

# On the ECI and CEI of Boron-Nitrogen Fullerenes

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## Abstract

The eccentric connectivity index and connective eccentricity index are important topological indices for chemistry. In this paper, we investigate the eccentric connectivity index and connective eccentricity index of boron-nitrogen fullerenes, respectively. And we give computing formulas of eccentric connectivity index and connective eccentricity index of all boron-nitrogen fullerenes with regular structure.

## Keywords

Eccentric Connectivity Index, Connective Eccentricity Index, Boron-Nitrogen Fullerenes

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## 1. Introduction

All graphs considered in this paper are simple connected graphs. Let  $G$  be a graph with vertex set  $V(G)$  and edge set  $E(G)$ . Let  $v \in V(G)$ ,  $d(v)$  denotes the degree of  $v$ . For vertices  $u, v \in V(G)$ , the *distance*  $d(u, v)$  is defined as the length of a 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.

The chemical information derived through the topological index has been found useful in chemical documentation, isomer discrimination, structure-property correlations, etc. For quite some time there has been rising interest in the field of computational chemistry in topological indices. The interest in topological indices is mainly related to their use in nonempirical quantitative structure-property relationships and quantitative structure-activity relationships. Among various indices, the eccentric connectivity index and connective eccentricity index involving eccentricity have attracted much attention.

Sharma *et al.* [1] introduced a distance-based molecular structure descriptor,

the *eccentric connectivity index* (ECI for short) defined as

$$\xi^c(G) = \sum_{v \in V(G)} d(v) \varepsilon(v). \quad (1)$$

The ECI was successfully used for mathematical models of biological activities of diverse nature, see [2]-[7] and the references cited therein.

A novel graph invariant for predicting biological and physical properties—*connective eccentricity index* (CEI briefly) was introduced by Gupta *et al.* [8], which was defined as:

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)}. \quad (2)$$

Some recent results on the CEI of graphs can be found in [9]-[14].

Boron-nitrogen fullerene is a member of the fullerene family, it has been extensively studied [15] [16] [17]. A boron-nitrogen fullerene is also called (4,6)-fullerene graph which is a plane cubic graph whose faces have sizes 4 and 6. Let  $G$  be a (4,6)-fullerene graph with  $n$  vertices. By Euler's formula,  $G$  has exactly six faces of size 4 and  $\frac{n}{2} - 4$  faces of size 6.

A (4,6)-fullerene graph is said to be of *dispersive structure* if has neither three squares arranged in a line nor a square-cap. According to the quadrilateral positional relationship, Wei and Zhang [18] given a classification of all (4,6)-fullerenes as follows.

**Lemma 1 [18]** *Let  $G$  be a (4,6)-fullerene graph. Then  $G$  can be of one of the following five types:*

- 1) a cube,
- 2) a hexagonal prism,
- 3) a tubular graph with at least one hexagon-layer,
- 4) a (4,6)-fullerene graph of lantern structure,
- 5) a (4,6)-fullerene graph of dispersive structure,

where the resulting graphs see **Figure 1**.

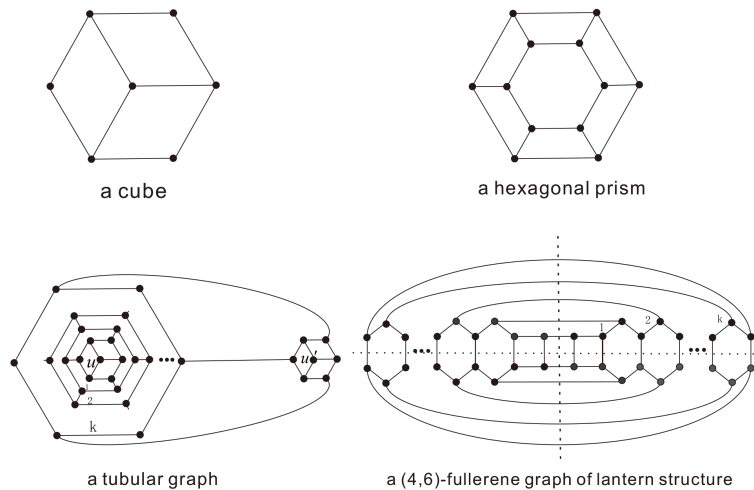
In this paper, we aim to investigate the ECI and CEI of a boron-nitrogen fullerene. In next section, we give computing formulas of ECI and CEI of a boron-nitrogen fullerene.

## 2. Computing Formula of ECI and CEI of a (4,6)-Fullerene

In this section, according the classification of all boron-nitrogen fullerenes in Lemma 1, we will give computing formula of CEI of a (4,6)-fullerene.

