Research article Available online www.ijsrr.org ISSN: 2279–0543

International Journal of Scientific Research and Reviews

Construction ofSpiral Conjecture and Its Utilization : C_{20} Fullerene

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ABSTRACT

Each carbon atom in fullerene is bonded to three other carbon atoms to give a polyhedron framework. In this paper some important properties of a fullerene molecules along with fullerene duals and fullerene graphs are discussed. Sprial conjecture is explained in terms of fullerene graph and its utility in fullerene isomer problems are discussed. During the entire discussion the simplest C_{20} fullerene molecule is chosen as an example.

KEY WORDS: Fullerene; Fullerene duals; Fullerene graphs; Sprial conjecture; Spiral sequence.

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A. INTRODUCTION

The first appearance of fullerene molecules in connection with an experiment i.e. graphite laser vapourization was proposed by Kroto,Heath, O'Brien, Curl and Smalley in the year of 1985[1].That proposoal was subsequently be confirmed by Krätschmer et.al. in 1990, in that paper a method was reported for bulk production of C_{60} molecule in a carbon-arc along with its structural evidence[2].In early graphite laser vapourization experiment, resulting carbon cluster obtained by, cooling and clustering the carbon vapour in a beam of helium, was analysed mass-spectrometrically[3]. Bimodal mass distribution i.e. even and odd C_n carbon cluster was ontained. The discivery of fullerenes from laser vapourization of graphite has opened up anew area or research to physicists, chemists and material scientists[4,5,6,7,18]. Fullerene (C_n) molecule are closed carbon-cage molecules containing pentagonal and hexagonal faces, of which C_{60} molecule is the most popular fullerene. C_{20} fullerene is the smallest fullerene and have dodecahedron structure with I_h point group symmetry. It is very difficult to synthesize but Prinzbach et.al. has succeeded in the synthesis of C_{20} fullerene via a chemical method[9].

I. Eulers's Polyhedron and Fullerene:

If v, f and e are the number of vertices , faces and edges of a spherical polyhedron then according to Euler's theorem[10] the following relation can be written as

$$v + f = e + 2 \qquad (1)$$

Fullerene molecules havealso spherical polyhedron structures thusEuler's theorem can be applied in caes of fullerene's structure. For a C_n fullerene molecule the number of verices is n, so $v = n$ and number of edges $e = 3n/2$.

From equation (1) we get the number of faces $f = (\frac{n}{2} + 2)$

So for any C_n fullerene molecules, spherical polyhedron with trivalent vertices the relation is given below

$$v = n,\ e = \boxed{3n/2 \text{ and } f = (\frac{n}{2} + 2)}$$

Let p and h are the number of pentagonal and hexagonal faces in a C_n fullerene molecule then total number of vertices will be as

$$n = \frac{(5p + 6h)}{3} \qquad (2)$$

Total number of faces will be given as

$$p+h=\frac{n}{2}+2 \qquad (3)$$

From equation (2) and (3) we get

$$p=12, h=(\frac{n}{2}-10) \qquad (4)$$

Thus any C_n fullerene molecule contains 12 pentagonal faces and $(\frac{n}{2}-10)$ hexagonal faces. Therefore C_{60} fullerene molecule has twelve pentagonal and rest twenty hexagonal faces.

II. Isolated Pentagon Rule (IPR):

The smallest fullerene polyhedron is the dodecahedron which has only 20 vertices. C_{20} fullerene fas only 12 pentagonal faces but no hexagonal faces. For C_{20} fullerene Isolated Pentagonal Rule (IPR) is not applicable. This rule was first proposed by Kroto in 1987[11]. The most important consequence of steric strain in fullerenes is the isolated pentagon rule. This rule states that the most stable fullerenes are those in which all the pentagons are isolated.

