Short communication

Third-Connectivity and Third-sum-Connectivity Indices of Circumcoronene Series of Benzenoid H_k

Mohammad Reza Farahani*

Department of Applied Mathematics of Iran University of Science and Technology, (IUST) Narmak, Tehran 16844, Iran

** Corresponding author: E-mail: Mr_Farahani@Mathdep.iust.ac.ir*

Received: 30-07-2012

Abstract

The m-connectivity index and m-sum connectivity index of a connected graph $G = (V,E)$ are ${}^m\chi(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}\dots d_{i_{m+1}}}}$ and ${}^mX(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+\dots+d_{i_{m+1}}}}$, where $v_{i_1}v_{i_2}\dots v_{i_{m+1}}$ runs over all paths of length m in G and d_i is the degree of vetex $v_i \in V(G)$. In this paper, we introduce a closed formula of the third-connectivity index and third-sum-connectivity index of molecular graph Circumcoronene Series of Benzenoid H_k $(k \geq 1)$.

Keywords: Benzenoid, m-connectivity index, m-sum-connectivity index, connected graph, Circumcoronene Series

1. Introduction

Let $G = (V,E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$ and $|V(G)| = n$, $|E(G)| = e$ are the number of vertices and edges of G. Also, if e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say „u and v are adjacent“. A connected graph is a graph such that there is a path between all pairs of vertices. For connected graph G, the m-connectivity index of G is defined as

$${}^m\chi(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}\dots d_{i_{m+1}}}}$$

where $v_{i_1}v_{i_2}\dots v_{i_{m+1}}$ runs over all paths of length m in G and d_i is the degree of vertex $v_i \in V(G)$.

Also in particular, *1-connectivity*, *2-connectivity* and *3-connectivity* indices are defined as

$$\chi(G)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_ud_v}},\quad {}^2\chi(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}}$$

and

$${}^3\chi(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}v_{i_4}}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}d_{i_4}}},$$

respectively.

In 1975, *Milan Randić*[1,2] introduced the *Randić connectivity index* (or 1-connectivity index) and uv runs over all pairs of adjacent vertices of G.

The m-sum connectivity index of G is defined as

$${}^mX(G)=\sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+\dots+d_{i_{m+1}}}},$$

where $v_{i_1}v_{i_2}\dots v_{i_{m+1}}$ runs over all paths of length m in G.

In particular, *1-sum-connectivity*, *2-sum-connectivity* and *3-sum-connectivity* indices are defined as

$$X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}},\quad {}^2X(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}}}$$

and

$${}^3X(G)=\sum_{v_{i_1}v_{i_2}v_{i_3}v_{i_4}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}+d_{i_4}}},$$

respectively.

In 2008, *B. Zhou* and *N. Trinajstić*[3,4] introduced a closely related variant of the Randić connectivity index and called the *sum-connectivity index*. Some mathematical properties of the (general) connectivity index and sum-connectivity index were given in references.[3–10] Since the *Circumcoronene Series of Benzenoid* is a connected molecular graph and has a very remarkable structure, we attend to general structure of this molecular graph. This family generates from *Benzene* C_6 and we denote k^{th} terms of this series by H_k $(k \geq 1)$, see Figure 1 and Figure 2. For further study and more detail of properties of this molecular graph, see paper series.[11–20]

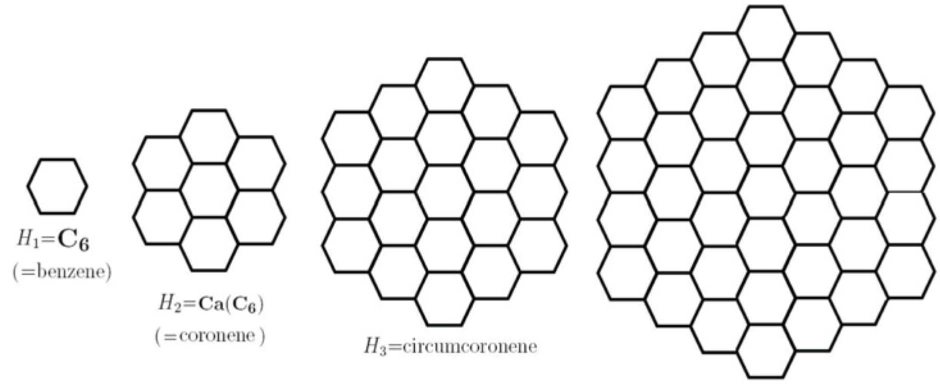

Figure 1. The first three graphs H_1, H_2, H_3 and H_4 from the circumcoronene series, such that H_1, H_2 are graphs C_6 and the Capra of planer benzenoid $Ca(C_6)$, respectively.

