with a hydrogen 1s orbital.

5. Free rotation

Rotation around carbon–carbon single bonds produces different spatial arrangements known as conformations.

- sp^3 carbon forms four σ bonds
- C–C and C–H bonds are σ bonds
- Tetrahedral angle ≈ 109.5°
- Rotation about C–C gives conformations

$$sp^3 + sp^3 \rightarrow \sigma(C–C)$$

$$sp^3 + 1s \rightarrow \sigma(C–H)$$

Isomerism of alkanes

Same molecular formula, different structure. Alkanes show chain and conformational isomerism; some branched ones also show optical isomerism.

Both are C_4H_{10}

Isomerism is the phenomenon in which two or more compounds have the same molecular formula but different structural arrangements or spatial configurations.
In alkanes, the most characteristic type of constitutional isomerism is chain isomerism, also called skeletal isomerism.

n-Butane

$CH_3–CH_2–CH_2–CH_3$

Straight chain

2-Methylpropane

$(CH_3)_3CH$

Branched chain

Isomers of pentane (C_5H_{12})

Pentane has the molecular formula C_5H_{12} and exists as three different structural isomers. These isomers contain the same number of carbon and hydrogen atoms but have different carbon skeletons.

More branching → lower boiling point

n-Pentane

Straight chain

36 °C

2-Methylbutane

Branched

28 °C

2,2-Dimethylpropane

Highly branched

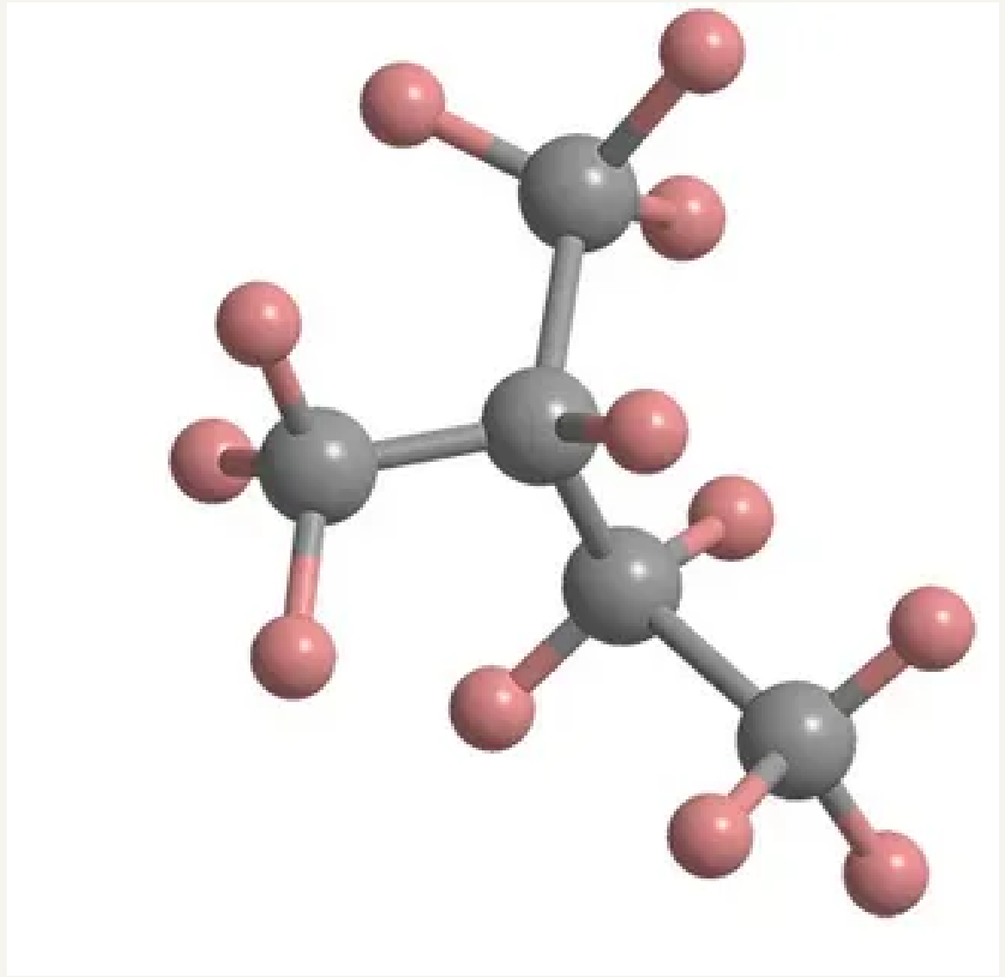
9.5 °C

IUPAC nomenclature

$CH_3–CH(CH_3)–CH_2–CH_3$

2-Methylbutane

1. Find the longest carbon chain
2. Name the parent alkane
3. Number for lowest locants
4. Name the substituents
5. Use di-, tri-, tetra- for repeats
6. List substituents alphabetically



Physical properties

The physical properties of alkanes are mainly determined by molecular mass, carbon-chain length, and molecular branching. Because alkanes are nonpolar molecules, their intermolecular attractions are dominated by London dispersion forces.

- Nonpolar; insoluble in water
- Soluble in nonpolar solvents
- Less dense than water
