

PHYSICAL CHEMISTRY OF NANOSTRUCTURED SYSTEMS

1

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LECTURE No. 2

CARBON BASED MATERIALS

OBJECTIVES

- To describe the structure and the most important characteristics of fullerenes, their formation and properties.
- To give the most important applications.

OUTLINE

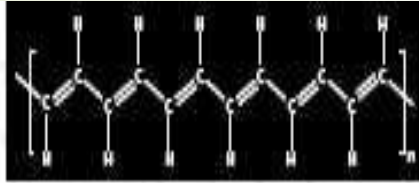
- ❑ Fullerenes. The structure and its characteristics.
- ❑ Types of fullerenes.
- ❑ Mechanism of formation.
- ❑ Chemical properties.
- ❑ Applications.

Importance of the carbon atoms

- ❑ The most studied chemical element
- ❑ Forms organic compounds with: H, O and N
- ❑ Applications in Medicine, Biology, energy production and conservation of environment
- ❑ Two types of materials: **graphite**, which we use in the pencil mines, and **diamond**, crystalline cubic structure.

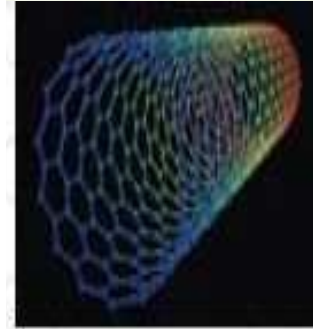


1940-1960. The graphite, semimetal with very anisotropic forms is investigated exhaustively.



1975-1978. The polyacetylene (CH)_n, doped, is synthesized. Metal polymers with a wide range of conductivities. Scientists receive the Nobel Prize for Chemistry, 2000.

1991. Carbon nanotubes are observed in a variety of forms that may be metallic or semiconducting.

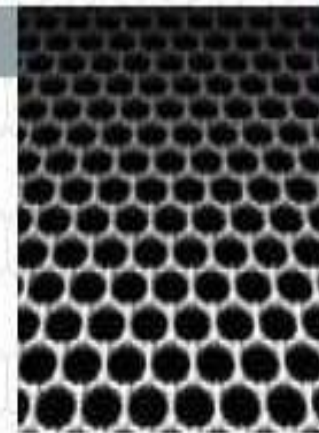


2004. Carbon monolayers. Initially one or more microns in length. Centimeter samples already exist.



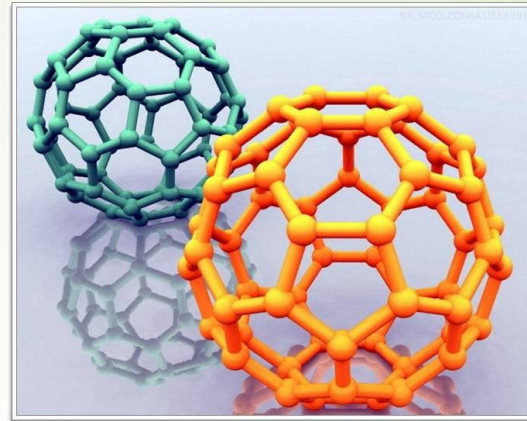
1960-1970. Graphite intercalations are characterized. They can be superconducting.

1985. Fullerenes are observed in outer space C₆₀ and larger structures. R.F.Curl Jr, H.Kroto and R.Smallley receive in 1996 the Nobel Prize for Chemistry.