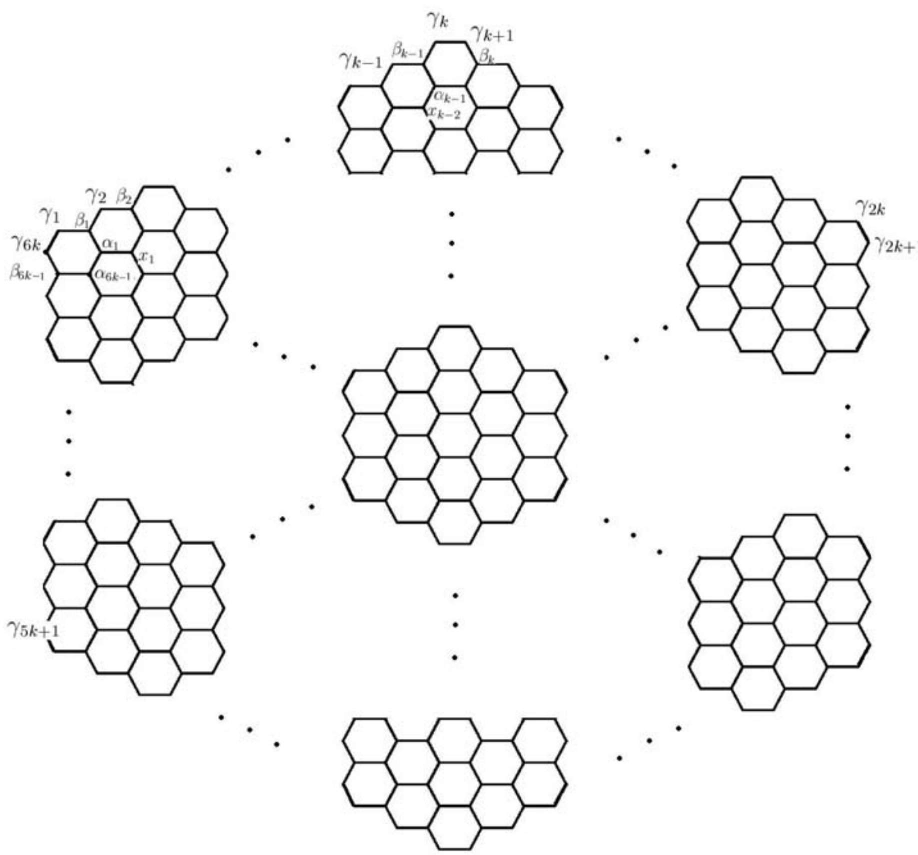

Figure 2. The circumcoronene series of benzenoid H_k $(k \geq 1)$.

In this paper, we focus on the structure of circumcoronene series of benzenoid and computing ${}^3\chi(G)$ and ${}^3X(G)$ of $G = H_k$.

2. Main Results and Discussion

According to the structure of H_k, we see that $|V(H_k)| = n_k = 6k^2$. Also, we have two partitions $V_3 = \{v \in V(H_k) | d_v = 3\}$ and $V_2 = \{v \in V(H_k) | d_v = 2\}$ of H_k with size $6k(k-1)$ and $6k$, respectively. Therefore

$$|E(H_k)| = e_k = \frac{3 \times 6k(k-1) + 2 \times 6k}{2} = 9k^2 - 3k.$$

Theorem 1.[20] consider the Circumcoronene Series of benzenoid H_k, $k \geq 1$. Then we have:

(i) The First-connectivity index of H_k is equal to:

$$\chi(H_k) = 3k^2 + (2\sqrt{6} - 5)(k - 1)$$

(ii) The First-sum-connectivity index of H_k is equal to:

$$X(H_k) = \frac{3}{2}\sqrt{6}k^2 + \left(\frac{12}{5}\sqrt{5} - \frac{5}{2}\sqrt{6}\right)k + \left(\sqrt{6} + 3 - \frac{12}{5}\sqrt{5}\right)$$

