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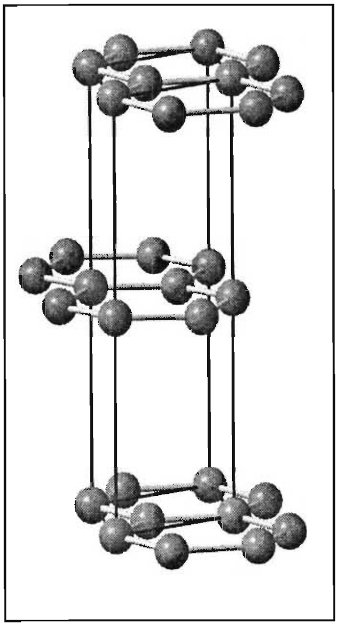
# Exploring the Fullerenes. How Geometrical Ideas Explain Strange Fullerene Structures

## Carbon the Wonder Atom

Nature is both beautiful and bountiful. An elegant testimony to this is provided by the wonderful world of atoms and molecules. The periodic table of elements lists some 92 different types of atoms occurring in nature. When atoms combine they form a myriad of molecular varieties. However in our daily life we deal mainly with about a few hundreds of these varieties, and that too made up mainly of hydrogen ($Z$ = 1), carbon ($Z$ = 6), nitrogen ($Z$ = 7) and oxygen ($Z$ = 8) together with a few other elements. Here again, it is carbon that enjoys a unique position in relation to our life and also in science and technology. The carbon atom with an electronic configuration $(1s)^2\ 2s^2\ 2p^2$, has four valence electrons viz., two each from the $2s$ and the $2p$ subshells. These electrons play a very vital role in the chemical bonding in molecules and also in solid state structures. In the solid state, carbon is known to exhibit two distinct kinds of structures. Thus we speak of two allotropic forms of carbon viz., graphite and diamond [1]. In the graphite structure these atoms are joined with each other in a hexagonal pattern forming a plane or a layer, as shown in *Figure* 1. Of course the different layers in a relatively weaker binding do give rise to a three dimensional solid. In the diamond structure, which is shown in *Figure* 2, the four valence electrons stretch out from a carbon atom tetrahedrally in space to form strong bonds, for which diamond is famous. Both these solid forms can join in principle an infinite number of carbon atoms.

***Figure 1. Structure of graphite.***



In this article we consider a new allotropic form involving a finite (e.g. 60) number of atoms, that was discovered rather accidentally in 1985 by Harold Kroto of UK and Richard Smalley of USA [2]. The new form has quickly achieved fame with the generic name 'fullerenes'. The fullerenes or bucky balls as they

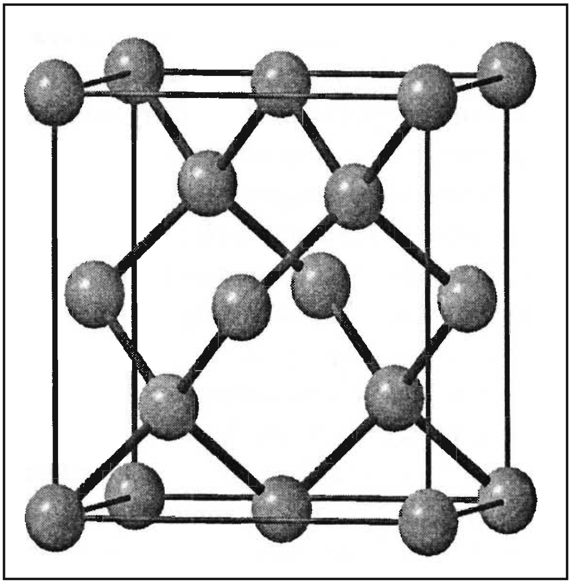
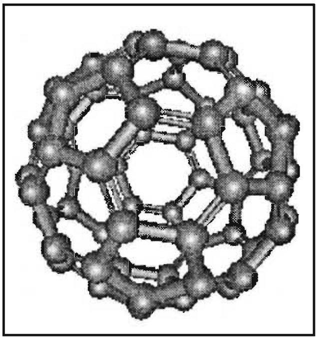


*Figure 2. Structure of diamond.*

are also called, are a class of big molecules (or clusters) that evolve out of three dimensional bonding of carbon atoms in a hollow closed structure, like a cage. Of them, the most abundant and the most popular is the $C_{60}$ molecule. This wonderful molecule consists of 60 carbon atoms and is depicted in *Figure* 3. It has a football like structure formed from intersecting hexagonal and pentagonal planes. The edges or line segments joining the C atoms represent the chemical bonds. The edges meet at the vertices i.e., the sites for the C atoms. *Figure* 3 shows that at some places there are double bonds (two parallel lines) connecting two sites , while there are single bonds elsewhere. From the geometrical point of view each site is the origin of three lines or edges. Now every edge represents a chemical bond, hence one of these three edges must actually correspond to a double bond, so that all the four valence electrons of the atom get involved in the bonding. For the present discussion however, we will consider the geometrical viewpoint only.

