Applied Mathematics, 2020, 11, 473-479
https://www.scirp.org/journal/am
ISSN Online: 2152-7393
ISSN Print: 2152-7385

On the ECI and CEI of (3, 6)-Fullerenes

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How to cite this paper: Wu, T.Z. and Lü, H.Z. (2020) On the ECI and CEI of (3, 6)-Fullerenes. *Applied Mathematics*, **11**, 473-479.
https://doi.org/10.4236/am.2020.116034

Received: May 14, 2020
Accepted: June 7, 2020
Published: June 10, 2020

Abstract

The eccentricity of a vertex in a graph is the maximum distance from the vertex to any other vertex. Two structure topological indices: eccentric connectivity index and connective eccentricity index involving eccentricity have a wide range of applications in structure-activity relationships and pharmaceutical drug design etc. In this paper, we investigate the eccentric connectivity index and the connective eccentricity index of a (3, 6)-fullerene. We find a relation between the radius and the number of spokes of a (3, 6)-fullerene. Based on the relation, we give the computing formulas of the eccentric connectivity index and the connective eccentricity index of a (3, 6)-fullerene, respectively.

Keywords

Eccentricity, Eccentric Connectivity Index, Connective Eccentricity Index, (3, 6)-Fullerene

1. Introduction

In this paper, we consider finite undirected simple connected graphs and follow the notation and terminology of [1].

Let $G=(V,E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Let $d(v)$ denote the degree of a vertex v. For vertices $u,v\in V(G)$, the *distance* $d(u,v)$ is defined as the length of the shortest path between u and v in G. The *eccentricity* $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex.

In organic chemistry, topological indices have a wide range of applications, such as isomer discrimination, structure-property relationships, structure-activity (SAR) relationships and pharmaceutical drug design etc. Recently, two topological indices involving eccentricity have attracted much attention. One is connective eccentricity index, the other is eccentric connectivity index. The *connective* *eccentricity index* (CEI briefly), denoted by $\xi^{ce}(G)$, is defined as follows:

$$\xi^{ce}(G)=\sum_{v\in V(G)}\frac{d(v)}{\varepsilon(v)}. \tag{1}$$

Gupta *et al.* [2] first used CEI to explore the antihypertensive activity of derivatives of N-benzylimidazole. For more background and some known results about CEI, we refer the reader to [3]-[10] and the references therein.

The *eccentric connectivity index* (ECI for short), denoted by $\xi^{c}(G)$, is defined as follows:

$$\xi^{c}(G)=\sum_{v\in V(G)}d(v)\varepsilon(v). \tag{2}$$

The ECI was first introduced by Sharma *et al.* [11], which has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature [12]-[18].

In the study of ECI and CEI, a natural problem is how to compute the ECI and CEI for a molecular graph. In this paper, our aim is to investigate the calculation formulas of ECI and CEI of a (3, 6)-fullerene.

An outline of the rest of the paper is to follows. In Section 2, we will present some properties of (3, 6)-fullerenes. In Section 3, we will give the computing formulas of ECI and CEI of a (3, 6)-fullerene.

2. Some Preliminaries

As a member of the fullerene family, (3, 6)-fullerenes has been extensively studied, see [19] [20] [21], among others. A (3, 6)-fullerene is a cubic plane graph whose faces have sizes 3 and 6. Let G be a (3, 6)-fullerene graph with n vertices. By Euler's formula, G has exactly four faces of size 3 and $\frac{n}{2}-2$ faces of size 6. And the connectivity of G is 2 or 3.

The structure of a (3, 6)-fullerene with connectivity 3 is well known, namely, it is determined by only 3 parameters *r*, *s* and *t*, where $r\geq 1$ is the radius (number of rings), s is the size (number of spokes in each layer and $s\geq 4$ is even), and t is the twist (torsion, $0<t\leq s$, $t\equiv r(\bmod 2)$). So we denote it by $F(r,s,t)$. For example, $F(2,4,2)$ and $F(2,4,0)$ are depicted in **Figure 1**, C is a cap of $F(2,4,2)$ and $F(2,4,0)$.