Theorem 2.[20] The Second-connectivity index and the Second-sum-connectivity index of H_k are equal to:

$$^{2}\chi(H_k)=(2k^2-3k+3)\sqrt{3}+(3k-4)\sqrt{2}$$

$$^{2}X(H_k)=6k^2+\left(\frac{9\sqrt{2}}{2}+\frac{6\sqrt{7}}{7}-12\right)k+\left(6-6\sqrt{2}+\frac{6\sqrt{7}}{7}\right)$$

Theorem 3. Let G be the circumcoronene series of benzenoid H_k $\forall$ $k \geq 1$. Then the third connectivity index and the third-sum-connectivity index of H_k are equal to:

$$^{3}\chi(H_k)=4k^2+\left(2+2\sqrt{6}-\frac{28}{3}\right)k+\left(\frac{11}{3}-\frac{4\sqrt{6}}{3}\right)$$

$$^{3}X(H_k)=6\sqrt{3}k^2+\left(\frac{6\sqrt{10}}{5}+\frac{36\sqrt{11}}{11}-14\sqrt{3}\right)k+\left(4+\frac{3\sqrt{10}}{5}-\frac{42\sqrt{11}}{11}+6\sqrt{3}\right)$$

Now, before prove Theorem 3, we introduce the general notation for vertices of circumcoronene series of benzenoid H_k in following denotation.

Denotation 1. Let $V(G)$ is the vertex set of $G = H_k$ with cardinality $6k^2$. So, we name all vertices as degree 2 by γ_i ($\forall i = 1, \dots ,6k$) and say these vertices by family $\boldsymbol{\Gamma}$, such that their adjacent vertices named by β_i (for $I = 1, \dots , 6k-1$ and $i \neq k, 2k, 3k, 4k, 5k$) and say family $\boldsymbol{B}$. In other words, $\gamma_{jk+1}\gamma_{(j+1)k}$, $\gamma_i\beta_i$ and $\gamma_{i-1}\beta_i \in E(H_k)$ Also for every allowable i, we name all β_i's adjacent vertices by α_i (say family **A**). α_i*'s* adjacent vertices named by x_i (for $I = 1, \dots, 6k-1$ and $i \neq k, 2k, 3k, 4k, 5k$) and say family $\boldsymbol{X}$. We name another vertices by y_j, $j = 1, \dots , 6k^2 – 24k + 24$, respectively and say family $\boldsymbol{Y}$.

In following proof, we attend to the degree of vertices γ_i, β_i, α_i, x_i and y_i. See Figure 2. So by use of above notations, we start proof of Theorem 3.

Proof of Theorem 3. Considered molecular graph $G = H_k$ on $6k^2$ vertices and $9k^2 – 3k$ edges. The maximum possible vertex degree in such a graph is n-1 and for H_k is 3. In other words, the vertices from family Γ have degree two and vertices from families B, A, X and Y have degree three. Suppose d_{ijkl} denote the number of 3-edges paths whose its four consecutive vertices have degree i, j, k and l respectively. Obviously $d_{ijkl} = d_{lkji}$.

By refer to reference [20], we can dividing all edge of circumcoronene series of benzenoid to three partitions E_4, E_5 and E_6, such that $|E_4| = 6 = d_{22}$, $|E_5| = 12(k\text{-}1) = d_{32}$ and $|E_6| = 9k^2 – 15k + 6 = d_{33}$. Obviously, an edge $e = uv \in E(G)$ is a member of edge set E_i if $d_u + d_v = i$.

Table 1. Categorization all 3-edges paths on based their first and end point, and the number of them. Notice that red color represent end point of diameter of cycles C_6.