III. Fullerene Duals:

It is well known that every spherical polyhedron fullerene has its dual. Now the relation between a fullerene and its dual is clearly explianed. The vertices of a polyhedron correspond to the faces of its dual and vice-versa. Nature of the faces is determined by the degrees of vertices of the polyhedron. The edges of these two correspond directly to one another. Icosahedron and dodecadron are common example of dual pairas shown in figure-1a. Octahedron and cube also bear such kind of relation as shown in figure-1b.

Figure-1:Two Dual Pairs (a) the Icosahedron and the Dodecahedron (b) the Octahedron and the Cube.

IV. Fullerene Graphs:

Fullerene graphs are two dimensional reprasentation of fullerenes. During the construction of a fullerene graph, the corresponding fullerene is to be flattened on a plane insuch a way that edges intersect only at the vertices. It is assumed that edges of a fullerene are elastic, so that any of the chosen face can be stretched to the outside of a graph. Vertices and edges of a fullerene graph represents atoms and bonds of the fullerene, similar to that in polyhedron. So many two dinmensional graphs are possible for a single polyhedron. Dodecafedron along with its planar representation is shown in figure-2.

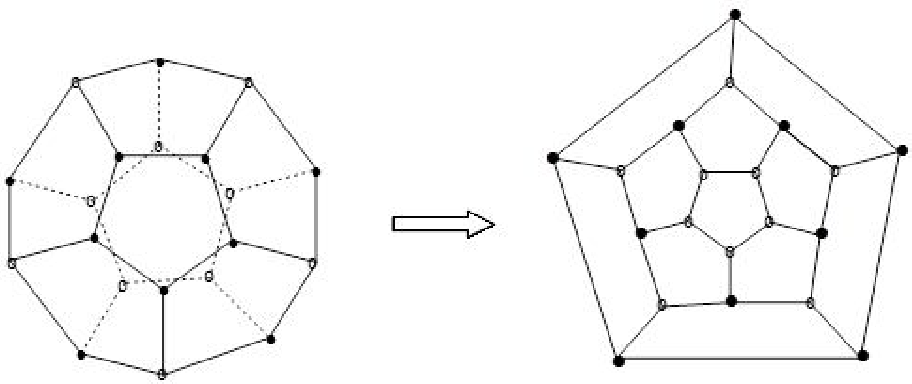

Figure-2: Dodecahedron Graph and Its Planar Graph

B. Spiral Conjecture of C_{20} Fullerene Molecule:

C_{20} molecule is the smallest fullerene has only twelve pentagonal faces as already mentioned. C_{20} fullerene graph is first constructed, then any one pentagonal face is stretched to the outside of the graph. Now the spiral can be started from any pentagonal face and it reaches to second one which is adjacent to previous face as well as it must have a open edge through which it proceeds to the next face. In this way sipral is drawn over the entire graph[12]. An unique spiral of dodecahedron is drawn over its planar representation as shownn in Figure-3.

For any fullerene any one face can be selected as a spiral start, again each edge of a given face is equally probable for spiral start. Spiral can be drawn clockwise and also anticlockwise. So considering all the factors total number of spirals would be :$12\times5\times2+(\frac{n}{2}-10)\times6\times2=6n$. So in case of C_{20} fullerene total number of spirals is $6\times20=120$.

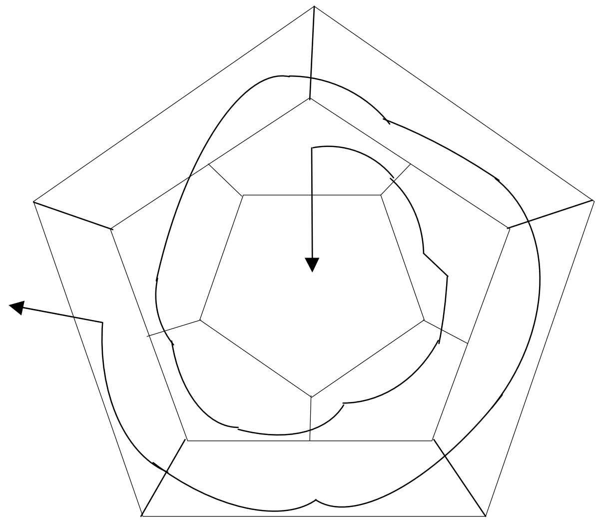

Figure-3: The Unique Spiral on Planar Graph of Dodecahedron.