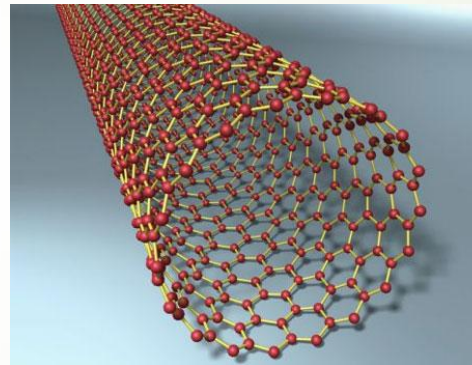


Carbon based materials

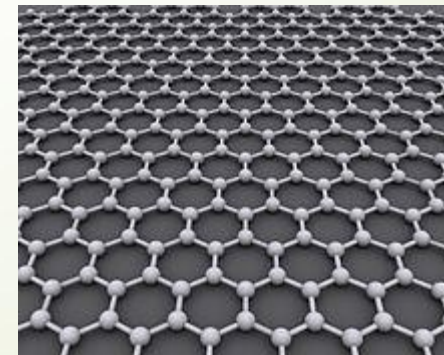
Fullerenes



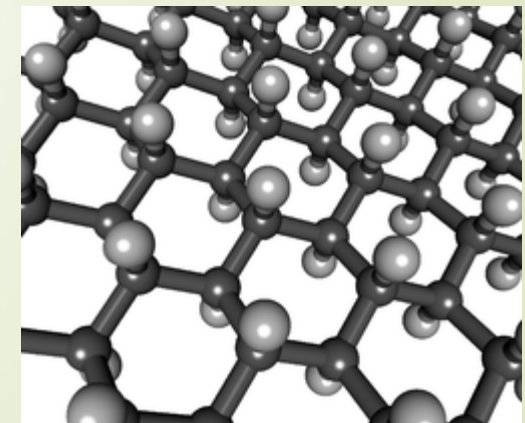
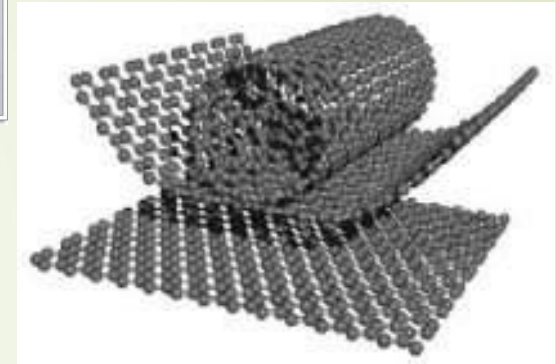
Nanotubes



Graphene

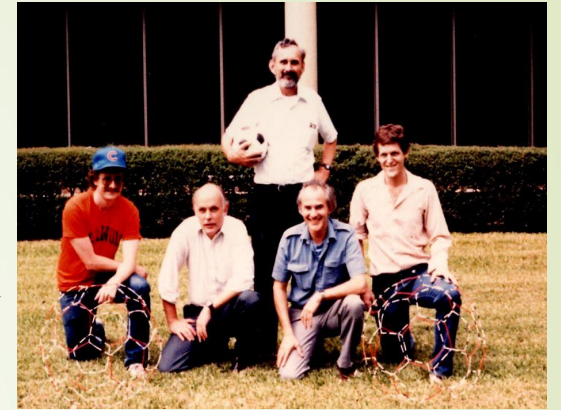


Graphane



Fullerenes

- They were discovered in 1985 by Harold **Kroto**, James R. Heath, Sean O'Brien, Robert **Curl**, and Richard **Smalley** at Rice University, USA (Nobel Prize in 1991).
- The unique electronic structure of fullerenes defines their unique properties including:
 - ✓ chemical resistance,
 - ✓ high strength,
 - ✓ thermal and electrical conductivity(Applications)



Characteristics of Fullerenes

- ❑ Structural beauty and versatility to form new compounds.
- ❑ Forms like spheres, ellipsoids or cylinders:
 - ✓ Sphericals → Bucky spheres
 - ✓ Cylindrical → Buckytubes or nanotubes

Characteristics of Fullerenes

Geodesic dome (Buckminster Fuller)



