Research & Reviews: Journal of Physics
ISSN: 2278-2265 (Online), ISSN: 2347-9973 (Print)
Volume 6, Issue 3
www.stmjournals.com

Fullerene: Properties, Synthesis and Application

Jyoti Yadav*
Department of Physics, Indira Gandhi University, Meerpur, Rewari, Haryana, India

Abstract
In this paper, a detailed study of fullerene is presented. Fullerene is the allotrope of carbon. These are also called as buckyballs. Their properties, synthesis and applications are discussed in this paper. Fullerene synthesis is done by arc discharge method and analysis is done by high performance liquid chromatography (HPLC). Synthesis process shows that C_{60} and C_{70} are produced at 1000 °C and that the concentration increases as pulse duration increases. The fullerenes can be utilized in organic photovoltaic (OPV), portable power, medical purpose, antioxidants and biopharmaceuticals.

Keywords: *Allotrope, hybridization, aromaticity, bonding, nanotechnology*

****Author for Correspondence*** E-mail: decentjyoti7@gmail.com

INTRODUCTION
Carbon has many allotropes like diamond, graphite, etc. Third allotropic form of carbon is fullerene. Any molecule made of only carbon atoms is fullerene. These can be of any shape like ellipsoid, sphere or tube. Fullerenes having spherical geometry are called buckyballs. Cylindrical fullerenes are given the name nanotubes. Graphite has layered structure in which hexagonal rings are linked to each other. Fullerene structure is like graphite but there may also be pentagonal rings in fullerene structure.

History
In the early 1970s, Osawa theoretically discussed the possibility of existence of polyhedral carbon cluster and predicted some of their properties. In 1985, Kroto et al. [2] studied the mass spectra of graphite vapour obtained by laser irradiation of a solid sample and observed peaks corresponding to masses 720 and 840. They suggested that these peaks corresponds to individual molecules C_{60} and C_{70}. The C_{60} molecule is a truncated icosahedron with an I_h symmetry while C_{70} has a more extended structure. In 1985, a new allotrope of carbon was discovered having atomic arrangement in closed shells. This allotrope has truncated icosahedrons structure. Buckminsterfullerene name was given to this allotrope after the name of architect Buckminster Fuller who fabricated cage like geodesic domes in 1960's [1].

Definition
Any molecule having only carbon atoms in various shapes like hollow sphere, tube or ellipsoid is called as fullerene. Fullerenes have interconnected carbon atoms in hexagonal and pentagonal rings. Fullerenes have similar structure like graphite except these may have pentagonal rings. Figure 1 shows the structural configuration and atomic arrangement of three allotropes of carbon.

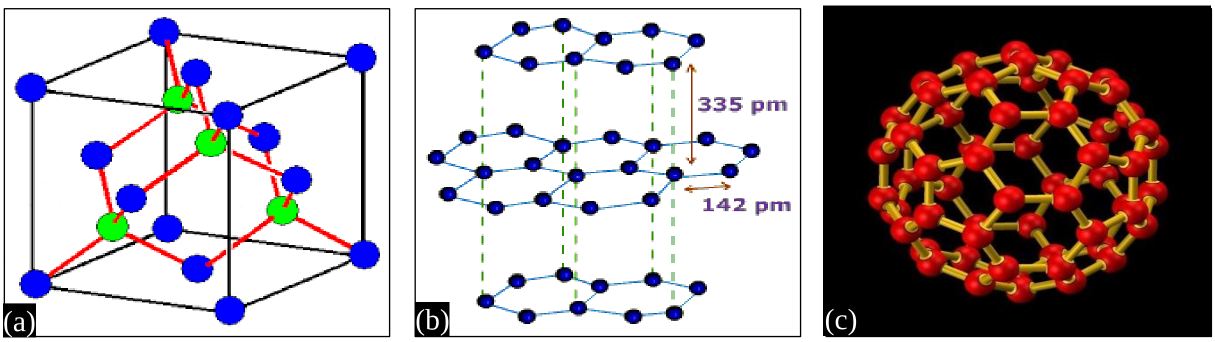

Fig. 1: (a) *Structure of Diamond,* ***(b)*** *Graphite,* ***(c)*** *Fullerene.*

Naming

Richard Buckminster Fuller was an architect who designed a geodesic dome having shape like interconnected rings. As fullerene also has interlinked rings structure, so these are given the name Buckminsterfullerene (C_{60}). After discovery of buckminsterfullerene, the fullerene family was discovered. The suffix "ene" tells that every carbon atom is bonded covalently to other three carbon atoms instead of four. It indicates that there are double bonds in fullerenes [2].