- Boiling point rises with mass
- Branching lowers boiling point

Carbon atoms	State
C_1–C_4	Gases
C_5–C_{17}	Liquids
C_{18} and up	Waxy solids

Natural sources and extraction

Alkanes are found naturally in large quantities in petroleum deposits and natural gas reservoirs.
These substances represent major sources of hydrocarbon fuels and chemical raw materials.

1. Natural gas

Natural gas consists mainly of methane, although it may also contain ethane, propane, butane, carbon dioxide, nitrogen, and other gases.
Methane is widely used for heating, electricity generation, and industrial chemical synthesis.

2. Crude petroleum

Crude petroleum is a complex mixture of hydrocarbons, including alkanes, cycloalkanes, aromatic compounds, and other organic substances.
Different hydrocarbons are separated according to their boiling-point ranges.

3. Associated petroleum gas

Associated gas is produced together with crude oil. It contains light hydrocarbons that can be recovered and used as fuels or chemical feedstocks.

Natural gas	Petroleum	Associated gas
Mainly methane	Alkanes, cycloalkanes, aromatics	Methane to butane

Crude oil and gas → processing → fractional distillation → hydrocarbon fractions

Laboratory preparation

Importance:
These reactions demonstrate how saturated hydrocarbons can be synthesized from different classes of organic compounds.

Although alkanes are mainly obtained from natural sources, several chemical methods are used to prepare them in laboratories.

Hydrogenation of alkenes

$CH_2{=}CH_2 + H_2 \rightarrow (Ni)\ CH_3{-}CH_3$

Wurtz reaction

$2CH_3Br + 2Na \rightarrow (\text{dry ether})\ C_2H_6 + 2NaBr$

Soda-lime decarboxylation

$CH_3COONa + NaOH \rightarrow (CaO, \Delta)\ CH_4 + Na_2CO_3$

Grignard hydrolysis

$CH_3MgBr + H_2O \rightarrow CH_4 + MgBrOH$

Chemical properties

Strong σ bonds and no polar groups make alkanes unreactive, but they still react under suitable conditions.