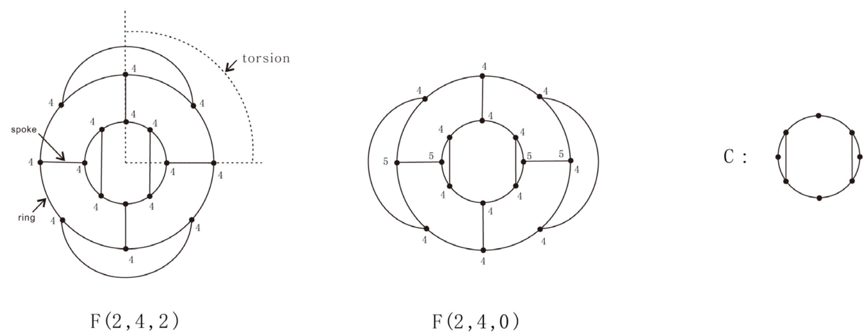

Figure 1. A (3, 6)-fullerene $F(r,s,t)$ with $r=2$, $s=4$, $t=2$ (or 0) and a cap C of them.

Yang and Zhang [22] characterized the structure of a (3, 6)-fullerene with connectivity 2.

Lemma 1. [22] *A* (3, 6)-*fullerene G has the connectivity* 2 *if and only if* $G \cong T_l$ *for some integer* $l \ge 2$, *where* T_l *is the tube consisting of l cyclic chains each of two hexagons, capped on each end by a cap of two adjacent triangles*, see Figure 2.

3. Main Results

Since a (3, 6)-fullerene is a 3-regular graph, if the eccentricity of every vertex of the (3, 6)-fullerene is known, then the ECI and CEI of the (3, 6)-fullerene can be computed. Thus, the following we will discuss the eccentricity of all vertices of $F(r,s,t)$.

Checking $F(r,s,t)$, it can be known that $F(r,s,t)$ consists of $r-1$ concentric layers of hexagons (*i.e.* each layer is a cyclic chain of s hexagons) and two caps with torsion t on ends. Thus, the radius, the number of spokes and the twist of $F(r,s,t)$ necessarily affects the eccentricity of every end of $F(r,s,t)$. As an example, we label the eccentricity of every vertex of $F(2,4,0)$ and $F(2,4,2)$, see Figure 1. Through a lot of illustrations, we find a relation between the radius r and the number of spokes s, and give the following result.

Theorem 1. *Let* $F(r,s,t)$ *be a* (3, 6)-*fullerene. If* $r \ge 2s-1$, *then*

$$\xi^{ce}\left(F(r,s,t)\right) = 6s\sum_{j=0}^{r-1}\frac{1}{r+j} \text{ and } \xi^{c}\left(F(r,s,t)\right) = 9sr^2 - 3sr.$$

Proof. Let $r \ge 2s-1$ in a (3, 6)-fullerene $F(r,s,t)$. Checking the structure of $F(r,s,t)$, we can obtain the following laws:

1) By the definition of eccentricity, we find that the eccentricity of every vertex of $F(r,s,t)$ do not change when the twist t changes. We give an example, see Figure 3.

2) Let u,v be two vertices of $F(r,s,t)$. The distance $d(u,v)$ attains the maximum value only when one of u and v belongs to a vertex of a cap of $F(r,s,t)$. If r is odd, then the eccentricity of every vertex of $\frac{r+1}{2}$-layer equal to r, and the eccentricity of every vertex of $\frac{r+1}{2}$-layer attain the minimum value in all vertices of $F(r,s,t)$. If r is even, then the eccentricities of the vertex pairs equal to r, and the eccentricities of the vertex pairs attain the minimum value in all vertices of $F(r,s,t)$, where the vertex pairs are adjacent, and one belongs to

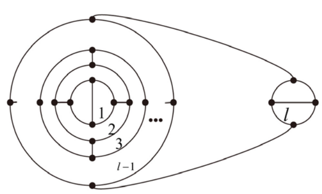

Figure 2. A (3, 6)-fullerene T_l.