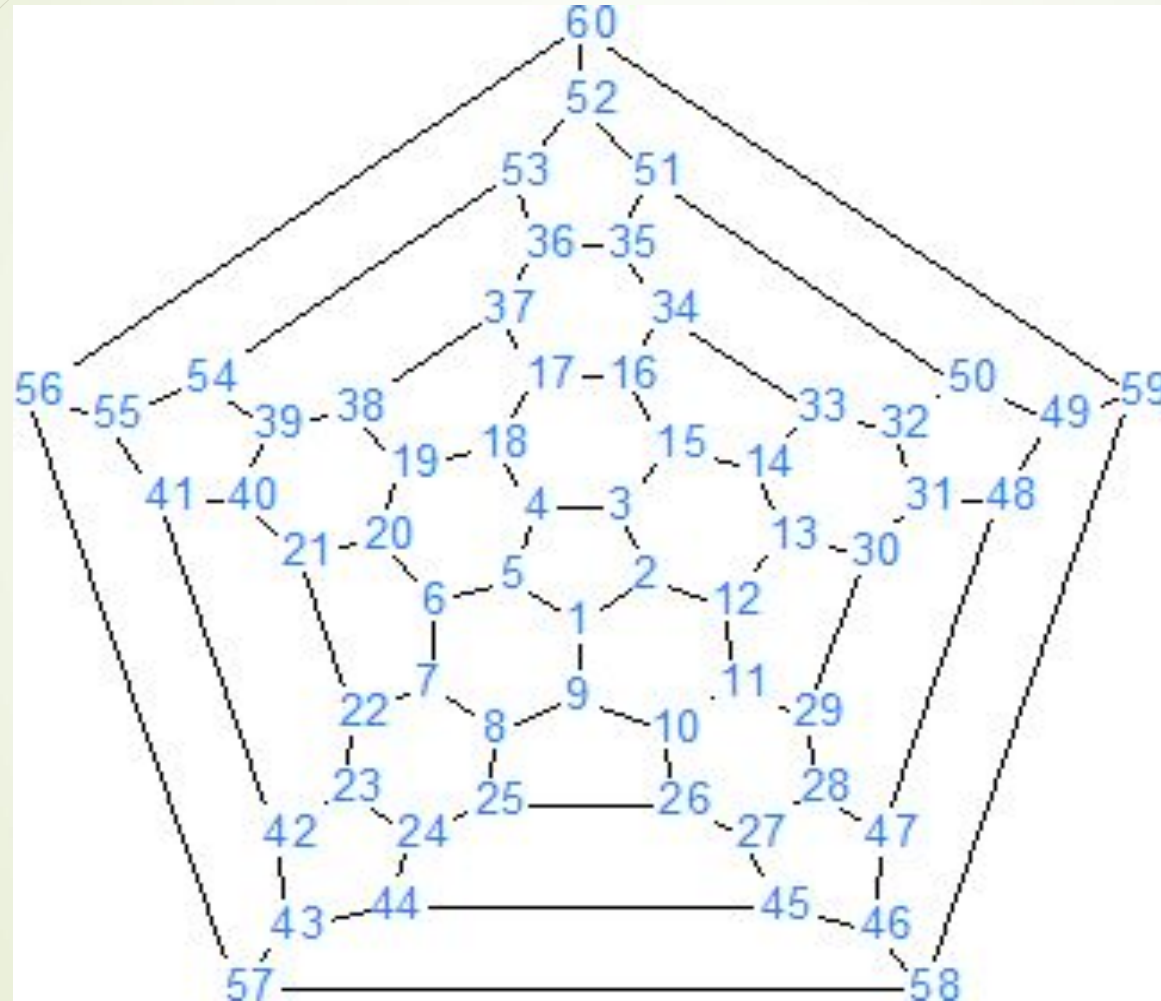
Characteristics of Fullerenes

Geodesic dome (Buckminster Fuller)