The first point of path with length 3	The families of end points	The number of these path
γ_{ik+1} and $\gamma_{(i+1)k}$ (I = 0,1, ... ,5)	Γ,B,A,A,X	$5 \times 12 = 60$
α_{ik+2} and $\gamma_{(i+1)k-1}$ (I = 0, 1, …, 5)	Γ,B,A,A,X,X	6 × 12 = 72
γ_{ik+j} (I = 0, 1, … , 5 and j = 3, … , k-2)	B,B,A,A,X,X	6 × 6(k 4) = 36k 144
β_{ik+1} and $\beta_{(i+1)k-1}$ (I = 0,1, ... ,5)	Γ,B,B,A,A,X,Y	7 × 12 = 84
β_{ik+j} (I = 0,1, ... , 5 and j = 2, ... , k-2)	Γ,Γ,A,A,A,A,Y,Y	8 × 6(k 3) = 48k 144
α_{ik+1} and $\alpha_{(i+1)k-1}$ (I = 0,1, ... , 5)	Γ,Γ,Γ,B,B,A,X,Y,Y,Y	10 × 12 = 120
α_{ik+j} (I = 0, 1, ... , 5 and j = 2, ... , k-2)	B,B,B,B,X,X,Y,Y,Y,Y	10 × 6(k 3) = 60k 180
$x_i \in X$	Γ,Γ,Γ,Γ,B,A,A,X,Y,Y,Y,Y	12 × 6(k 2) = 72k 144
$y_i \in Y$	B,A,X,Y,Y,Y,Y,Y,Y,Y,Y,Y	$12 \times 6(k\text{-}2)^2 = 72k^2 – 288k + 288$

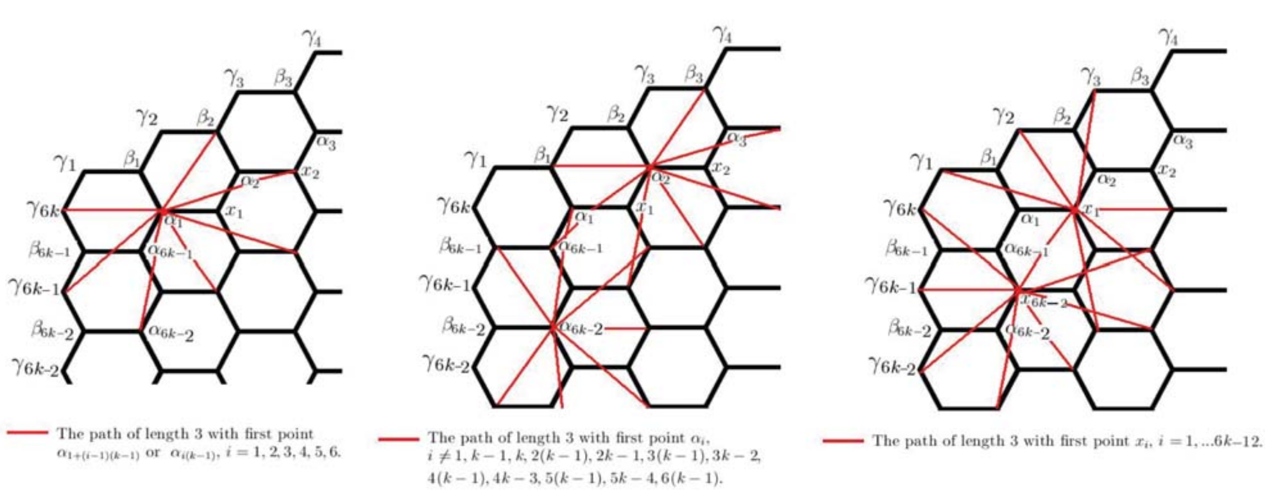

Figure 3. Example: The path with length 3 of H_k, which their first point is α_1, α_2 and x_1.

So, since a 3-edges path $v_i\, v_j\, v_k\, v_l$ pass on edge $e = v_j v_k$, thus the number of 3-edges paths of H_k is equal to $d^3(H_k) = (3\text{-}1)(3\text{-}1)|E6| + (3\text{-}1)(2\text{-}1)|E5| + (2\text{-}1)(2\text{-}1)|E_4| = 2 \times 2 \times (9k^2\text{-}15k + 6) + 2 \times 1 \times 12(k\text{-}1) + 1 \times 1 \times 6 = 36k^2 - 36k + 6$. Now, if we according to 3-edges paths of circumcoronene series of benzenoid H_k in Figure 3 and Figure 4, it is easy to see that $9k(k\text{-}1) + 3$ number of 3-edges paths are diameters of cycles C_6 and other 3-edges paths are non-diameter. In other words,

$$d^3(H_k)=36k^2\text{-}36k+6=\underbrace{2(9k\,(k-1)+3)}_{\text{diameters of cycles } C_6}+\underbrace{18k\,(k-1)}_{\text{non-diameter}}$$

Of course, we denote the number of C_6 in the molecular graph $G = H_k$ by ζ_k and $\zeta_k = 3k(k - 1) + 1$. Now, by using above terminologies and Denotation 1, we can categorize the paths with length 3 (all 3-edges paths) on based their first and end point in following table.

