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The Remarkable Properties of C_{60}: in Chemistry, Symmetry and Graph Theory

INTRODUCTION

Among all the elements, Carbon is the backbone to life. An entire branch of chemistry, Organic Chemistry, is devoted to this element and its bonding natures with other elements. Since Carbon has only four valent electrons it is able to produce long homoatomic stable chains, molecular chains containing one element or atom. Up until 1985 diamond and graphite were the only known forms of molecules entire composed of Carbon; however, a new form of an entirely Carbon composed molecule exists. Its shape is a spherical closed pentagonal/hexagonal homoatomic shell, which is based from geodesic domes that are based on hexagons and pentagons. Hence, it is no surprise that these homoatomic shells are called Fullerenes, after the American architect Richard Buckminster Fuller, who was renowned for his geodesic domes (Figure 1).

Figure 1. Richard Buckminster Fuller[1]

[1] Taken from http://www.diamondimages.com/bucky/bucky.html

Although there are other fullerenes, the primary focus of this paper will be of the fullerene C_{60} (Figure 2). C_{60}, given the nickname Bucky Ball, has remarkable properties in chemistry, rotational symmetry, and graph theory.

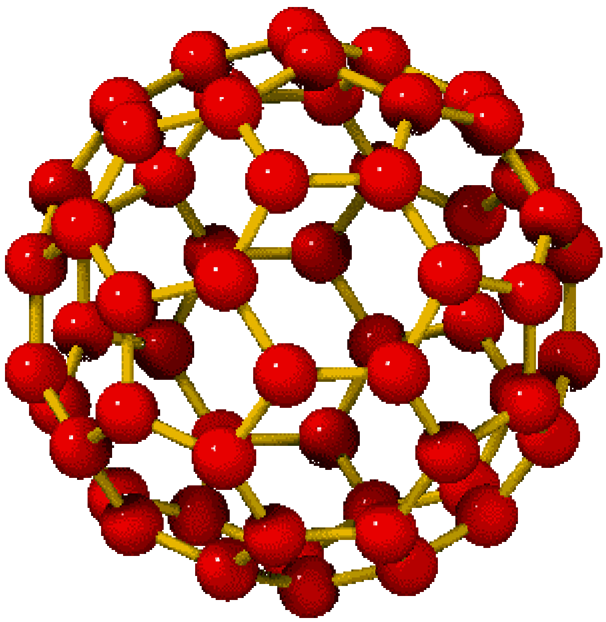

Figure 2. The Fullerene C_{60}: a Bucky ball[2]

HISTORY

In 1985, Harold Kroto of the University of Sussex and Richard Smalley of Rice University reported the discovery of stable structures consisting only of carbon atoms. The most abundant and stable of these new structures was the C_{60} molecule. For their discovery of the Buckyball, Kroto, Smalley, and their colleague, Robert Curl, won the 1996 Nobel Prize in Chemistry. Initially, C_{60} could only be produced in tiny amounts, but soon things began to change dramatically. In 1990, Wolfgang Kratschmer, Lowell Lamb, Konstantinos Fostiropoulos, and Donald Huffman discovered how to produce pure C_{60} in much larger quantities. With the discovery of C_{60}, new branches of Fullerene-Chemistry have opened, instantly capturing the imagination of chemists and have since been the subject of intensive research. By 1997, 9,000 Fullerene compounds were known.

[2] Taken from http://www.psyclops.com/bucky.shtml

CHEMISTRY

The C_{60} species is a new form of carbon, adding to the two other forms known, graphite and diamond (Figure 3). The new form of carbon, C_{60}, is different from graphite and diamond in that it consists of discrete molecules rather than networks of carbon atoms. In graphite, the carbon atom layers are held in place with van der Waals interactions, which causes them to slip past each other under pressure. Diamond, on the other hand, consists of carbon atoms that are covalently bonded to each other by σ (single) bonds in a three-dimensional network, which gives extraordinary rigidity and hardness to the structure. C_{60}, which has a molecular weight of 720 amu (atomic mass units), is a mustard-colored solid that is soluble in common organic solvents, especially solvents containing benzene or toluene. Although C_{60}, is soluble in organic solvents, it dissolves relatively slowly, indicating that the molecules pack together very well in their crystals, and has a very high melting point.

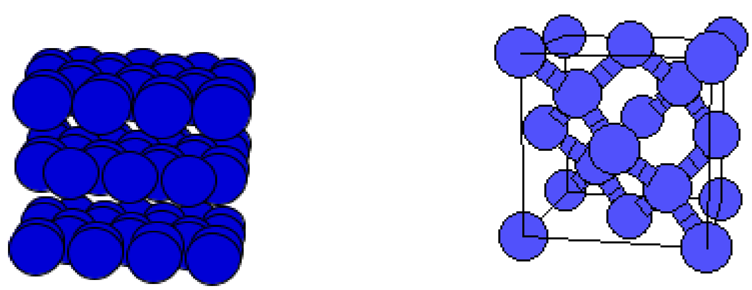

Figure 3. The three-dimensional structures of graphite (left) and diamond (right).[3]