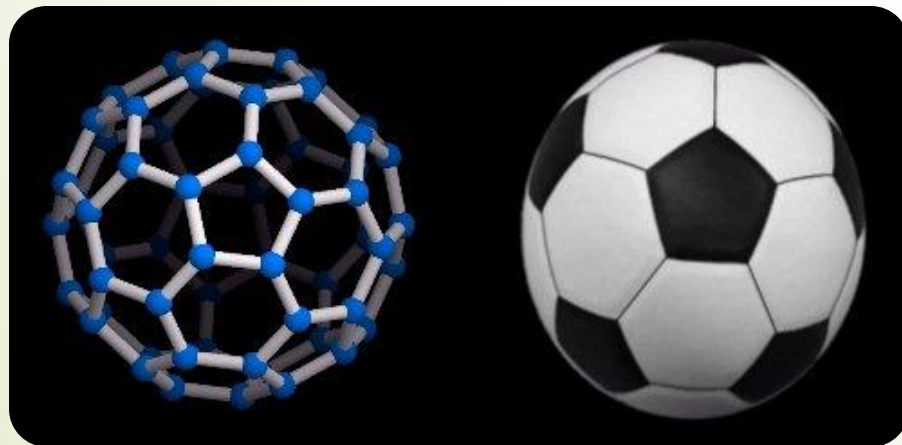
(Buckminsterfullerenes)

The most common form of fullerenes: C_{60}



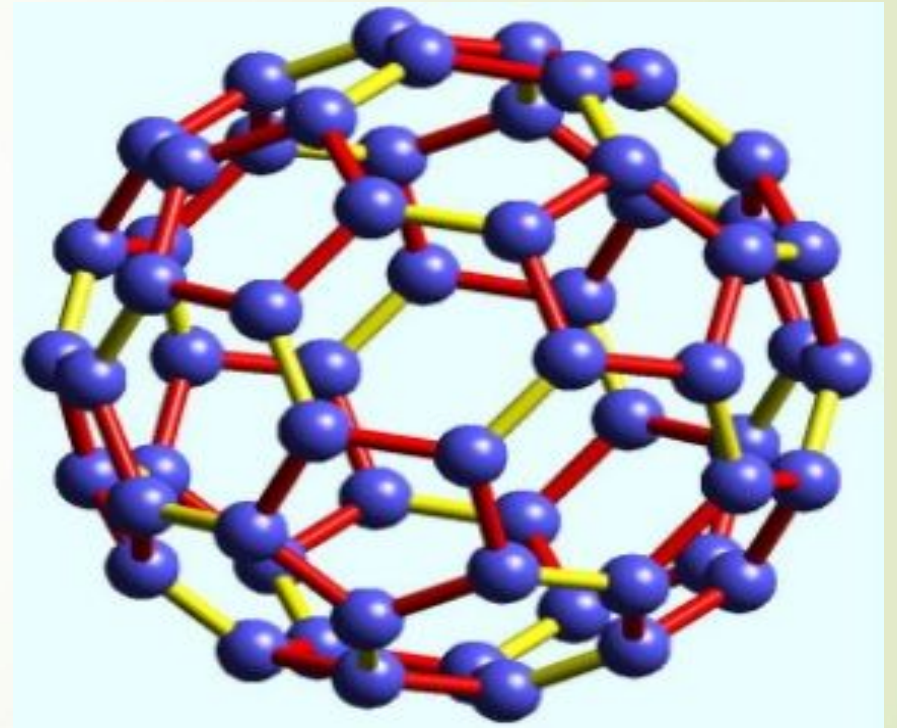
Characteristics of C_{60}

- ❑ There are 60 carbon atoms bonding together like hexagons and pentagons in a soccer ball.
- ❑ It consists in 20 hexagons and 12 pentagons.



Characteristics of C₆₀

- ❑ Each carbon atom is bonded to three others.
- ❑ Yellow bonds represent double bonds and red bonds, single.
- ❑ Pentagonal rings contain only single bonds and hexagonal, double and single bonds.



