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A discussion of fullerene structures

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Abstract

We aim to highlight and present various interesting aspects of structures of fullerenes, including a theorem about the number of pentagons in spherical fullerenes [1], and use that discussion to present a few points about truncated polyhedra [2], and finally conclude by talking about truncated icosahedral C_{60} fullerenes[1][2].

1 Introduction

Fullerenes are a very interesting group of compounds which constitute an intense field of research due to their unique structures and electronic properties, and also because of their potential applications in nanotechnology and material sciences.[1] In this article we will discuss various aspects of its structures from a graph theoretic and topological point of view.[3] Then we will proceed onto a mathematical treatment of various truncated polyhedra[2] and take a cursory glance at truncated icosahedral C_{60} fullerenes[1][2].

2 Theory

Before beginning to talk about fullerenes, we present some mathematical preliminaries.
Though the scope of the theorem we wish to present is more general, we present only the portions relevant to our study:
For any polyhedron with V vertices, E edges and F faces, the relation $V - E + F = 2$ holds true.[3] One may verify it for simple examples: A cube has 8 vertices, 12 edges and 6 faces, and $8 - 12 + 6 = 2$.A tetrahedron has 4 vertices, 6 edges and 4 faces, and $4 - 6 + 4 = 2$.
The "2" in the equation $V - E + F = 2$ is known as **Euler's Characteristic**, which basically is an **invariant** in topology, basically meaning that any "spherical" (convex) polyhedron will necessarily have its Euler's characteristic to be 2.Although we shall not explore that avenue here, Euler's characteristics help determine the structures of non-spherical fullerenes as mentioned below.For example, the Euler's characteristic of a **torus** (a doughnut) is zero, for a **polygonal tiling** of a torus, $V - E + F = 0$.

With this basic introduction, we now move onto our main area of interest, fullerene structures.Fullerenes are allotropes of carbon having various structures and shapes.Although there are ellipsoidal and "tube" shaped fullerenes too (they are the well known carbon nanotubes)[4], and scientists regard the planar graphene as being an extreme, as in asymptotic, case of fullerenes, the main class of fullerenes (C_n) discovered are shaped as hollow spheres.Graph theory forces any spherical structure composed of polygons to include pentagons or heptagons within its tiling of polygons[1], and as actual fullerenes do have pentagons in them, then some more mathematics forces that n be even (that's why we never encounter something like C_{61} composed only of pentagons and hexagons).Moreover, each carbon in these fullerenes have 3 σ bonds emanating from it, and one π bond too, with one of its neighbours (**the π bonds are arranged so as to make the hexagonal rings aromatic**).As mentioned earlier, the whole C_n molecule is composed of hexagonal and pentagonal rings.In fact, the first topic of our discussion will be to prove a conterintuitive result about the number of pentagons and hexagons contained in a fullerene, as described below:

2.1 Numbers of polygons in spherical fullerenes

So lets suppose we have a fullerene C_n composed entirely of pentagons and hexagons, more specifically, say p pentagons and h hexagons.Suppose we try to express the number of vertices (which we already know to be n) in terms of p and h as follows: $5p + 6h$ is the total number of vertices there would've been if the polygons were freely arranged in space instead of being joined together as they are in the fullerene.But as we know, in the process of coming together to form a fullerene, every carbon links up with 3 others, ie:-**every vertex is a member of exactly 3 polygons**.Thus $5p + 6h$ over-counts the number of vertices by a factor of 3, and hence:

$$5p + 6h = 3n \qquad (1)$$

(1)

Now, for the second equation we need to use the theorem introduced earlier: V is clearly n, and F is $p+h$.For E, observe that each edge in a fullerene is shared between two polygons: Thus the number of edges is $\frac{5p+6h}{2}$ (Why? $5p+6h$ over-counts the number of edges by a factor of 2), which, from equation 1 is known to be $\frac{3n}{2}$ (One may observe that since E is an integer, that's why n needs to be even .This was the mathematics mentioned above which was forcing n to be even). Thus,

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

(2)

Solving the equations yields $p = 12$ and $h = \frac{n-20}{2}$. Here comes the interesting part: **Every spherical fullerene composed of only pentagons and hexagons has 12 pentagons in it irrespective of the number of carbons in it.[1]**

Quickly calculating the number of hexagons in the most common fullerenes, C_{60} and C_{70} yields that they have 20 and 25 hexagons respectively.

Although one may continue to present more facts about the number of vertices, polygons etcetera, at this point the reader might wish to actually visualise the structures of at least the common fullerenes such as C_{60}.This takes us towards our next topic, that of truncated polyhedra[2], as described below.

2.2 Truncated Polyhedra

By virtue of the definition of polyhedra being broad, the domain of truncated polyhedra is broad too.But here we shall concern ourselves with the truncated polyhedra of the **platonic solids** only.
A truncated polyhedron is derived from its parent polyhedron by "chopping" of **small** sections from all its vertices: Note that we aren't concerned with the "metric" properties such as volume etcetera of our truncated polyhedra, only its **topological properties**. The image of a truncated tetrahedron[2] is given below for clearer understanding:

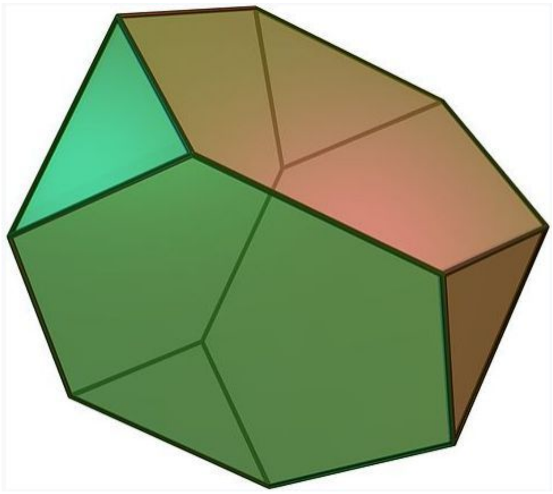

Figure 1: Truncated Tetrahedron, en route to the explanation of appearance of truncated polyhedra in chemical structures