Types of Fullerene

Fullerenes were discovered in 1985. After that, various types of fullerenes were discovered on the basis of structural variations. These are following:

Buckyball Clusters

The most common buckyball is C_{60} but C_{20} is the smallest member in buckyball clusters [3]. Figure 2 shows the structure of smallest buckyball.

Nanotubes

Nanotubes have very small dimensions. These are hollow from inside like a tube with single or multiple boundaries. Nanotubes are mostly used in electronic industries. Figure 3 shows structure of nanotube [4].

Megatubes

Megatubes have larger diameter as compared to nanotubes. They have walls of various sizes. Megatubes are mainly used for the transportation of different sized molecules [5].

Polymers

Polymers are formed under high temperature and high pressure. These can have different structures like one dimensional chain, two-dimensional and three-dimensional shapes [6]. Figure 4 shows structure of polymers.

Nano-onions

Nano-onions are spherical in shape. They have multiple carbon layered structure with a buckyball core between the layers. Nano-onions are utilized as good lubricants [7]. Figure 5 shows the structure of nano-onions.

Buckminsterfullerene (C_{60})

C_{60} is a molecule having 60 carbon atoms. These atoms are arranged in a cage like structure having 12 pentagons and 20 hexagons. The shape of C_{60} is like a soccer ball. The black portions of soccer ball are pentagons and white are hexagons. If we put carbon atoms at all these 60 points, then we get structure of buckminsterfullerene. If we imagine that the C_{60} molecule has size of the order of soccer ball, then size of soccer ball will be equal to earth size. C_{60} molecule is the most symmetric molecule having symmetries like reflection symmetry, rotational symmetry etc. [8]. A geodesic dome has the similar structural view like a buckminsterfullerene as shown in Figure 6.

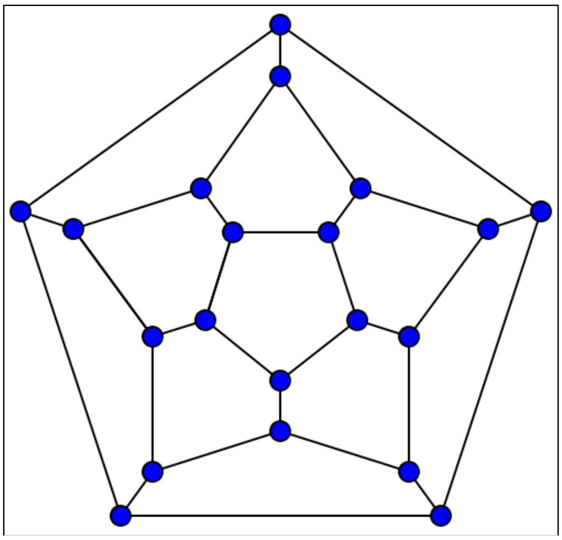

Fig. 2: *Structure of 20-Fullerene (Dodecahedral Graph).*

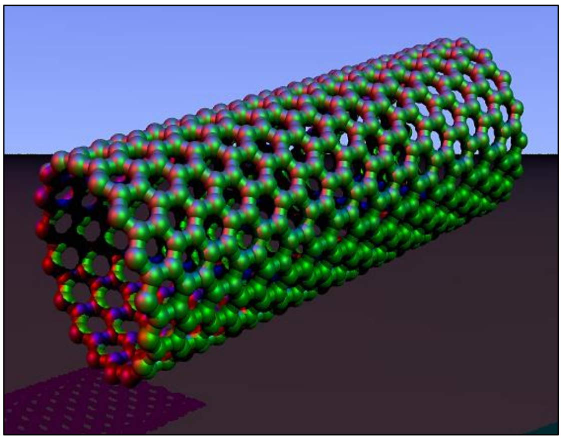

Fig. 3: *Structure of Nanotube.*

Structure of C_{60}

In C_{60}, each carbon atom is covalently bonded to three neighbouring carbon atoms. Hence it has sp^2 hybridization [9]. Hybridization of carbon atoms in C_{60} is shown in Figure 7.