*Figure 3. Structure of $C_{60}$.*



The building blocks of a $C_{60}$ molecule are 12 pentagons and 20 hexagons. For other fullerenes (e.g. $C_{70}$) these building blocks vary in number and sometimes in shape too. Fullerenes have attracted the attention of not only physicists and chemists but

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biologists and mathematicians as well. Quite a few elementary facts about the structure of the fullerenes can be understood by applying the fundamental ideas of geometry, and that is what we aim to do presently. One may wonder, at the outset, as to why pentagons in addition to hexagons are involved in this structure. Does it not suffice to have only hexagons here, as in graphite (*Figure* 1)? The answer to this question is 'no', since *Figure* 3 is actually three dimensional, unlike the planar arrangement of *Figure* 1 for graphite. Just try to curl up a plane paper into a sphere. You may end up with a closed surface, but it will have either voids i.e. gaps, or overlaps. A plane graphite layer cannot be simply folded up into a sphere. We need therefore, pentagons together with hexagons to curl up and form a hollow round cage perfectly. Still one wonders why only certain numbers of these polygons are needed to build up that particular shape of the fullerene molecule. The basic requirement here is that the structure must be closed perfectly without gaps or overlaps. This is elegantly laid down in a general way through a famous geometrical result that was given by the mathematician Euler about two hundred years ago.

**Geometric Considerations**

According to Euler's famous result [3] if a convex polygon has $V$ (number of) vertices, $E$ edges and $F$ faces, then one must have,

$$V + F - E = 2. \tag{1}$$

The fullerene architecture must also follow (1). We wish to find the consequences of this fundamental relation, but let us first note down simpler relations as obtained presently. *Figure* 3 showing a typical fullerene indicates that each of the $V$ vertices is the origin of three edges. But the total number of edges $E$ is not $3V$. Each edge connects two vertices so that,

$$E = 3V/2. \tag{2}$$

Further, if there are $x$ number of pentagons and $y$ number of hexagons that build up this structure, then in all, the total number of faces would be,

$$F = x + y \tag{3}$$

Now, again each edge connects two faces, hence the total number of edges can also be written as,

$$E = (5x + 6y)/2 \tag{4}$$

For $C_{60}$ we have $V = 60, x=12$ (pentagons) and $y = 20$ (hexagons). Thus in this case the total edges calculated from (2) or (3) are $E=90$. (By the way, how many single bonds and double bonds should be there in $C_{60}$?) Further, the total faces in that case are $F = 12 + 20 = 32$. Thus, with $V=60, F=32$ and $E=90$, Euler's result i.e. (1) is satisfied for $C_{60}$ structure.

One also notes that, owing to the relations like (2) and (3) the number of atoms (or vertices $V$) in such a closed cage must be even. The number of pentagons must also be even.
Let us now explore the geometry further.

**Pentagons and Hexagons**

The $C_{60}$ is just one (but the most important) member of a class of big molecules or clusters. Can we use the basic relations stated above to 'construct' others? The answer is yes: and let us see how that can be done. Consider in general a closed cage made up of $x$ pentagons and $y$ hexagons. We use $E = 3V/2$ in (4) and obtain,

$$5x + 6y = 3V \tag{5}$$

Euler's result (1) together with (2) and (3) turns out to be,

$$x + y = V/2 + 2 \tag{6}$$

Equations (5) and (6) can be solved simultaneously to yield $x=12$. Now, with $y$ as a positive integer this means that geometrically one can construct a fullerene out of 12 pentagons and any number $y = 0, 1, 2, 3, ...$ of hexagons. For example, in $C_{70}$ – another well-known fullerene – we have a system of 70 carbon atoms. Here $V=70$, $x=12$ and $y=25$, as required. In other words, considerations of geometry indicate that $C_{70}$ should be made up of 12 pentagons and 25 hexagons, such that $E = 105$. One can also infer in this way, the geometrical structures of other fullerenes like $C_{20}$, $C_{22}$, ... and $C_{20+2n}$ in general, with $n$ as the number of hexagons. The pentagons will of course be 12. Yet another example of this type is $C_{84}$, where $V = 84, E = 126, x = 12$ and $y = 32$. We must remember all the same, that we will be led to geometrical possibilities only. The question of the stability of a particular fullerene must be addressed separately through considerations of chemical bonding.

