Breaking of Icosahedral Symmetry: $C_{60}$ to $C_{70}$

Mark Bodner¹, Jiří Patera¹,²*, Marzena Szajewska²**

¹ MIND Research Institute, Irvine, California, United States of America, ² Centre de Recherches Mathématiques, Université de Montréal, Montréal, Québec, Canada

Abstract

We describe the existence and structure of large fullerenes in terms of symmetry breaking of the $C_{60}$ molecule. Specifically, we describe the existence of $C_{70}$ in terms of breaking of the icosahedral symmetry of $C_{60}$ by the insertion into its middle of an additional $I_2$ decagon. The surface of $C_{70}$ is formed by 12 regular pentagons and 25 regular hexagons. All 105 edges of $C_{70}$ are of the same length. It should be noted that the structure of the molecules is described in exact coordinates relative to the non-orthogonal icosahedral bases. This symmetry breaking process can be readily applied, and could account for and describe other larger cage cluster fullerene molecules, as well as more complex higher structures such as nanotubes.

Introduction

Fullerenes are molecules composed entirely of carbon, taking the form of a cage or tube. The family of cage cluster fullerenes is also commonly referred to as buckyballs. The most stable and commonly occurring member of this family is the molecule $C_{60}$, which consists of 60 carbon atoms arranged in a structure of truncated icosahedrons, made of hexagons and pentagons, with carbon atoms at the corners of each hexagon and a bond along each edge (creating the well-known soccer ball structure - Fig. 1). This structure has been investigated and determined experimentally in both the solid state [1] and in the gas phase [2].

Much effort has been directed to answer why the fullerenes are so stable and which other higher fullerenes with different sizes and shapes can be formed as stable entities [2,4–6]. It should be noted that the structure of the molecules is described in exact coordinates relative to the non-orthogonal icosahedral bases. This symmetry breaking process can be readily applied, and could account for and describe other larger cage cluster fullerene molecules, as well as more complex higher structures such as nanotubes.

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The second most commonly occurring cage structure fullerene is the molecule $C_{70}$, composed of 70 carbon atoms. Electron diffraction and theoretical studies have verified that this molecule possesses a “rugby ball” structure with a pinching of the waist as the bond lengths follow a simple pattern determined by their relationship to the 5- and 6-membered rings [2,3] - Fig. 1.

In the present work we consider the existence and structure of higher fullerenes as a symmetry breaking problem, starting from the $C_{60}$ molecule which possesses the highest degree of symmetry. Guided by the common practices in particle physics, we consider the description specifically of the $C_{70}$ molecule as a symmetry breaking problem, with the additional twist that the usual branching rule for the icosahedral symmetry group $H_3$ to the dihedral symmetry group $H_2$ is enhanced by adding to it one more decagonal term. The group $H_2$ is the lowest noncrystallographic finite reflection group. We consider the icosahedral symmetry group $H_3$ of order 120 of certain carbon molecules as the exact symmetry that is broken to its subgroup $H_2$ or order 10 dihedral symmetries. We also suggest within this framework how higher order structures such as nanotubes may naturally arise. This provides a framework for understanding of the observed even carbon number rule and for predicting higher order structures which may be assembled.

The paper is unique in providing exact coordinates of the vertices of the fullerenes thus eliminating any additional numbering conventions used elsewhere [16]. This opens the possibility of defining special functions of 3 variables generated by the vertices (see Example 3), to study their possible orthogonality, and conceivably even the corresponding orthogonal polynomials defined by the fullerene structures.