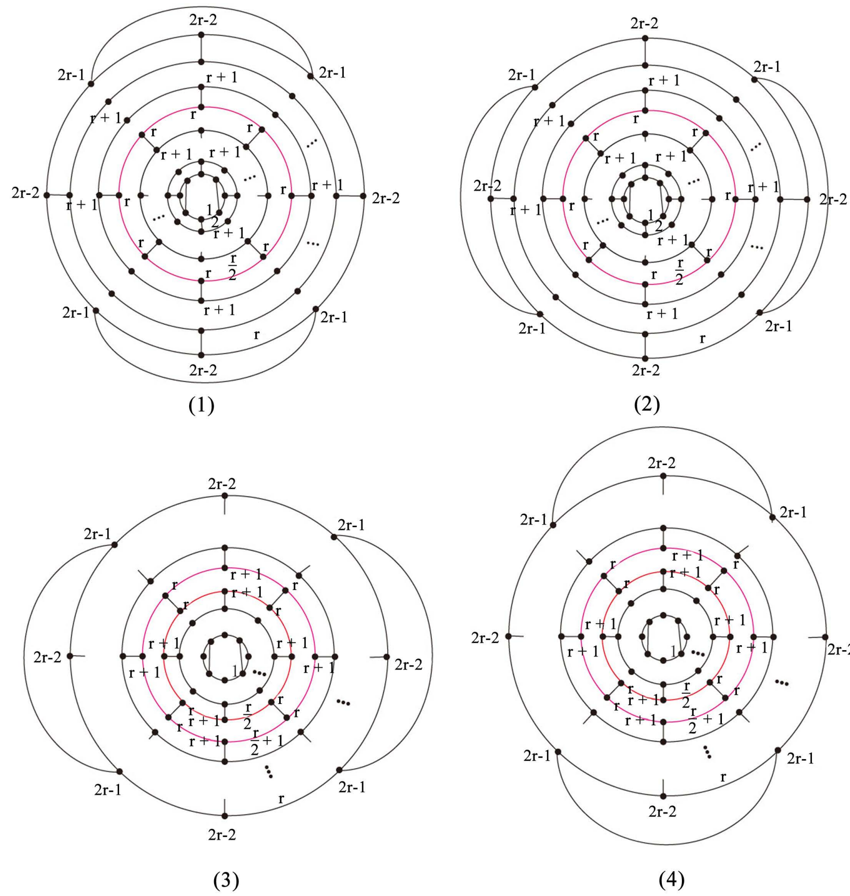

Figure 3. The eccentricity of every vertex of a (3, 6)-fullerene $F(r,s,t)$.

$\frac{r}{2}$-layer, the other belongs to $\frac{r}{2}$-layer. Thus, the eccentricity sequence of $F(r,s,t)$ is $\overbrace{r,\cdots,r}^{2s},\overbrace{r+1,\cdots,r+1}^{2s},\cdots,\overbrace{2r-1,\cdots,2r-1}^{2s}$.

Combining (1), (2) and arguments above, we have

$$\xi^{ce}(G) = 3\times 2s\times\left(\frac{1}{r}+\frac{1}{r+1}+\cdots+\frac{1}{2r-1}\right) \tag{3}$$

$$= 6s\left(\frac{1}{r}+\frac{1}{r+1}+\cdots+\frac{1}{2r-1}\right) \tag{4}$$

$$= 6s\sum_{j=0}^{r-1}\frac{1}{r+j} \tag{5}$$

and

$$\xi^{c}(G) = 3\times 2s\times\left[r+(r+1)+\cdots+(2r-1)\right] \tag{6}$$

$$= 6s\left(r^2+\frac{r^2-r}{2}\right) \tag{7}$$

$$= 9sr^2-3sr. \tag{8}$$

The proof is completed.

Theorem 2. *Let* $T_l\,(l\geq 1)$ *be a* (3, 6)-*fullerene. Then*

$$\xi^{ce}(T_l)=\begin{cases}12 & \text{if } l=1,\\ 8 & \text{if } l=2,\\ 12\sum_{j=0}^{l-1}\frac{1}{l+j} & \text{if } l\ge 3.\end{cases} \text{ and } \xi^{c}(T_l)=\begin{cases}12 & \text{if } l=1,\\ 72 & \text{if } l=2,\\ 18l^2-6l & \text{if } l\ge 3.\end{cases} \tag{9}$$

Proof. Checking T_l, it is easy to see that the eccentricity of every vertex of T_l is 1. By (1) and (2), we have $\xi^{ce}(T_1)=12$ and $\xi^{c}(T_1)=12$.