Characteristics of C_{60}

- ❑ Double bonds have shorter bond length:
 - ❑ Instability in the pentagonal rings
 - ❑ Poor delocalization of electrons

Molecule reactivity

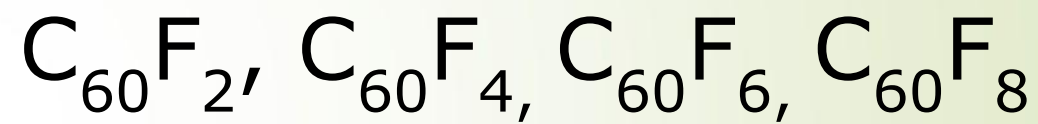
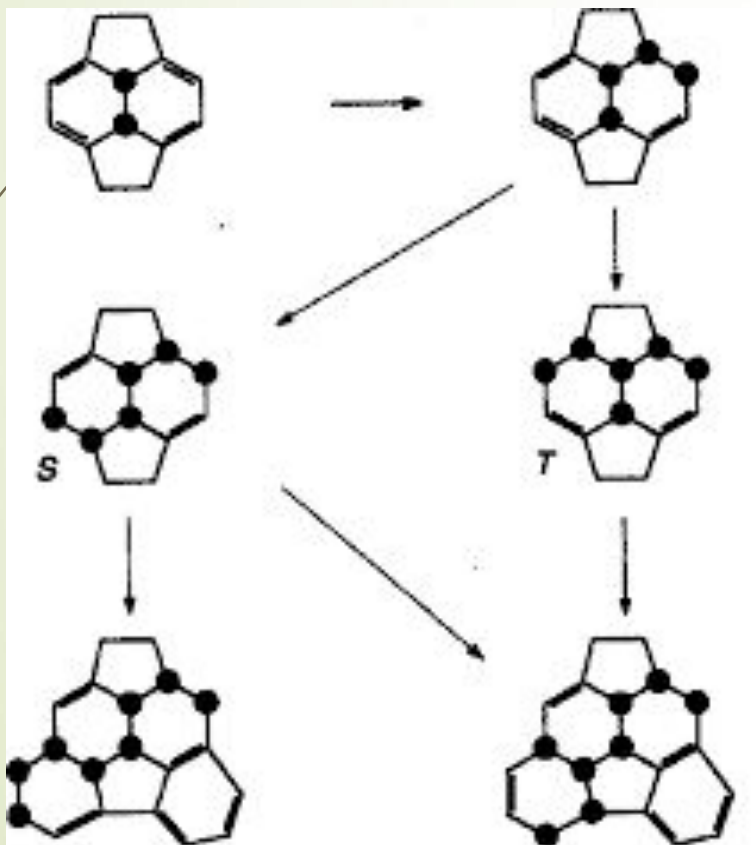
- ❑ Strong and resistant carbon macromolecule. It resists extraordinary pressures.
- ❑ There are different structures: C_{20} , C_{26} , C_{36} , C_{50} ,
 C_{60} , C_{70} , C_{72} , C_{76} , C_{80} , C_{82} , C_{84} , up to C_{540} .

Physical properties

- Density: $1,72 \text{ g/cm}^3$
- Poorly soluble in most solvents (toluene and carbon disulfide).
- Solutions of pure buckminsterfullerene have an intense purple color.
- Thermal conductivity (300 K): $0.4 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$
- Electrical conductivity: $1.7 \cdot 10^{-7} \text{ Cm}$
- Boiling temperature: $1180 \text{ }^\circ\text{C}$
- Great tensile strength

Chemical properties.

Reactions of addition. Halogenation.
Fluorides.