Icosahedral bases in $\mathbb{R}^3$

In order to get exact coordinates of polytopes related to icosahedral symmetry, one has to use bases in the real 3-dimensional space $\mathbb{R}^3$ that reflects the symmetry, namely the simple roots $\varpi_1$, $\varpi_2$, $\varpi_3$ of the icosahedral group and their duals [17]. The geometric relations of the vectors in the $z$-basis are described by the matrix of scalar products.
Figure 1. The structure of the $C_{60}$ molecule. (a) The polytope $C_{60}$ is formed by 60 vertices equidistant from its center. Its surface consists of 12 regular pentagons and 20 regular hexagons. All 90 edges are of the same length. (b) The $C_{60}$ polytope viewed in the direction almost parallel to the plane spanned by $\omega_2$ and $\omega_3$, which makes the $H_2$ orbits (pentagons and decagons) easy to identify. (c) The $C_{60}$ polytope viewed in the direction parallel to the $H_2$ plane spanned by $\omega_0$ and $\omega_1$. Surface edges of $C_{60}$ are omitted in (b) and (c). Horizontal segments are projections of the $H_2$ orbits. The number in a row shows the $z_k$ coordinate of the $H_2$ orbit. The vertical direction is that of $z_1$.

doi:10.1371/journal.pone.0084079.g001

The dual or reciprocal $\omega$-basis is defined by

$$C_{jk} = \langle \omega_j, \omega_k \rangle = \frac{1}{\det C} \begin{pmatrix} 3 - \tau & 2 & \tau \\ 2 & 4 & 2\tau \\ \tau & 2\tau & 3 \end{pmatrix}$$

It follows from Eq.(2) that the $x$- and $\omega$-bases are related by the matrix equality $x = C \omega$, and $\omega = C^{-1} x$. Explicitly we have

$$\begin{align*}
x_1 &= 2\omega_1 - \omega_2 & \omega_1 &= (1 + \frac{1}{2}\tau)z_1 + (1 + \tau)z_2 + (\frac{1}{2} + \tau)z_3 \\
x_2 &= -\omega_1 + 2\omega_2 - \tau\omega_3 & \omega_2 &= (1 + \tau)z_1 + (2 + 2\tau)z_2 + (1 + 2\tau)z_3 \\
x_3 &= -\tau\omega_2 + 2\omega_3 & \omega_3 &= (\frac{1}{2} + \tau)z_1 + (1 + 2\tau)z_2 + (3 + \frac{3}{2}\tau)z_3
\end{align*}$$

For the $\omega$-basis of $H_2$ we choose $\omega_2$ and $\omega_3$ of $H_3$. By Eq.(2), the direction orthogonal to the plane spanned by $\omega_2$ and $\omega_3$, is that of $x_1$.

The reflections $r_1$, $r_2$, and $r_3$ in $\mathbb{R}^3$ generate the icosahedral group of order 120. Their action on any vector $x \in \mathbb{R}^3$ is given by

$$r_k x = x - \langle x, x_k \rangle x_k, \quad k = 1,2,3, \quad x \in \mathbb{R}^3.$$  

In particular, $r_1 0 = 0$ and $r_2 x_k = -x_k$, and also $r_2 \omega_0 = \omega_0 - \delta_k x_k$.

$C_{60}$

Repeated application of the three reflections to the seed point $(1,1,0) = \omega_1 + \omega_2$ of $C_{60}$, according to Eq.(5), yields the 60 vertices of $C_{60}$ in the $\omega$-basis:

Figure 2. The structure of the $C_{70}$ molecule. (a) The polytope $C_{70}$ has 105 edges and 12 pentagonal and 25 hexagonal faces. (b) $C_{70}$ viewed from a direction almost parallel to the plane of $\omega_2$ and $\omega_3$. (c) The $H_2$ structure of $C_{70}$ viewed from a direction parallel to the plane of $\omega_2$ and $\omega_3$. The column of numbers shows the $z_1$-coordinate of the $H_2$ orbits of vertices of $C_{70}$. The inserted decagon has the $z_1$-coordinate equal to 0. Surface edges are omitted in (b) and (c).

doi:10.1371/journal.pone.0084079.g002
The straight line containing special positions also in \( C \) points of which have 0 as their second or third coordinate, are the dominant coordinates are positive dominate the decagons. The boxed points, and decagons). Boxed points in which the second and third dominant point of \( C \) of the hexagon generated by \( r \) center of opposite pentagons on the surface of \( C \). Their relative angles and lengths are read from the matrix \( \begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \end{pmatrix} \) come up naturally from the classification of its 2-faces as one orbit of the seed pentagon. The symmetry group of the seed pentagon is generated by the reflections \( r_2 \) and \( r_3 \).