STRUCTURE AND SYMMETRY

The ^{13}C nuclear magnetic resonance spectrum of C_{60} shows a single peak at 142.68 ppm in the aromatic region of the spectrum. Since only one peak appeared in the nuclear magnetic resonance spectrum, all the carbons in the atoms in C_{60} are equivalent to each other. This is possible only with a highly symmetrical structure, also indicated by the high melting point and close

[3] Taken from http://cst-www.nrl.navy.mil/lattice/struk/carbon.html

packing of the crystal structure. The structure proposed for C_{60} (Figure 2) is that of a truncated icosahedron, or more familiarly that of a soccer ball (Figure 4). The truncated icosahedron is believed to have been conceived by Archimedes as one of his 13 solids known as the "Archimedean solids." The molecule itself consists of 60 carbons atoms, arranged as 12 pentagons and 20 hexagons, which were formed by cutting off or truncating the 12 vertices of the icosahedron and thus replacing them with a pentagonal face. Thus in this structure, every carbon atom is at the juncture of two six-membered rings, which contain three double bonds, and one five-membered ring. The most striking property of its structure is its high symmetry.

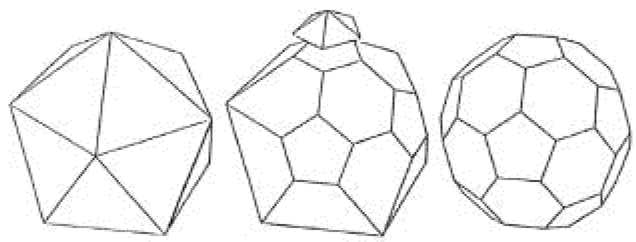

Figure 4. Truncating an icosahedron.[4]

For the C_{60} molecule there are three rotation axes (Figure 5). Perhaps, the most intriguing of these is the 5-fold axis, which is through the centers of two facing pentagons. The term 5-fold refers to the number of times that the molecule can be rotated around its axis, which in this case is 5, and look the same as it did previous to rotation. By looking down on one of the pentagons, one can see that the molecule is symmetric under rotations of 360°/5 = 72 degrees. Next, the rotation axis for the 3-fold model is through the center of two facing hexagons. Unlike the 5-fold axis, the 3-fold axis takes a rotation of 120 degrees to map the molecule onto itself. Lastly, there is a 2-fold axis, which is through the centers of the edges between two hexagons. This axis takes a rotation of 180 degrees to map the molecule onto itself.

[4] Taken from http://www.mpi-stuttgart.mpg.de/andersen/fullerene/intro.html

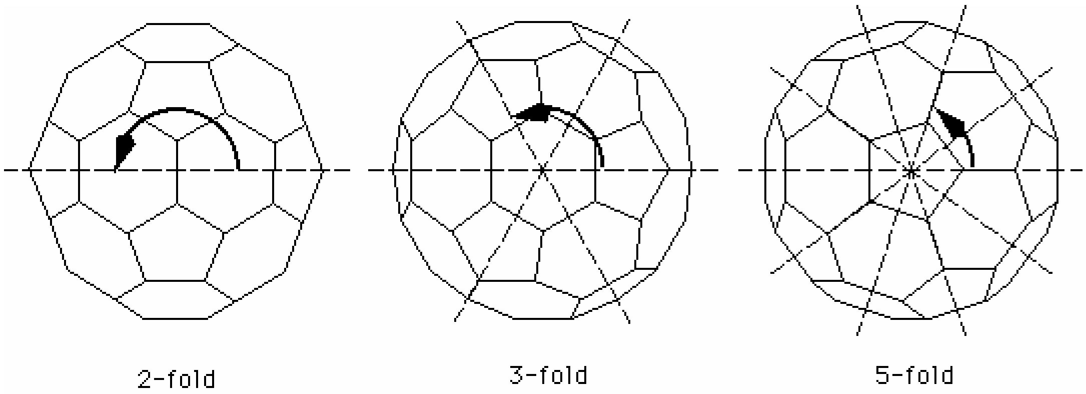

Figure 5. The rotational axes of the C_{60} molecule.[5]

Since each axis passes through two pentagons, and since there are 12 pentagons in the molecule, there are only 6 different 5-fold axes. Similarly, since there are 20 hexagons, there are only 10 different 3-fold axes. The number of differing 2-fold axes is 15, since each hexagon is neighbored by three other hexagons, so there are 30 edges between two hexagons, i.e. 15 different 2-fold axes. Thus, by combining all those transformations, 120 different symmetry operations can be found. This makes C_{60} the molecule with the largest known number of symmetry operations, the most symmetric of molecules.