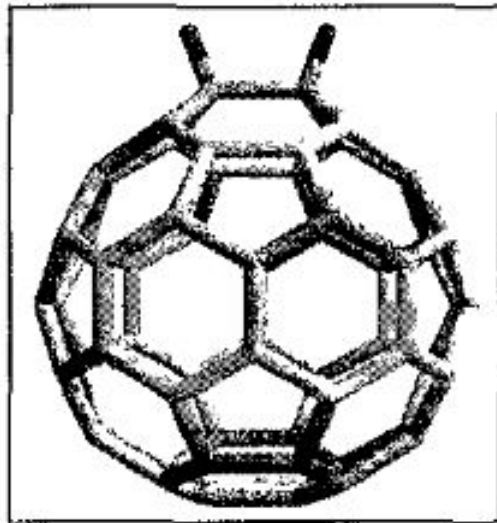
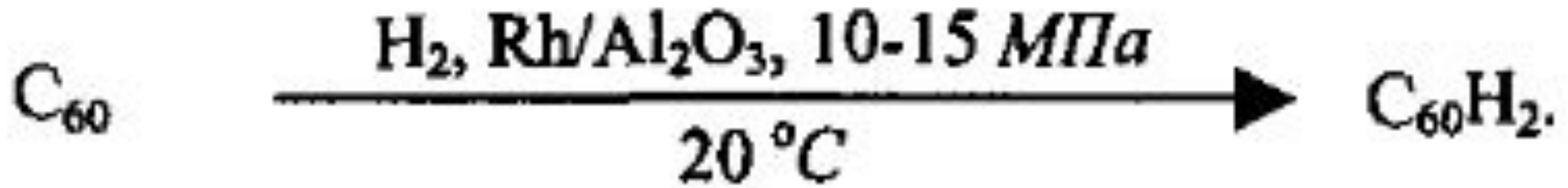
Chemical properties.

Reactions of addition. Halogenation.
Chlorides.



Chemical properties.

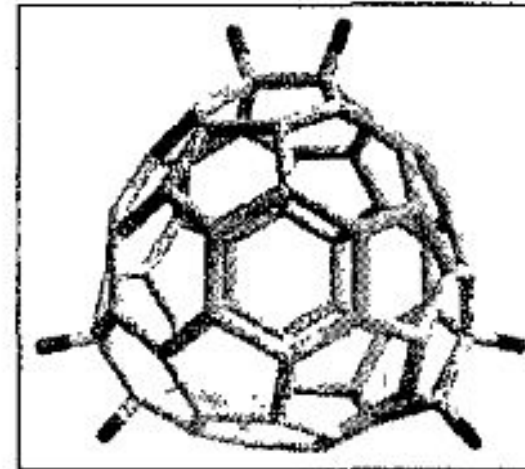
Reactions of addition. Hydrogenation.



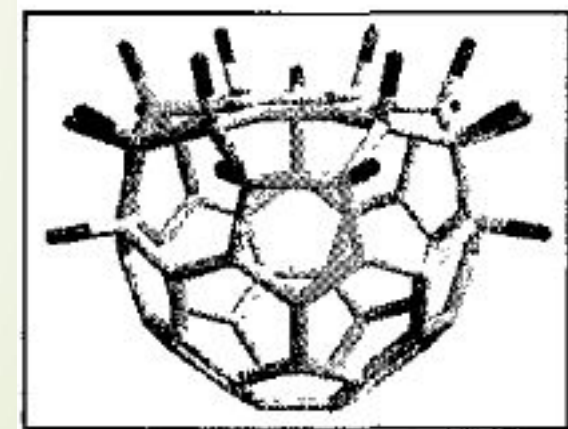
Строение C_{60}H_2



Строение
основного изомера C_{60}H_4



Строение
основного изомера C_{60}H_6



Строение $\text{C}_{60}\text{H}_{18}$

Chemical properties.

Endohedral fullerenes

They are fullerenes that have additional atoms, ions, or clusters enclosed within their inner spheres.