Let us illustrate the construction of the seed hexagon and of the seed pentagon, starting from the dominant point of \( C_60 \):

\[
\begin{align*}
(1,1,0) & \quad r_1 & \quad (1,0) \\
(-1,0,0) & \quad r_2 & \quad (2,-1,\tau) \\
(1,2,\tau) & \quad r_3 & \quad (2,1,\tau) \\
(-1,2,\tau) & \quad r_4 & \quad (2,-1,\tau) \\
(-1,-1,2\tau) & \quad r_5 & \quad (2,1,\tau) \\
(1,-1,2\tau) & \quad r_6 & \quad (2,-1,\tau)
\end{align*}
\]

The vertices of a hexagon and pentagon of the surface of \( C_60 \) are shown here in the \( \tau \)-basis.

Example 2
The three simple roots, \( x_1, x_2, x_3 \), of the icosahedral group form a special basis in \( \mathbb{R}^3 \). Their relative angles and lengths are read from the matrix \( C \) (Eq.1). Those values define the icosahedral group \( H_3 \). Therefore they take special positions also in \( C_60 \).

Let us show that (i) the straight line containing \( \pm x_1 \) passes through the center of opposite pentagons on the surface of \( C_60 \). To show it, one needs to take the seed generated by \( r_1 \) and \( r_2 \), and add its vertices to verify that coordinates of the sum are zero in the plane spanned by \( \omega_2 \) and \( \omega_3 \),

\[
x_1 \sim (1,1,0) + (2,-1,\tau) + (2,\tau,-\tau) + (2-\tau,-\tau,1) + (1,2\tau,0,0) = 0
\]

(ii) The straight line containing \( \pm x_2 \) passes through the center of opposite edges on the surface of \( C_60 \) that separate two hexagons.

Example 3
In this example let us view each point \( x \) of Eq.(1) as an exponential function, \( \lambda \to e^{2\pi i \langle \lambda, x \rangle} \), where \( x \in \mathbb{R}^3 \), and then add up all \( 60 \) such exponentials. Call such a sum \( C(\lambda, x) \). Since each \( \lambda \) comes with both signs in Eq.(1), we have \( C(\lambda, x) \) equal to the sum of 8 orbits of \( 60 \) to the cosines \( \cos(2\pi \langle \lambda, x \rangle) \).

Properties of \( C(\lambda, x) \) deserves further study. The function ‘remembers’ the structure of \( C_60 \) in the entire 3-space and shows intricate interferences of the cosines with a clear maximum when \( x \) is at the origin of \( \mathbb{R}^3 \). On the spherical surface of the \( C_60 \) shell, the function \( C(\lambda, x) \) depends periodically on the radius of \( C_60 \).

The general idea, we pursue here for the modification \( C_60 \to C_70 \), is first to decompose \( C_60 \) into the sum of 8 orbits of \( H_3 \), then to insert another \( H_2 \) decagon into its middle. In Fig. 3 it can be seen that the upper and lower half of \( C_60 \) are connected by a ring of 5 hexagons. Replacing that ring by a larger one that is

\[
x_2 \sim (1,1,0) + (1,2,0) \quad (0,3,0)
\]

(iii) The straight line containing \( \pm x_3 \) passes through the center of opposite hexagons on the surface of \( C_60 \).

\[
x_3 \sim (1,1,0) + (1,2,0) + (2,1,\tau) + (1,2,\tau) + (1,1,2\tau) = (0,0,6\tau)
\]

Figure 3. The 12 pentagons of the surface of \( C_60 \) are shown without the hexagons. The 60 dots are the vertices of \( C_60 \). The polytope is oriented as in Fig. 1. doi:10.1371/journal.pone.0084079.g003
made out of 10 hexagons (see Fig. 4), one gets the polytope $C_{70}$. It is shown in Fig. 2 in three different views analogous to the presentation of $C_{60}$ in Fig. 1.