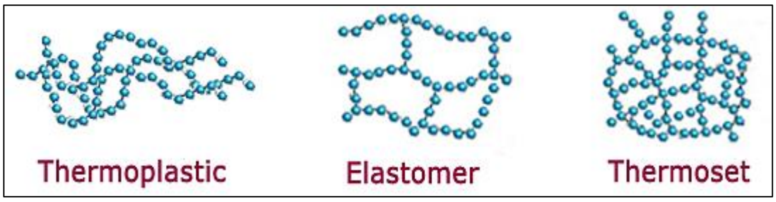

Fig. 4: *Structure of Polymers.*

Fig. 5: *Structure of Nano-Onions.*

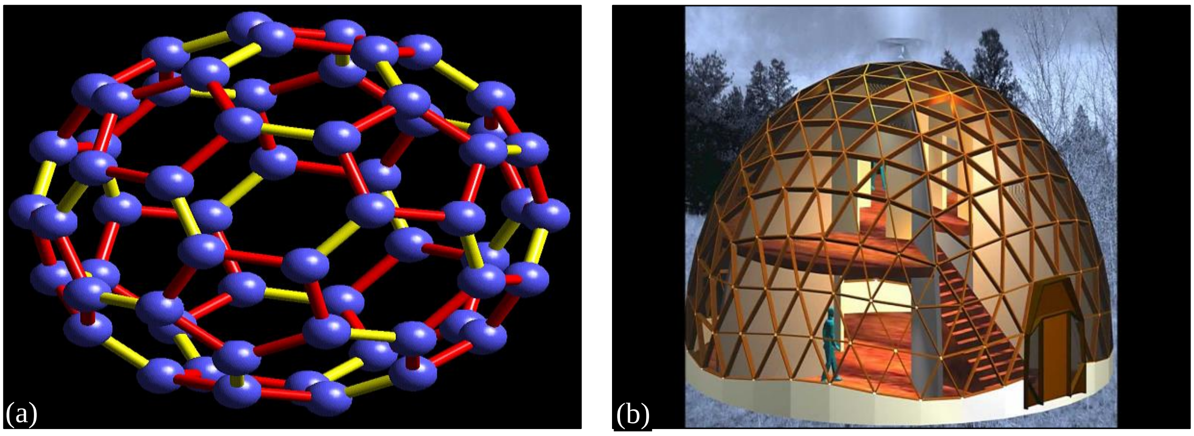

Fig. 6: (a) *A Buckminsterfullerene,* ***(b)*** *A Geodesic Dome.*

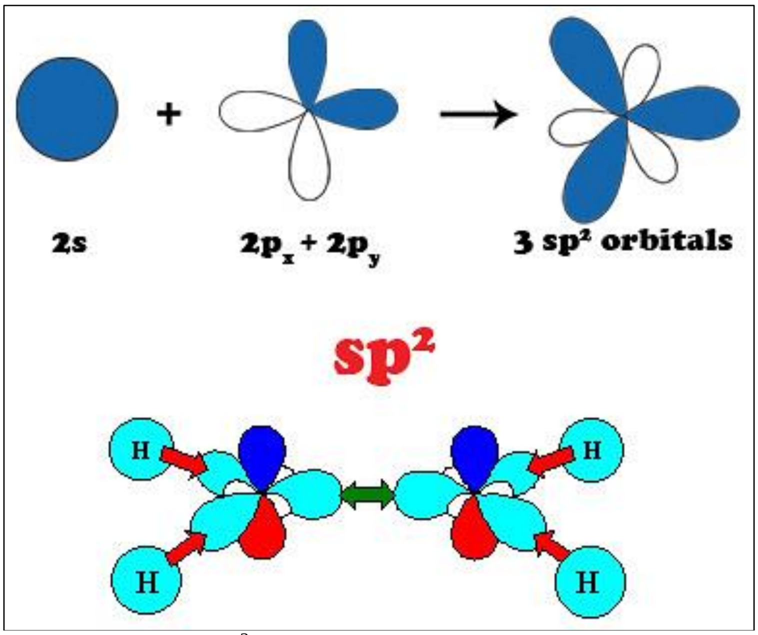

Fig. 7: *sp^2 Hybridization of C-Atom in C_{60}.*

Fullerenes have 20 hexagonal and 12 pentagonal rings. On every polygon's vertices, there is a carbon atom and along edge of each polygon, there is a bond. It has two bond lengths and average bond length of C_{60} is 1.4 Å. C_{60} is not super-aromatic. It is an alkene having electron deficiency property. It reacts with species which are rich of electrons. There can be an infinite number of fullerenes on the basis of number of pentagonal and hexagonal rings. C_{60} has face center cubic lattice structure. The van-der Waals diameter and nucleus to nucleus diameter of this molecule are 1.1 and 0.71 nm respectively [10].