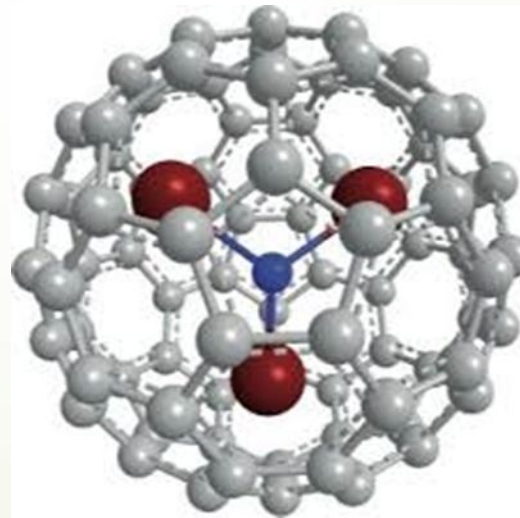
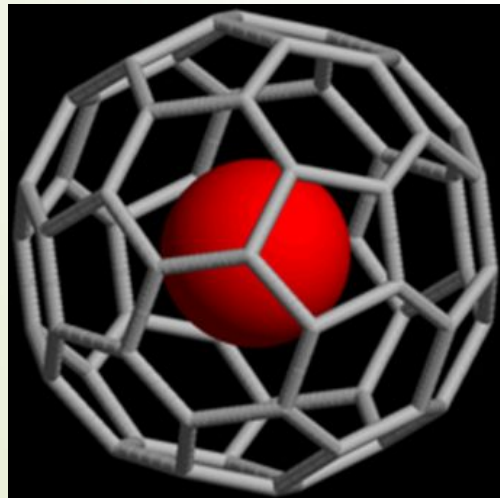
Molecular containers



Chemical properties.

Endohedral fullerenes

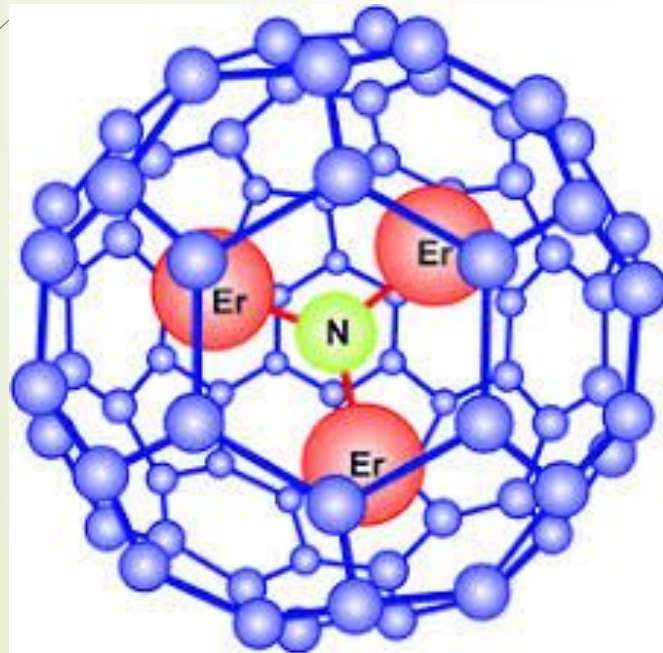
1. Within the carbon skeleton can be one or more metal atoms.



Chemical properties.

Endohedral fullerenes

2. Atoms of inert gases and nitrogen.



Chemical properties.

Endohedral fullerenes

The first C_{60} complex was synthesized in 1985 and called lanthanum C_{60} $La@C_{60}$



Applications

- ❑ Electronics, chemistry, medicine, optics
- ❑ As the basis to produce batteries
- ❑ Optical gates
- ❑ As additives for rocket fuel, lubricant.

Control questions

1. Describe in briefly what is fullerenes?
2. Mention the main characteristics of fullerenes.
3. Explain the structure of C_{60}
4. Mention some physical properties of fullerenes.
5. Mention some chemical properties of fullerenes and explain one of them.

**THANK YOU FOR YOUR
ATTENTION!**