So, Table 1 implies that $d_{2232} = ½(12 + 12) = 12$, $d_{3223} = ½(2(6)) = 6$, $d_{3232} = ½(24k\text{-}48) = 12k\text{-}24$, $d_{3322} = ½(12 + 12) = 12$, $d_{3323} = ½(24k\text{-}48) = 12k\text{-}24$, $d_{2333} = ½(48k\text{-}36) = 24k\text{-}18$ and $d_{3333} = 36k^2\text{-}84k + 42$.

Now, computations of the third-connectivity index and third-sum-connectivity index of H_k are easy and we will have:

$$^3\chi(H_k) = \sum_{v_i v_j v_k v_l} \frac{1}{\sqrt{d_i d_j d_k d_l}}$$

$$= \sum_{i\times j\times k\times l=16}^{81} \frac{d_{ijkl}}{\sqrt{i \times j \times k \times l}}$$

$$= \frac{d_{2232}}{\sqrt{2\times2\times3\times2}} + \frac{d_{2323}}{\sqrt{2\times3\times2\times3}} + \frac{d_{2233}}{\sqrt{2\times2\times3\times3}} + \frac{d_{3223}}{\sqrt{3\times2\times2\times3}}$$

$$+ \frac{d_{2333}}{\sqrt{2\times3\times3\times3}} + \frac{d_{3233}}{\sqrt{3\times2\times3\times3}} + \frac{d_{3333}}{\sqrt{3\times3\times3\times3}}$$

$$= \frac{12}{\sqrt{24}} + \frac{12k-24+12+6}{\sqrt{36}} + \frac{12k-24+24k-18}{\sqrt{54}} + \frac{36k^2-84k+42}{\sqrt{81}}$$

$$= \frac{12}{\sqrt{24}} + \frac{12k-24+12+6}{\sqrt{36}} + \frac{12k-24+24k-18}{\sqrt{54}} + \frac{36k^2-84k+42}{\sqrt{81}}$$

$$= \sqrt{6} + 2k - 1 + 2\sqrt{6}k - \frac{7\sqrt{6}}{3} + 4k^2 - \frac{28}{3}k + \frac{14}{3}$$

$$= 4k^2 + \left(2 + 2\sqrt{6} - \frac{28}{3}\right)k + \left(\frac{11}{3} - \frac{4\sqrt{6}}{3}\right)$$