For C_{20} fullerene 120 possible ways of starting the spirals are of identical symmetry. Often all spirals of a given C_n fullerene can not successfully unwind the faces, these are called failingspirals. If we have to find out the total number of successful spirals (N_t) then two things are to be considered, one is symmetry distinct spiral (N_s) and other is order of the piont group ($|G|$) of that fullerene. Relation is given as follows

$$N_t = N_s|G| \qquad (5)$$

For C_{20} fullerene (dodecahedron) number of symmetry distinct sprial is one i.e. $N_s = 1$ and point group of dodecafedron is I_h thus order is 120. So for C_{20} fullerene $N_t = 120$. It specifices that dodecahedron has no failing spiral.

C. Utility of Spiral Conjecture:

Spiral conjecture concept or diagram is straightforwardly utilized in fullerene isomer problems. Fullerene spiral can be represented by a one-dimensional sequence of 5s and 6s which indiicates the position of pentagons and hexagons along its path. For dodecahedron, (as shown in figure) spiral unwind twelve pentagons successively therefore spiral should be represented as 555555555555. In this way all probable one-dimensional spiral sequence of pentagons and hexagons can be generated to wind them up into fullerenes. The failing spirals must be rejected. Each unique spiral sequence represents one isomer of a given C_n fullerene. In this metthod isolated pentagon rule

(IPR) should be followed. In such way spiral conjecture can be used to calculate the number of fullerene isomers successfully.

CONCLUSION:

Computer programme can used to generate all probable spiral sequenes of 5s and 6s theoretically. After obtaining the tentative spiral sequences, it is to check whether they are successfully wind up to generate a fullerene maintaining all constrains.

REFERENCES:

1. KrotoH. W, HeathJ. R, O'BrienS. C, CurlR. F, SmalleyR. E. C60 Buckminsterfullerene.Nature.1985; 318:3-162.
2. Kratschmer W, Lamb L. D, Fostiropoulos K, Huffman D. R.Solid C_{60}: a new form of carbon. Nature.1990; 347: 354-358.
3. RohlfingE. A, CoxD. M, KaldorA.Production and characterization of supersonic carbon cluster beams. J. Chem. Phys.1984; 81: 3322-3330.
4. Klein D. J, Seitz W. A, Schmatz T. G.Symmetry of infinite tubular polymers: application to buckytubes. Nature, 1993; 97: 1231-1236.
5. BillupsW. E, CiufoliniM. A. (Eds.).Buckminsterfullerenes. VCH Publishing: New York; 1993.
6. DresselhausM. S, DresselhausG, EklundP. C. Science of Fullerenes and Carbon Nanotubes. 1. Academic Press: Boston, USA; 1996.
7. KrotoH. W, FischerJ. E, Cox D. E. (Eds.). The Fullerenes. Pergamon Press: Oxford, UK; 1993.
8. AndreoniW. (Ed.), The Chemical Physics of Fullerenes 10 Years Later, Kluwer Academic Publ: Dordrecht, The Netherlands; 1996.
9. PrinzbachH, WeilerA, LandenbergerP, WhalF, WörthJ, ScottL. T, GelmontM, OlevanoD, von IssendorffB.Gas-phase production and photoelectron spectroscopy of the smallest fullerene, C20. Nature. 2000; 407:3-60.
10. FowlerP. W, ManolopoulosD. E. Adetailed discussion of Euler's theorem. Cambridge University Press: Cambridge; 1976.
11. H. W. Kroto, The stability of the fullerenes C_n, with n = 24, 28, 32, 36, 50, 60 and 70. Nature.1987; 329: 529-531.
12. FowlerP. W, ManolopoulosD. E. An Atlas of Fullerenes. Clarrendon press: Oxford; 1995.