Combustion

Oxidation by oxygen

Pyrolysis

Thermal decomposition

Cracking

Breaking C–C bonds

Dehydrogenation

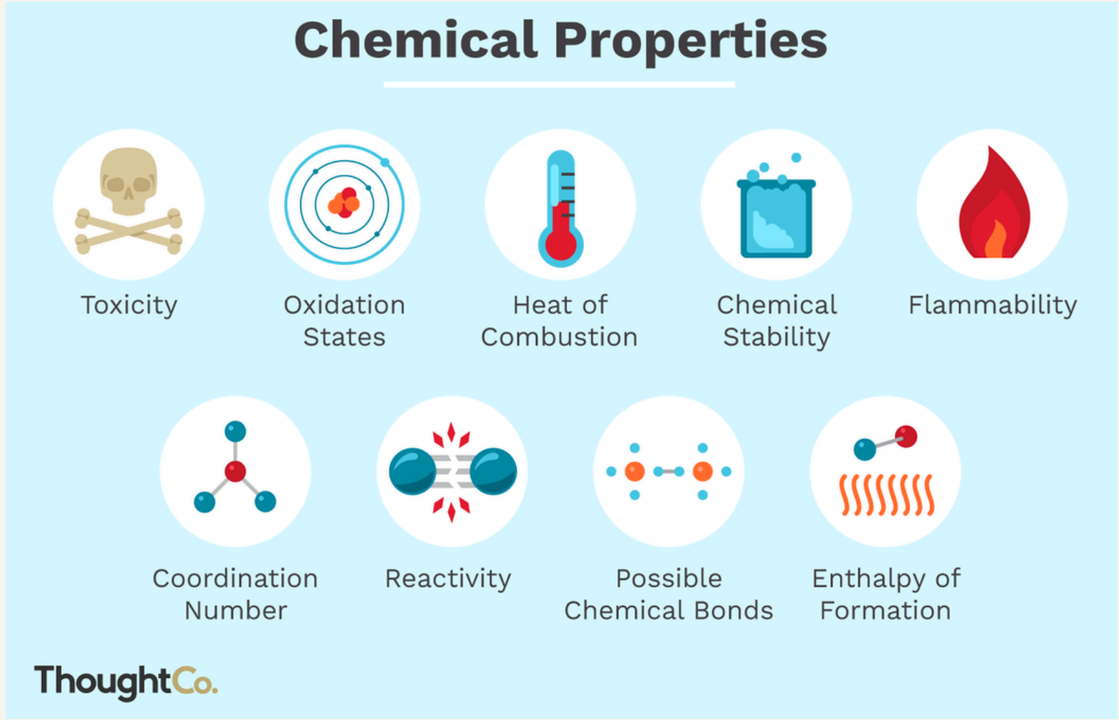
Removal of hydrogen

Halogenation

Radical substitution

Isomerization

Skeleton rearrangement



Combustion

Complete

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + Q$

$2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O + Q$

$C_nH_{2n+2} + (3n+1)/2\ O_2 \rightarrow nCO_2 + (n+1)H_2O$

Incomplete

$2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O$

CO or soot forms when oxygen is short

Uses: heating, electricity, vehicle fuel, industry



Halogenation

$CH_4 + Cl_2 \rightarrow (hv)\ CH_3Cl + HCl$

Further chlorination gives CH_2Cl_2, $CHCl_3$, CCl_4

Initiation

$Cl_2 \rightarrow 2Cl\bullet$

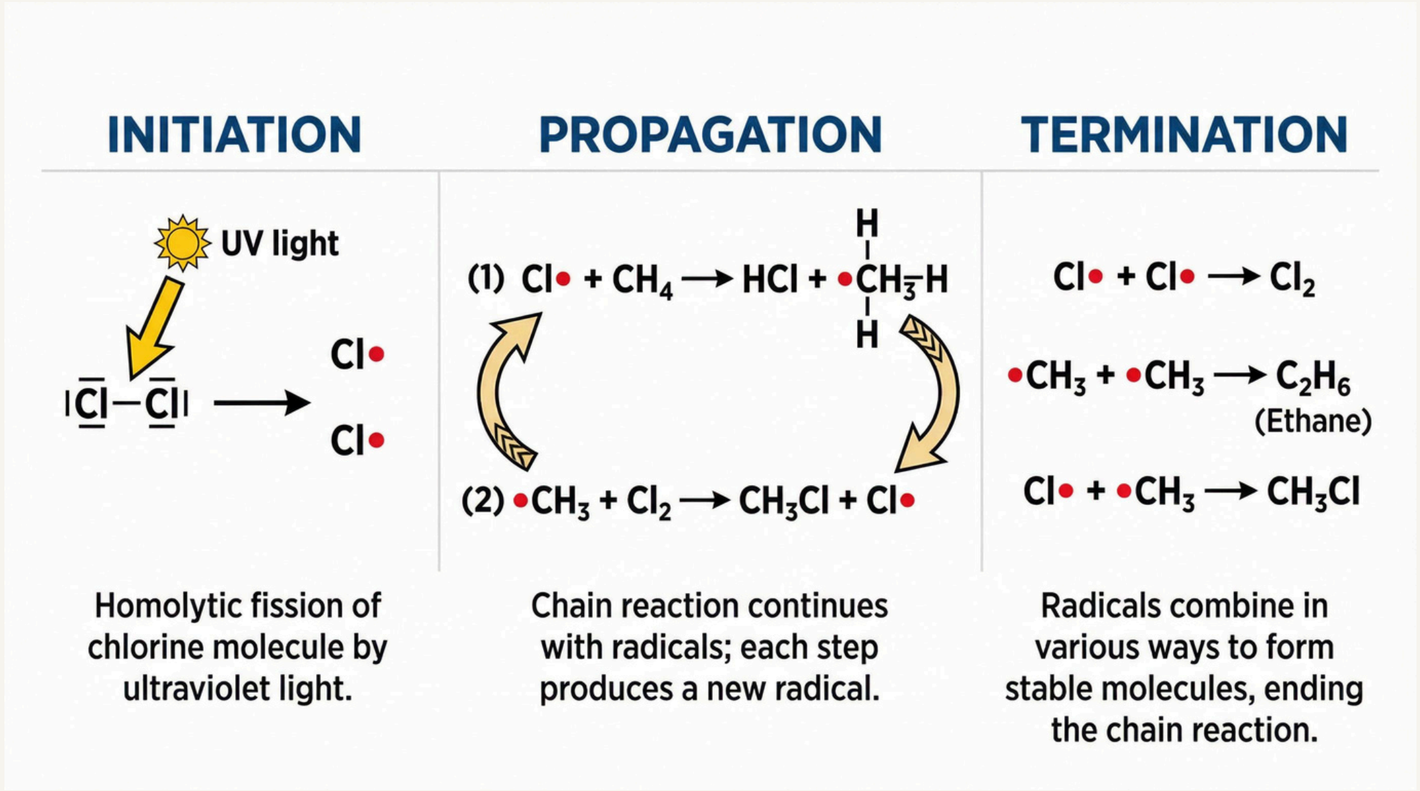
Propagation

$Cl\bullet + CH_4 \rightarrow HCl + CH_3\bullet$

$CH_3\bullet + Cl_2 \rightarrow CH_3Cl + Cl\bullet$

Termination

$CH_3\bullet + Cl\bullet \rightarrow CH_3Cl$



Cracking, dehydrogenation, isomerization

Several industrial reactions are used to convert alkanes into more valuable chemical products.

1. Cracking

Cracking is a process in which large hydrocarbon molecules are broken into smaller molecules.

It may occur through thermal or catalytic processes.

2. Dehydrogenation

Dehydrogenation involves the removal of hydrogen from saturated hydrocarbons to form unsaturated compounds..

3. Isomerization

Isomerization converts a straight-chain alkane into a branched-chain isomer without changing its molecular formula.

Reaction	**Equation**	**Purpose**
Cracking	$C_{10}H_{22} \rightarrow (\Delta)\ C_5H_{12} + C_5H_{10}$	Lighter hydrocarbons
Dehydrogenation	$CH_3CH_3 \rightarrow (\text{cat.}, \Delta)\ CH_2{=}CH_2 + H_2$	Alkenes
Isomerization	$n\text{-}C_4H_{10} \rightarrow (\text{cat.})\ (CH_3)_3CH$	Higher octane gasoline

Conclusion

- General formula C_nH_{2n+2}; sp^3 carbons; single bonds only
- Chain isomerism gives different skeletons
- IUPAC rules name alkanes systematically
- Sources: petroleum, natural gas, lab synthesis
- Reactions: combustion, halogenation, cracking, dehydrogenation, isomerization
- Essential fuels and industrial raw materials