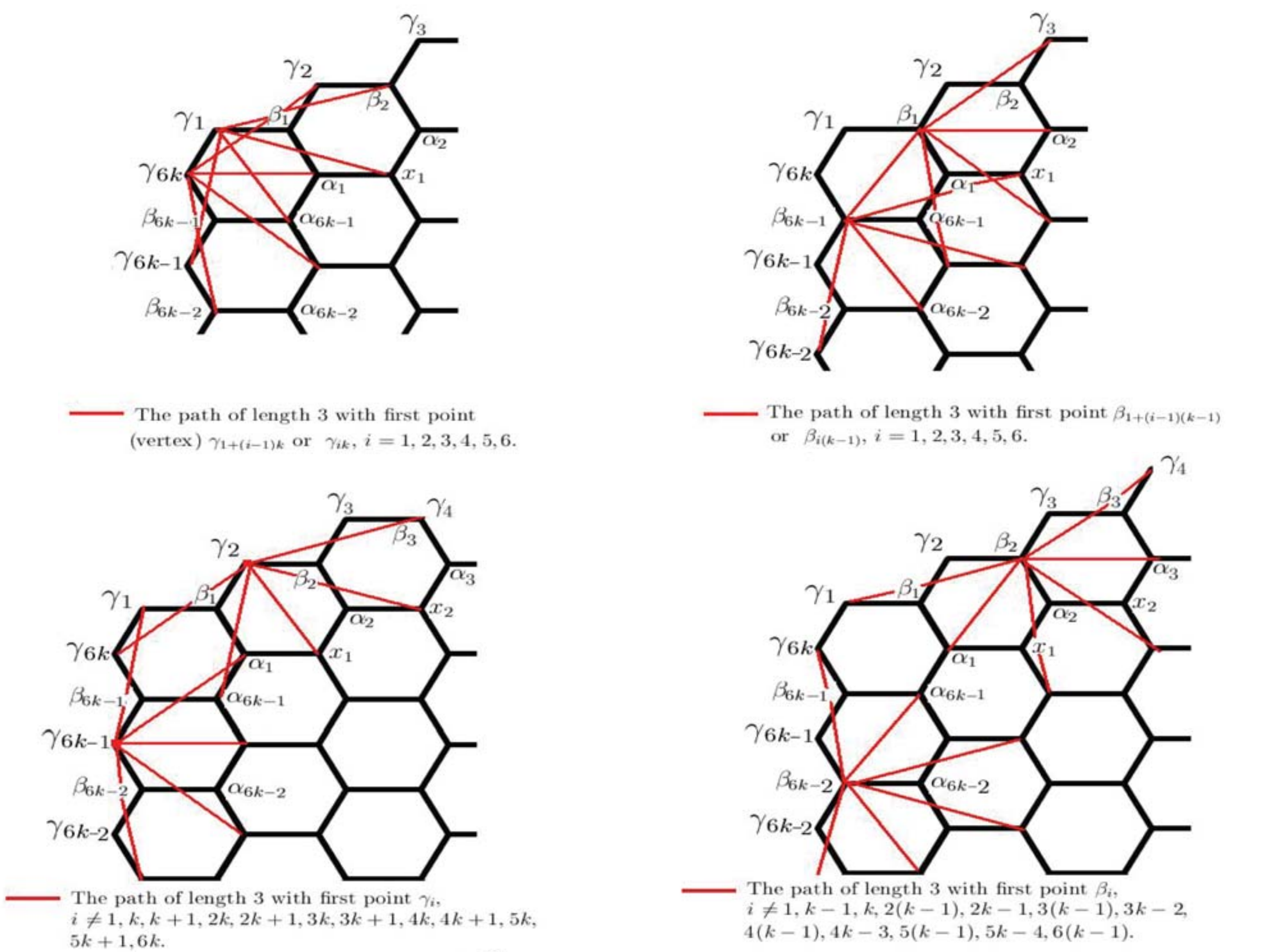

Figure 4. Example: The path with length 3 of H_k, which their first point is γ_1, γ_2, β_1 and β_2.

Also, the third-sum-connectivity index of H_k is equal to

$$
\begin{aligned}
{}^3\chi(H_k) &= \sum_{v_i v_j v_k v_l} \frac{1}{\sqrt{d_i+d_j+d_k+d_l}} \\
&= \sum_{i+j+k+l=8}^{12} \frac{d_{ijkl}}{\sqrt{i+j+k+l}} \\
&= \frac{d_{2232}}{\sqrt{2+2+3+2}} + \frac{d_{2323}}{\sqrt{2+3+2+3}} + \frac{d_{2233}}{\sqrt{2+2+3+3}} + \frac{d_{3223}}{\sqrt{3+2+2+3}} \\
&\quad + \frac{d_{2333}}{\sqrt{2+3+3+3}} + \frac{d_{3233}}{\sqrt{3+2+3+3}} + \frac{d_{3333}}{\sqrt{3+3+3+3}} \\
&= \frac{12}{\sqrt{9}} + \frac{12k-6}{\sqrt{10}} + \frac{36k-42}{\sqrt{11}} + \frac{36k^2-84k+42}{\sqrt{12}} \\
&= 4 + \frac{6\sqrt{10}k - 3\sqrt{10}}{5} + \frac{36\sqrt{11}k - 42\sqrt{11}}{11} + 6\sqrt{3}k^2 - 14\sqrt{3}k + 6\sqrt{3} \\
&= 6\sqrt{3}k^2 + \left(\frac{6\sqrt{10}}{5} + \frac{36\sqrt{11}}{11} - 14\sqrt{3}\right)k + \left(4 + \frac{3\sqrt{10}}{5} - \frac{42\sqrt{11}}{11} + 6\sqrt{3}\right)
\end{aligned}
$$

Here, we complete the proof of Theorem 3.