**Theorem 2** *Let  $G$  be a (4,6)-fullerene graph. Then*

- 1)  $\xi^{ce}(G) = \begin{cases} 8 & \text{if } G \text{ is a cube,} \\ 9 & \text{if } G \text{ is hexagonal prism.} \end{cases}$
- 2)  $\xi^c(G) = \begin{cases} 72 & \text{if } G \text{ is a cube,} \\ 144 & \text{if } G \text{ is hexagonal prism.} \end{cases}$



**Figure 1.** The (4,6)-fullerenes in Lemma 1.

*Proof.* Let  $G$  be a cube. Checking the structure of  $G$ , we obtain that the eccentricity of every vertex in  $G$  is 3. By (1) and (2), we have

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(G)} \frac{3}{3} = 8, \tag{3}$$

and

$$\xi^c(G) = \sum_{v \in V(G)} d(v)\varepsilon(v) = \sum_{v \in V(G)} 3 \times 3 = 72. \tag{4}$$

Similarly, let  $G$  be a hexagonal prism. Checking the structure of  $G$ , we obtain that the eccentricity of every vertex in  $G$  is 4. By (1) and (2), we obtain

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)} = \sum_{v \in V(G)} \frac{3}{4} = 9, \tag{5}$$

and

$$\xi^c(G) = \sum_{v \in V(G)} d(v)\varepsilon(v) = \sum_{v \in V(G)} 3 \times 4 = 144. \tag{6}$$

□

**Theorem 3** Let  $G$  be a tubular graph, and let the number of hexagon-layer in  $G$  be  $k \geq 1$ . Then

$$\xi^{ce}(G) = 18 \sum_{i=3}^{k+4} \frac{1}{k+i} + \frac{6}{2k+5}; \tag{7}$$

$$\xi^c(G) = 27k^2 + 129k + 156. \tag{8}$$

*Proof.* Let  $v$  be a vertex of  $G$ . By the structure of  $G$  (see **Figure 1**), we know that the eccentricity of  $v$  equal to the distance between  $v$  and  $u$  (or  $u'$ ). Thus, the eccentricity sequence of  $G$  is  $(\overbrace{2k+5, 2k+5}^2, \overbrace{2k+4, \dots, 2k+4}^6, \overbrace{2k+3, \dots, 2k+3}^6, \dots, \overbrace{k+4, \dots, k+4}^6, \overbrace{k+3, \dots, k+3}^6)$ . By (1) and (2), we obtain

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)} \tag{9}$$

$$= 3 \left[ \left( \frac{1}{2k+4} + \frac{1}{2k+3} + \dots + \frac{1}{k+3} \right) \times 6 + \frac{1}{2k+5} \times 2 \right] \tag{10}$$

$$= 18 \sum_{i=3}^{k+4} \frac{1}{k+i} + \frac{6}{2k+5}. \tag{11}$$

and

$$\xi^c(G) = \sum_{v \in V(G)} d(v) \varepsilon(v) \tag{12}$$

$$= 3 \left[ 2(2k+5) + 6 \left[ (k+3) + (k+4) + \dots + (2k+4) \right] \right] \tag{13}$$

$$= 3 \left[ 2(2k+5) + 6 \frac{[(k+3) + (2k+4)](k+2)}{2} \right] \tag{14}$$

$$= 27k^2 + 129k + 156. \tag{15}$$

This completes the proof.  $\square$

**Theorem 4** Let  $G$  be a (4,6)-fullerene graph having lantern structure, and let the number of hexagon-layer in  $G$  be  $k \geq 1$ , see **Figure 1**. Then

$$\xi^{ce}(G) = 24 \sum_{i=3}^{k+3} \frac{1}{k+i}; \tag{16}$$

$$\xi^c(G) = 36k^2 + 108k + 72. \tag{17}$$

*Proof.* Checking  $G$ , we see that  $G$  is symmetry. By the symmetry of  $G$ , it is easy to obtain that the eccentricity sequence of  $G$  is  $(\overbrace{2k+3, \dots, 2k+3}^8, \overbrace{2k+2, \dots, 2k+2}^8, \dots, \overbrace{k+4, \dots, k+4}^8, \overbrace{k+3, \dots, k+3}^8)$ . By (1) and (2), we have

$$\xi^{ce}(G) = \sum_{v \in V(G)} \frac{d(v)}{\varepsilon(v)} \tag{18}$$

$$= 3 \left[ \left( \frac{1}{2k+3} + \frac{1}{2k+2} + \dots + \frac{1}{k+3} \right) \times 8 \right] \tag{19}$$

$$= 24 \sum_{i=3}^{k+3} \frac{1}{k+i}. \tag{20}$$

and

$$\xi^c(G) = \sum_{v \in V(G)} d(v) \varepsilon(v) \tag{21}$$

$$= 3 \left[ 8 \left[ (k+3) + (k+4) + \dots + (2k+2) + (2k+3) \right] \right] \tag{22}$$

$$= 3 \left[ 8 \frac{[(k+3) + (2k+3)](k+1)}{2} \right] \tag{23}$$

$$= 36k^2 + 108k + 72. \tag{24}$$

The proof of the theorem is now complete.  $\square$

### 3. Conclusion

In this note, we give calculation formulas of ECI and CEI of all (4,6)-fullerenes

with regular structures, respectively. In the future, we will discuss the calculation of ECI and CEI of a (4,6)-fullerene graph of dispersive structure, and try to give an algorithm.

### Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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