GRAPH THEORY

In order to use graph theory to represent a molecule, it is necessary to define a representation for points and lines. The point of a graph represents each atom of a chemical structure and lines represent the atomic bonds as shown in Figure 5. The two graphs in this figure have the same chemical formula of C_3H_7OH, yet they are different molecules that exhibit different physical properties. These chemical compounds are isomers. In 1857, the mathematician A. Cayley observed that many of these graphs have theoretic representations, which have the property that there is a unique path of lines between each pair of points. A graph with this property is called a tree. Cayley attempted to use this work to enumerate the possibilities for certain isomers, which are

[5] Taken from http://www.mpi-stuttgart.mpg.de/andersen/fullerene/symmetry.html

trees.[6] Furthermore, the number of edges from a given point, in this case a given atom, is dependent on the number of valance electrons the atom has. For example in figure 6, Carbon has four vertices since it has four valence electrons. Hydrogen, on the other hand, has only one vertex, which corresponds to its one valence electron.

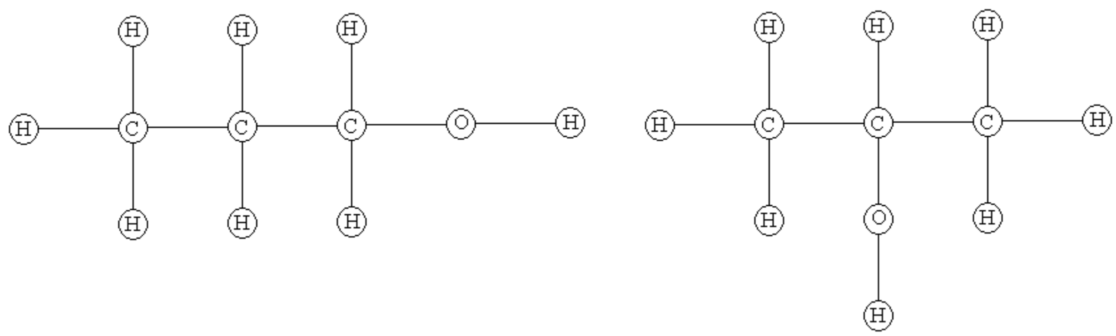

Figure 6. Chemical Isomers of C_3H_7OH. [7]

For more geometrically complicated molecules, a theorem of the mathematician Leonhard Euler can be used to show that the spherical surface of a molecule that is entirely built from pentagons and hexagons must have exactly 12 pentagons. Since the Euler characteristic is a number, C, which characterizes the various classes of geometric figures, it can be calculated from the number of vertices V, edges E, and faces F.

$$C = V - E + F \qquad (1)$$

For simple polyhedra, Euler showed that the Euler characteristic is C = 2. This is easily seen to be true for a cube. In a cube V = 8, E = 12 and F = 6, hence C = 8 – 12 + 6 = 2. Showing C is an invariant for all simple polyhedra is much harder.[8]

[6] L.R. Foulds, *Graph Theory Applications*, Springer-Verlag, New York, NY, 1992, 7.

[7] Figure drawn by author.
[8] http://www.mpi-stuttgart.mpg.de/andersen/fuller/euler.html

For the case of the geometry of C_{60}, the Euler formula (1) can be greatly simplified. Since the structure is made only from pentagons and hexagons, let P be the number of pentagons, and H be the number of hexagons. Thus the number of faces is

$$F = P + H.$$

Since each edge is shared by two polygons the number of edges is

$$E = (5P + 6H)/2.$$

For the number of vertices, we know that at least three polygons share a vertex and that for a convex polyhedron the sum of the internal angles of the polygons must not exceed 360 degrees. Since the internal angle for a pentagon is 108 degrees and for a hexagon is 120 degrees, there must not be more than three polygons sharing a vertex. Thus, there are exactly three polygons meeting at each vertex, so

$$V = (5P + 6H)/3.$$

Inserting all this into (1) and assuming C = 2, we end up with

$$P = 12$$

Thus, a simple polyhedron made entirely from pentagons and hexagons must contain exactly 12 pentagons. The number of hexagons can be arbitrarily given. With the number of hexagons known, the number of vertices can be easily calculated using:

$$V = 20 + 2H$$

Yet, with a Fullerene, the number of vertices is just the number of carbon atoms in the molecule. Therefore, Fullerenes must contain an even number of carbon atoms and must contain at least 20 Carbons, making C_{20} the smallest Fullerene.

CONCLUSION

The discovery of C_{60} in experiments with a purpose other than making a new form of carbon is a good example of how fundamental scientific research produces unexpected results with unforeseen consequences. As a result of this discovery, no chemist can look at the structure of C_{60} without imagining some other chemical species encapsulated in the cavity in side the ball. Buckyballs, because of their perfect spherical shape, and ability to form lattices with the alkali metals to fill electron gaps, could be the key to the next generations of computers.[9]

Furthermore, since their discovery, a broad range of uses for Buckyballs has been found. Among them is using them as impervious to laser beams, which could be useful in the military. [10] They may also be important in fighting the HIV virus; it has been found that the water-soluble buckyballs can inhibit an enzyme (HIV-1 protease), which is critical to the development of the virus. Industrially it is significant as a superconductor. They can also be used as lubricants as the balls can roll between surfaces.[11]

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[9] http://linc.cs.vt.edu/schools/bhs/projects/John%20Gabrysch/conclusion.htm
[10] http://www.bfi.org/bucky_balls.htm
[11] http://www.spacedaily.com/news/carbon-01e.html

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