3. Conclusions

We present the topological indices called »third-connectivity index« and »third-sumconnectivity index« of molecular graphs of Circumcoronene Series of Benzenoid H_k. These connectivity indices have been successfully correlated with physico-chemical properties of organic molecules. The first connectivity index was introduced by M. Randic and demonstrated very good correlation with boiling points of alkanes; since then the connectivity indices have been extended and applied in numerous structure – activity relationship models. The two connectivity indices introduced in this work have a potential application in structure – activity models whenever the benzenoid H_k structures are included in the data sets.

4. Acknowledgments

The author is thankful to Prof. *Mircea V. Diudea* from Faculty of Chemistry and Chemical Engineering Babes-Bolyai University (Romania) for helpful comments and suggestions.

5. References

1. M. Randić and P. Hansen. *J. Chem. Inf. Comput. Sci.* **1988**, *28*, 60.
2. M. Randić. *J. Am. Chem. Soc.* **1975**, *97*, 6609.
3. B. Zhou and N. Trinajstić. *J. Math. Chem.* **2009**, *46*, 1252–1270.
4. B. Zhou and N. Trinajstić. *J. Math. Chem.* **2010**, *47*, 210–218.
5. B. Zhou and N. Trinajstić. *Acta Chim. Slov*. **2010**, *57*, 518–523.
6. B. Lucic, N. Trinajstić and B. Zhou. *Chem. Phys. Lett.* **2009**, *475*, 146–148.
7. Z. Du, B. Zhou and N. Trinajstić. *J. Math. Chem*. **2010**, *47*, 842–855.
8. Z. Du, B. Zhou and N. Trinajstić. *Appl. Math. Lett.* **2010**, *24*, 402–405.
9. F. Ma and H. Deng. *Mathematical and Computer Modelling.* **2011**, February.
10. R. Xing, B. Zhou and N. Trinajstić. *J. Math. Chem.* **2001**, *48*, 583–591.
11. J. Brunvoll, B. N. Cyvin and S. J. Cyvin. *J. Chem. If. Comput. Sci.* **1987**, *27*, 171–177.
12. V. Chepoi and S. Klavžar. *Discrete Mathematics.* **1998**, *192*, 27–39.
13. J. R. Dias. *MATCH Commun. Math. Comput. Chem.* **1996**, *4*, 57–85.
14. M. V. Diudea. *Studia Univ. Babes-Bolyai*. **2003**, *4*, 3–21.
15. A. Dress and G. Brinkmann. *MATCH Commun. Math. Comput. Chem.* **1996**, *33*, 87–100.
16. M. Goldberg. *Tohoku Math. J*. 43, 104–108. **1937**.
17. S. Klavžar and I. Gutman. *J. Chem. Inf. Comput. Sci.* **1997,** *37(4),* 741–744.
18. S. Klavžar. *MATCH Commun. Math. Comput. Chem.* **2008**, *60*, 255–274.
19. A. Soncini, E. Steiner, P. W. Fowler, R. W. A. Havenith, and L. W. Jenneskens. *Chem. Eur. J.* **2003**, *9*, 2974–2981.
20. M. R. Farahani. *Studia Univ. Babes-Bolyai*., **2011**, Submitted for publish.

Povzetek

m-ti povezovalni indeks in m-ti vsotno povezovalni indeks povezanega grafa $G = (V, E)$ definiramo takole:

${}^m\chi(G) = \sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1}d_{i_2}\dots d_{i_{m+1}}}}$ ter ${}^mX(G) = \sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1}+d_{i_2}+\dots+d_{i_{m+1}}}}$, kjer $v_{i1} v_{i2} \dots v_{i_{m+1}}$ teče prek vseh poti dolžine m v grafu G in

je d_i stopnja vozlišča $v_i \in V(G)$. V tem prispevku prikažemo sklenjeno formulo za tretji povezovalni in tretji vsotno povezovalni indeks molekularnega grafa za neskončno družino cirkumkoronenov H_k $(k \geq 1)$.