(Courtesy:Wikipedia, refer [2])

By virtue of this definition, if suppose our platonic polyhedra has E edges, then its truncated daughter will have $2E$ **vertices,** $3E$ **edges and** $E+2$ **faces**: Why? A justification of this statement is given below:

(a) **Faces** Note that our truncated polyhedron will have $V+F$ faces because apart from the F faces of the parent polyhedron, each of the parent's vertices will also become a face of the daughter polyhedron.By the mathematical theorem given above, $V+F=E+2$.

(b) **Vertices** Let the number of edges leaving a particular vertex V_i of the parent polyhedron be d_i, also known as the **degree** of that vertex. Then

note that the number of vertices of our daughter polyhedron is Σd_i: Why? Because every vertex V_i of the parent polyhedron was converted into a d_i sided polygon in the daughter polyhedron.But also note that Σd_i is twice the number of edges of the parent polyhedron, because in the process of counting the total degree of all vertices of a polyhedron, all edges are counted twice, once each for their endpoints.Thus Σd_i=$2E$, and we rest our case here.
Note how all carbons in all the spherical fullerenes (under our study) are of degree 3.

(c) **Edges** Once number of vertices and faces are known, number of edges is the sum of the numbers of vertices and faces minus 2.

Note the fact that we were able to calculate the number of vertices, edges and faces of the truncated polyhedron just by knowing the number of edges of the parent polyhedron only.
Returning to fullerenes, we now introduce the fact that a fullerene is a **truncated icosahedron**[2].Before analysing what a truncated icosahedron is though, we first mention a few things about icosahedra first.The image of a icosahedron is given (Fig.2):

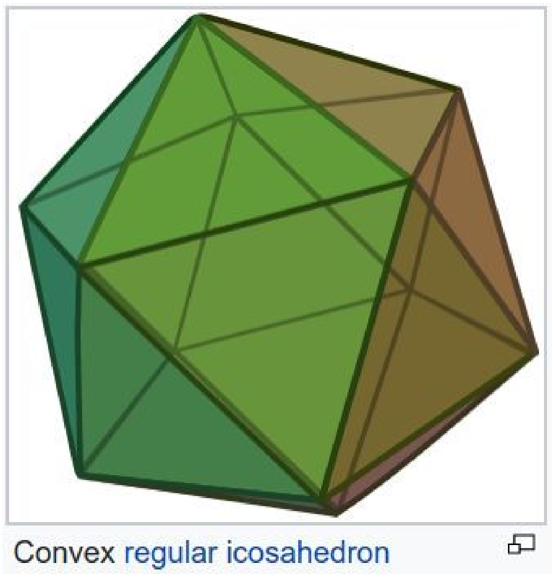

Figure 2: Icosahedron, as a precursor to its truncated version (Courtesy:Wikipedia, refer [2])

An (regular convex) icosahedron has 20 faces (all of them being triangles), 30 edges and 12 vertices[2].

Moving on to truncated icosahedra, they, by our derived formula will have 60 vertices (the 60 carbons of C_{60}), 90 edges and 32 faces (12 pentagons + 20 hexagons), as shown (Fig.3):

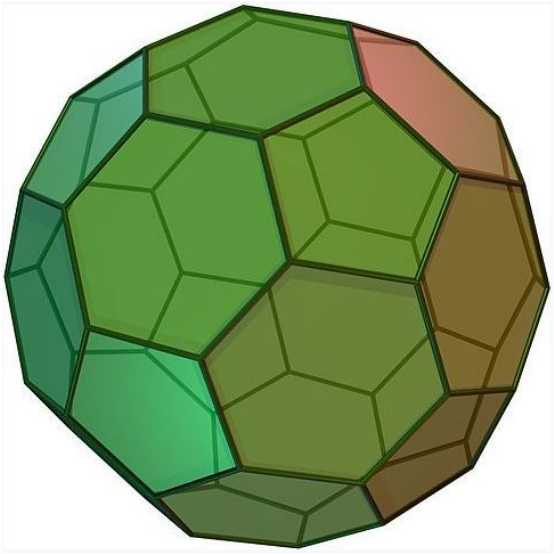

Figure 3: Truncated Icosahedron, to better illuminate the structure of C_{60} (Courtesy:Wikipedia, refer [2])

As mentioned earlier, the hexagonal rings of fullerenes are aromatic[1], leading to different bond lengths between carbon atoms in the compound.Also note however, that fullerenes don't exhibit **superaromaticity**. The aromatic π cloud of a hexagonal ring is not delocalised over the entire framework (unlike the "asymptotic" fullerene graphene, where there does exist a delocalised π cloud over the entire planar structure), and rightly so because of the strain in the carbon atoms which are most stable being planar but are forced to wrap themselves up in a spherical framework.In fact, this strain is the cause of some minor reactivity displayed by fullerenes, which are otherwise quite chemically inert.

3 Conclusions

In this article we wished to present various interesting facts about the geometry of fullerenes, like the fact that **any spherical fullerene composed only of pentagons and hexagons will always have exactly 12 pentagons in it**, and then proceeded to study of truncated polyhedra, mentioning a formula to readily calculate the numbers of vertices, edges and faces of truncated polyhedra from the number of edges of the parent polyhedron using the topological formula mentioned at the beginning of the article, finally concluding by passing a cursory glance at fullerene reactivity.

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