PROPERTIES OF C_{60} MOLECULE

Symmetry Property

C_{60} molecule is known for its symmetry property. C_{60} molecule has three types of rotation axes. 5-fold rotational symmetry is the most common. It is through the centers of two pentagons which are facing each other. 3-fold rotation symmetry axes are from the central point of 2-hexagonals which are facing each other. At last, 2-fold symmetric axes are through the edge centers of 2-hexagons. Hence it is called the most symmetric molecule [11]. 2-fold, 3-fold and 5-fold rotation symmetries of C_{60} are shown in Figure 8.

Physical Properties

Density (g.cm^{-3}): 1.65
Refractive index (600 nm): 2.2
Boiling point: Sublimation occurs at 800 K
Resistivity (ohms m^{-1}): 1014
Vapour pressure (Torr): 5×10^{-6} at room temperature: 8×10^{-4}at 800 K

Chemical Properties

Aromaticity

Japanese workers Yoshinda and Osawa have proposed a definition of a new class of conjugated molecules, which they called super-aromatics. They assigned to this class of compounds molecule of polyhedral form which contain electrons in molecular orbital delocalised on the surface of a three dimensional structure having an almost spherical symmetry. They suggested that C_{60} molecule has the structure of truncated icosahedron. This C_{60} molecule possesses a system of mobile electron which contributes additional stabilisation to polyhedron as in benzene molecule. They produced the first quantitative estimates of resonance energy for this unusual type of conjugated molecule and concluded that C_{60} cluster has great resonance energy than benzene molecule. Hence C_{60} molecule was assigned to a new class of aromatic system [12].

SYNTHESIS OF FULLERENES

Arc Discharge Method

This is a pulsed arc discharge method of synthesis operated at high temperature. Parts of the apparatus are furnace for heating purpose, a tube made up of quartz, electrodes of carbon, a trap which is water cooled and a high voltage pulsed power input. For annealing process of carbon clusters, a buffer gas is allowed to pass through the quartz tube. The tube temperature is between 25 and 1000°C. The flow rate of the buffer gas is maintained at 300 cm^3/s. Pressure of the buffer gas is maintained at 500 Torr.

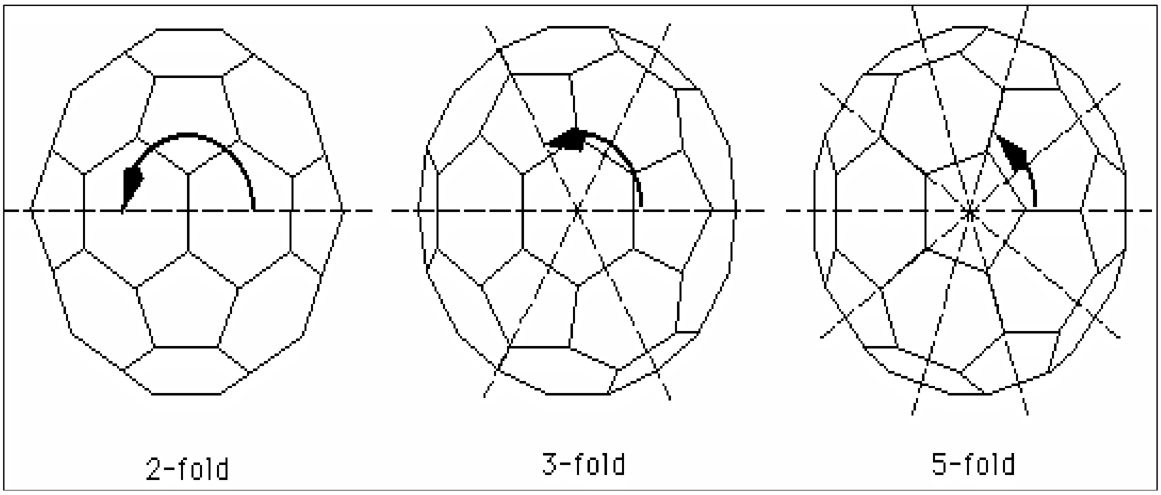

Fig. 8: *Rotation Symmetries of C_{60}.*

The input power supply provides pulsated high voltage of 1.1 kV, 22 A and 50–300 sec duration. By this method, electrode at negative terminal is consumed. Then the carbon after condensation is annealed to form fullerenes. The fullerene and other carbon particles are then collected on the water cooled trap. Analysis of fullerenes is done by high performance liquid chromatography (HPLC). The present HPLC system can detect fullerenes at low concentrations. Dependencies of fullerene concentration on temperature, HV pulse duration and buffer gas species are measured.