Similarly, checking T_l, if $l=2$, then the eccentricity of every vertex of T_l equals to 3. By (1) and (2), we have $\xi^{ce}(T_1)=8$ and $\xi^{c}(T_1)=72$.

Let $l\ge 3$ in T_l. By the structure of T_l, it is easy to know that the eccentricity sequence of T_l is $\left(\overbrace{l,l,l,l}^{4},\overbrace{l+1,l+1,l+1,l+1}^{4},\cdots,\overbrace{2l-1,2l-1,2l-1,2l-1}^{4}\right)$. By (1) and (2), we have

$$\xi^{ce}(G)=3\times 4\times\left(\frac{1}{l}+\frac{1}{l+1}+\cdots+\frac{1}{2l-1}\right) \tag{10}$$

$$=12\left(\frac{1}{l}+\frac{1}{l+1}+\cdots+\frac{1}{2l-1}\right) \tag{11}$$

$$=12\sum_{j=0}^{l-1}\frac{1}{l+j}, \tag{12}$$

and

$$\xi^{c}(G)=3\times 4\times\left[l+(l+1)+\cdots+(2l-1)\right] \tag{13}$$

$$=12\left(l^2+\frac{l^2-l}{2}\right) \tag{14}$$

$$=18l^2-6l. \tag{15}$$

For notation consistency, T_l can be denoted by $F(r,s)$ with $r=l$ and $s=2$, where r is the radius and s is the number of spokes of a (3, 6)-fullerene.

By Theorems 1 and 2, we can obtain the following result.

Theorem 3. *Let G be a* (3, 6)-*fullerene with the radius r and the number of spokes s. If* $r\ge 2s-1$. *Then*

$$\xi^{ce}(G)=6s\sum_{j=0}^{r-1}\frac{1}{r+j} \text{ and } \xi^{c}(G)=9sr^2-3sr. \tag{16}$$

4. Discussions

In this paper, we investigate the ECI and CEI of a (3, 6)-fullerene. We obtain an important relation between radius r and the number of spokes s of a (3, 6)-fullerene. That is, if $r\ge 2s-1$, then the twist of a (3, 6)-fullerene does not change the eccentricity of every vertex of the (3, 6)-fullerene. Based on the relation, we give the computing formulas of ECI and CEI of a (3, 6)-fullerene, respectively.

Let us conclude this paper with a question:

Question. How to compute the ECI and CEI of a (3, 6)-fullerene when

$r < 2s - 1$?

Acknowledgements

This research is supported by the National Natural Science Foundation of China (No. 11761056), the Natural Science Foundation of Qinghai Province (No. 2016-ZJ-947Q), the Scientific Research Innovation Team in Qinghai Nationalities University.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

[1] Bondy, J.A. and Murty, U.S.R. (1976) Graph Theory with Applications. Macmillan, London. https://doi.org/10.1007/978-1-349-03521-2

[2] Gupta, S., Singh, M. and Madan, A.K. (2000) Connective Eccentricity Index: A Novel Topological Descriptor for Predicting Biological Activity. *Journal of Molecular Graphics and Modelling*, **18**, 18-25. https://doi.org/10.1016/S1093-3263(00)00027-9

[3] Azari, M. and Iranmanesh, A. (2013) Computing the Eccentric-Distance Sum for Graph Operations. *Discrete Applied Mathematics*, **161**, 2827-2840. https://doi.org/10.1016/j.dam.2013.06.003

[4] Geng, X., Li, S. and Zhang, M. (2013) Extremal Values on the Eccentric Distance Sum of Trees. *Discrete Applied Mathematics*, **161**, 2427-2439. https://doi.org/10.1016/j.dam.2013.05.023

[5] Li, S., Zhang, M., Yu, G. and Feng, L. (2012) On the Extremal Values of the Eccentric Distance Sum of Trees. *Journal of Mathematical Analysis and Applications*, **390**, 99-112. https://doi.org/10.1016/j.jmaa.2012.01.022

[6] Yu, G. and Feng, L. (2013) On the Connective Eccentricity Index of Graphs. *MATCH Communications in Mathematical and in Computer Chemistry*, **69**, 611-628.