Symmetry breaking

The $H_3$ symmetry gets broken when the additional decagon is inserted into the middle of its decomposition into $H_2$-orbits. The $H_3$ symmetry remains exact.

$$C_{70} : \quad 5 + 5 + 10 + 10 + \mathbb{R} + 10 + 10 + 5 + 5, \quad (7)$$

The enlarged structure is $C_{70}$ which has lost the spherical symmetry of $C_{60}$. It has 70 vertices, and in the middle of it there are 5 consecutive parallel decagons centered at the $z_1$-axis.

There are still two questions to be answered however before one can call it $C_{70}$. The answers to these questions must assure that the exterior surface of $C_{70}$ is composed of pentagons and hexagons of the same size as it is for $C_{60}$. From Fig. 3 we see that the upper and lower halves of $C_{60}$ are bound by a ring of hexagons. (i) What are the distances between the five decagons, and (ii) what is the orientation of the inserted decagon in the $z_1$-plane?

The answers to the questions are found by making two observations from Fig. 4, where the additional decagon is placed in the middle, so that its $z_1$ coordinate is zero.

(i) In order to keep the distances between the five decagons of $C_{70}$ equal to what they are in $C_{60}$, we have to shift correspondingly the upper and the lower halves of what used to be $C_{60}$. Their $z_1$ coordinates are increased and decreased by 0.5$r$ respectively.

(ii) The first row of hexagons in Fig. 4 (right), belonged to the upper half of $C_{60}$. The second row in Fig. 4 (right) is situated as was the second row in Fig. 4 (left). There it was the top row for the lower part of $C_{60}$. In Fig. 4 (right) it is the inserted middle row of $C_{70}$. The third row of hexagons in Fig. 4 (right) is the top row of the lower half of $C_{60}$. However, its position matches the hexagons of the first row. Hence the dominant points of the first and third rows differ by the sign of the first coordinate only.

Summarizing, below are the exact coordinate of the 70 vertices of $C_{70}$ in the basis $\{z_1, \omega_2, \omega_3\}$:

$$(8)$$

According to [19] the carbon polytope $C_{70}$ is slimmer in the middle. Such data can be matched by choosing a smaller radius for the decagon $(0,1,2)$ in Eq.(8) in the middle of $C_{70}$. Also the edges leading to that decagon may have to be changed correspondingly. The boxed points in Eq.(8) are the dominant points.

In the present work we have described the existence of the molecule $C_{70}$ in terms of a symmetry breaking process of the insertion of an $H_3$ decagon (or equivalently inserting a ring of surface hexagons), thus breaking the icosahedral symmetry of $C_{60}$. There is nothing to prevent however, the insertion of three or more rings of hexagons into the $C_{60}$ structure creating ones that are larger and more complex. Thus the mechanism enables the creation from $C_{60}$, the fullerene $C_{70}$, $C_{80}$, $C_{90}$ and so on. From the continuation of the process of the insertion of hexagon rings in this fashion, it can also readily be seen that it enables the creation of nanotubes of any length.

Acknowledgments

M.S. is grateful to CRM, Université de Montréal, for the hospitality extended to her during her postdoctoral fellowship. The authors would like to thank Dr. M. Angelova for stimulating discussions and comments.

Author Contributions

Conceived and designed the experiments: MB JP MS. Performed the experiments: MB JP MS. Analyzed the data: MB JP MS. Wrote the paper: MB JP MS.
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