RESULTS

HPLC chromatograms of the fullerenes are observed which show that peak area depends on the temperature and duration of discharge. It is resulted that C_{60} and C_{70} both are produced at 1000°C. Also, the concentration increases with increase in pulse duration. At 1 ms discharge duration time, the concentration of C_{60} in the soot is 0% in He, 1.54% in Ar and 1.12% in Kr buffer gases. Therefore, Ar and Kr are more effective buffer gases for production of fullerene than the buffer gas [13].

APPLICATIONS OF FULLERENE (C_{60})

Fullerenes are used in many more applications in various fields. Some are mentioned below [14]:

- As organic photovoltaics (OPV),
- As antioxidants and biopharmaceuticals,
- As polymer additives,
- As catalysts,
- As water purification and bio-hazard protection catalysts,
- In portable power devices,
- As vehicles compounds, and
- For medical purposes.

CONCLUSIONS

This article gives the basic information of structural configuration of fullerenes, their various properties, synthesis and useful applications. Synthesis of fullerenes is done by using arc discharge method and analyzed by using high performance liquid chromatography. These can be used in organic photovoltaic (OPV), vehicles compound, medical purpose, antioxidants and biopharmaceuticals and polymer additives.

REFERENCES

1. Henson RW. *The History of Carbon 60 or Buckminsterfullerene*. Archived from The Original on 15 Jun 2013.
2. Kroto HW, Heath JR, Obrien SC, *et al*. C_{60}: Buckminsterfullerene. *Nature*. 1985; 318(6042): 162–163p.
3. Atkinson Nancy. Buckyballs Could Be Plentiful in the Universe. *Universe Today*. 2010.
4. Iijima Sumio. Helical Microtubules of Graphitic Carbon. *Nature*. 1991; 354: 56–58p.
5. Mitchel DR, Brown R, Malcolm Jr. The Synthesis of Megatubes: New Dimensions in Carbon Materials. *Inorg Chem*. 2001; 40(12): 2751–5p.
6. Shvartsburg AA, Hudgins RR, Gutierrez Rafael, *et al*. Ball-and-Chain Dimers from a Hot Fullerene Plasma (PDF). *J Phys Chem A*. 1999; 103(27): 5275–5284p.
7. Sano N, Wang H, Chhowalla M, *et al*. Synthesis of Carbon 'Onions' in Water. *Nature*. 2001; 414(6863): 506–7p.
8. Buseck PR, Tsipursky SJ, Hettich R. Fullerenes from the Geological Environment. *Science*. 1992; 257(5067): 215–7p.
9. Iijima S. Direct Observation of the Tetrahedral Bonding in Graphitized Carbon Black by High Resolution Electron Microscopy. *J Cryst Growth*. 1980; 50(3): 675–683p.
10. Schultz HP. Topological Organic Chemistry: Polyhedranes and Prismanes. *J Org Chem*. 1965; 30(5): 1361–1364p.
11. Li Y, Huang Y, Du Shixuan, *et al*. Structures and Stabilities of C_{60}-Rings. *Chem Phys Lett*. 2001; 335(5–6): 524–532p.
12. Osawa E. Superaromaticity. *Kagaku*. 1970; 25: 854–863p.
13. Sugai T, Omaote H, Bandow S, *et al*. Production of Fullerenes and Single-Wall Carbon Nanotubes by High-Temperature Pulsed Arc Discharge. *J Chem Phys*. 2000; 112(13). https://doi.org/10.1063/1.481172

14. Yadav BC, Kumar R. Structure, Properties and Applications of Fullerenes. *Int J Nanotechnol Appl.* 2008; 2(1): 15–24p.

Cite this Article
Jyoti Yadav. Fullerene: Properties, Synthesis and Application. *Research & Reviews: Journal of Physics*. 2017; 6(3): 1–6p.