[7] Yu, G., Feng, L. and Ilić, A. (2011) On the Eccentric Distance Sum of Trees and Unicyclic Graphs. *Journal of Mathematical Analysis and Applications*, **375**, 99-107. https://doi.org/10.1016/j.jmaa.2010.08.054

[8] Yu, G., Qu, H., Tang, L. and Feng, L. (2014) On the Connective Eccentricity Index of Trees and Unicyclic Graphs with Given Diameter. *Journal of Mathematical Analysis and Applications*, **420**, 1776-1786. https://doi.org/10.1016/j.jmaa.2014.06.050

[9] Xu, K., Das, K. and Liu, H. (2016) Some Extremal Results on the Connective Eccentricity Index of Graphs. *Journal of Mathematical Analysis and Applications*, **433**, 803-817. https://doi.org/10.1016/j.jmaa.2015.08.027

[10] Xu, K., Liu, M., Das, K., Gutman, I. and Furtula, B. (2014) A Survey on Graphs Extremal with Respect to Distance-Based Topological Indices. *MATCH Communications in Mathematical and in Computer Chemistry*, **71**, 461-508.

[11] Sharma, V., Goswami, R. and Madan, A.K. (1997) Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure-Property and Structure-Activity Studies. *The Journal for Chemical Information and Computer Scientists*, **37**, 273-282. https://doi.org/10.1021/ci960049h

[12] Ashrafi, A.R., Došlić, T. and Saheli, M. (2011) The Eccentric Connectivity Index of TUC4C8(R) Nanotubes. *MATCH Communications in Mathematical and in Computer Chemistry*, **65**, 221-230.

[13] Došlić, T., Saheli, M. and Vukicevic, D. (2010) Eccentric Connectivity Index: Extremal Graphs and Values. *Iranian Journal of Mathematical Chemistry*, **1**, 45-56.

[14] Dureja, H., Gupta, S. and Madan, A.K. (2008) Predicting Anti-HIV-1 Activity of 6-Arylbenzonitriles: Computational Approach Using Superaugmented Eccentric Connectivity Topochemical Indices. *Journal of Molecular Graphics*, **26**, 1020-1029. https://doi.org/10.1016/j.jmgm.2007.08.008

[15] Ilić, A. and Gutman, I. (2011) Eccentric Connectivity Index of Chemical Trees. *MATCH Communications in Mathematical and in Computer Chemistry*, **65**, 731-744.

[16] Morgan, M.J., Mukwembi, S. and Swart, H.C. (2011) On the Eccentric Connectivity Index of a Graph. *Discrete Mathematics*, **311**, 1229-1234. https://doi.org/10.1016/j.disc.2009.12.013

[17] Zhang, J., Zhou, B. and Liu, Z. (2012) On the Minimal Eccentric Connectivity Indices of Graphs. *Discrete Mathematics*, **312**, 819-829. https://doi.org/10.1016/j.disc.2011.10.006

[18] Zhou, B. and Du, Z. (2010) On Eccentric Connectivity Index. *MATCH Communications in Mathematical and in Computer Chemistry*, **63**, 181-198.

[19] DeVos, M., Goddyn, L., Mohar, B. and Šámal, R. (2009) Cayley Sum Graphs and Eigenvalues of (3, 6)-Fullerenes. *Journal of Combinatorial Theory*, *Series B*, **99**, 358-369.

[20] Shi, L. and Zhang, H. (2016) Forcing and Anti-Forcing Numbers of (3, 6)-Fullerenes. *MATCH Communications in Mathematical and in Computer Chemistry*, **76**, 597-614.

[21] Yang, R. and Zhang, H. (2015) 2-Resonant Fullerenes. *European Journal of Combinatorics*, **49**, 13-24. https://doi.org/10.1016/j.ejc.2015.02.025

[22] Yang, R. and Zhang, H. (2012) Hexagonal Resonance of (3, 6)-Fullerenes. *Journal of Mathematical Chemistry*, **50**, 261-273. https://doi.org/10.1007/s10910-011-9910-8