### Pentagons and Heptagons

Let us next imagine a fullerene consisting of $x$ pentagons and $y$ heptagons. To see whether such a structure is allowed geometrically, we note first that in this case the total number of edges would be given by

$$E = (5x + 7y) / 2. \tag{7}$$

The equation (6) expressing the Euler result still holds. Proceeding as earlier we solve (6) and (7) to obtain the following condition,

$$x - y = 12. \tag{8}$$

In the literature some authors [4] prefer to use a transparent notation, and denote the number of pentagons by $n_5$, with $n_7$ denoting the number of heptagons in a structure. Equation (8) then becomes,

$$n_5 = n_7 + 12. \tag{9}$$

Thus, if a fullerene is made up of pentagonal and heptagonal rings, then the number $n_5$ must be more than $n_7$ by 12.

### Pentagons, Hexagons and Heptagons

Now, let us think of a hollow surface enclosed by joining $x$ hexagons and $y$ heptagons perfectly, without any pentagons. The edges in this case, as compared to (4) and (7), would be,

$$E = (6x + 7y)/2 \quad (10)$$

Already we have the other relation between $x$ and $y$ in the form of (6). Simultaneous solution of (6) and (10) does not yield a positive integer for $y$, the number of heptagons. Let us therefore, invite a few pentagons to also join a coalition of carbon atoms. Suppose that in a closed cage the numbers of pentagons, hexagons and heptagons are $n_5$, $n_6$ and $n_7$, respectively. The total number of faces will now be

$$F = n_5 + n_6 + n_7. \quad (11)$$

And the total number of edges $E = 3V/2$, will also be given by,

$$E = 5n_5 + 6n_6 + 7n_7 \quad (12)$$

Using (1) we can eliminate two of the three variables $n_5$, $n_6$ and $n_7$ to arrive at the following two conditions,

$$n_5 = n_7 + 12, \; n_5 >= 12 \quad (13)$$
$$n_6 = V/2 - 10 - 2n_7 \quad (14)$$

Finally, it is possible to have here structural isomers, i.e. different combinations of the building blocks of different shapes and numbers, giving rise to a fullerene with a certain number of carbon atoms $V$. Separate considerations would be required to explain the relative stability of a particular isomer.

### Summing Up

The experimental discovery of fullerenes about a decade and a half back, has thrown open a world of hollow 3D molecules formed by carbon atoms. We have been able to explore in this article some of the structural properties of these systems on the basis of elementary geometry. We have shown that Euler's result imposes conditions, with (6), (9), (13) and (14) for these 3D cage structures to exist. We must note that these conditions are necessary but not sufficient. Once a structure is allowed by these conditions, the next question is regarding its stability. The bond strengths tend to reduce as the angular strain of the bond, i.e. the deviation from its natural direction increases. In view of this, the building blocks of shapes other than 5, 6 and/or 7

**Box 1. About Euler**

Leonhard Euler (1707–783) was a Swiss mathematician who made great contributions in various branches of mathematics. He showed that, for a convex polygon having $V$ vertices, $F$ faces and $E$ edges, the following relation always holds:

$$V + F = E + 2.$$

Readers would find it interesting to verify this relation various 3D objects like a box, a pyramid, a prism, etc. Euler is remembered for the fundamental developments he made in algebra, differential calculus and mathematical analysis.

He also discovered theoretically, the so-called 'libration points' the points in space where all competing gravitational forces are perfectly balanced. Generally the credit for this discovery is given entirely to mathematician Lagrange.

member rings are not likely to occur in a stable cage. Hence the discussion was restricted to pentagons, hexagons and heptagons only. Some guidelines to the stability are provided from the wealth of organic molecules having hexagonal and pentagonal rings.

There is much more to fullerenes than that touched upon here. Small carbon clusters containing less than 20 atoms are not fullerenes; rather they are linear or cyclic. One can stretch imagination further and try to fold a hexagonal graphite layer (*Figure* 1) in a cylindrical or a tube form, and that can exist geometrically. However, if we wish to cap this so-called ' nano-tube' at the ends, then again pentagonal rings are required there, for an efficient enclosure. Very big carbon cage structures of increasingly complicated geometry have come to be known as hyperfullerenes. They can have $C_{60}$ at the core, surrounded by as many as 540 or even more carbon atoms [4].

## Suggested Reading


[1] S K Kulkarni and A W Joshi, Diamond, Carbon and all that, *Physics Education*, April-June, p. 31, 1997.

[2] R F Curl and R E Smalley, Fullerenes, *Scientific American*, p. 32, October 1991.

[3] R Ananthaiah, Discovery of fullerenes, *Resonance*, Vol. 2, No. 1, p. 68, 1997.

[4] K H Paranjape, Geometry IV, *Resonance*, Vol. 1, No. 8, p. 28, 1996.

[5] T G Smalz, W A Seitz, D J Klein and G E Hite, *J. Am. Chem. Soc.*, Vol.110, p.1113, 1988.