DOI: 10.2478/awutm-2013-0013

VERSITA

Analele Universităţii de Vest, Timişoara
Seria Matematică – Informatică
LI, 2, (2013), 29– 37

Computing Eccentricity Connectivity Polynomial of Circumcoronene Series of Benzenoid H_k by Ring-Cut Method

Mohammad Reza Farahani

Abstract. Let $G = (V, E)$ be a simple connected molecular graph. In such a simple molecular graph, vertices represent atoms and edges represent chemical bonds, we denoted the sets of vertices and edges by $V = V(G)$ and $E = E(G)$, respectively. If $d(u, v)$ be the notation of distance between vertices $u, v \in V$ and is defined as the length of a shortest path connecting them. Then, Eccentricity connectivity polynomial of a molecular graph G is defined as $ECP(G, x) = \sum_{v \in V} d_G(v) x^{ecc(v)}$, where $ecc(v)$ is defined as the length of a maximal path connecting to another vertex of v. $d_G(v)$ (or simply d_v) is degree of a vertex $v \in V(G)$, and is defined as the number of adjacent vertices with v. In this paper, we focus on the structure of molecular graph *circumcoronene series of benzenoid* H_k *(*$k \geq 2$*)* and counting the eccentricity connectivity polynomial $ECP(H_k)$ and eccentricity connectivity index $\xi(H_k)$, by new method (called *Ring-cut Method*).

AMS Subject Classification (2010). Primary 05C12; secondary 05A15

Keywords. Eccentricity connectivity polynomial; Eccentricity connectivity index; Ring-cut Method; Circumcoronene Series; benzenoid.

1 Introduction

In mathematics chemistry, $G = (V, E)$ is a simple connected molecular graph, such that its vertices correspond to the atoms and the edges to the chemical bonds, we denoted the vertex set and edge set of G by $V = V(G)$ and $E = E(G)$, respectively. We denote the number of vertices and the number of edges of G by n and e, respectively ($n = |V|$ and $e = |E|$).
We know that there exits at least one path between all pairs vertices $u, v \in V(G)$, because we suppose that G be the connected graph. Therefore, the distance $d(u, v)$ between vertices u and v is defined as the length of a minimum (or shortest, exactly) path connecting u and v. And alternatively, the eccentricity $eec(v)$ is the length of a maximal path connecting to another vertex of v. In other works, is maximum distance with first-point v in G ($eec(v) = Max\{d(u, v)|\forall u \in V(G)\}$). Two special cases of eccentricity $eec(v)$ is the radius ($r(G)$) and diameter ($d(G)$) of G, and are defined as the minimum and maximum eccentricity among vertices of G, respectively.
In 1997 [1], *Sharma, Goswami* and *Madan* introduced the eccentric connectivity index of the molecular graph G, $\xi(G)$. It is defined as

$$\xi(G) = \sum_{v \in V} d_G(v) \times ecc(v),$$

where $d_G(v)$ denotes the degree of the vertex v in V and is defined as the number of adjacent vertices with v.
The eccentric connectivity polynomial of a graph G,

$$ECP(G, x) = \sum_{v \in V} d_G(v) x^{ecc(v)}.$$

Then the eccentric connectivity index is the first derivative of $ECP(G, x)$ evaluated at $x = 1$. See [2-5] for details.
The circumcoronene series of benzenoid is a famous family of molecular graph, which consist several copy of benzene C_6 on circumference. It be presented in many papers, some its report obtain from paper series [6-15]). Benzene C_6 (or H_1) is first member from this family. Of curse in chemical science, benzene is an important hydrocarbon C_6H_6. But in mathematics graph theory, hydrogen atoms are often omitted (vertex as degree 1). And other first terms of this series are $H_2 = coronene$, (or $Ca(C_6)$ Capra of benzenoid [16-22]) $H_3 = circumcoronene$, $H_4 = circumcircumcoronene$ and general view of H_k, see Figure 1, Figure 2 and Figure 3 (where they are shown).

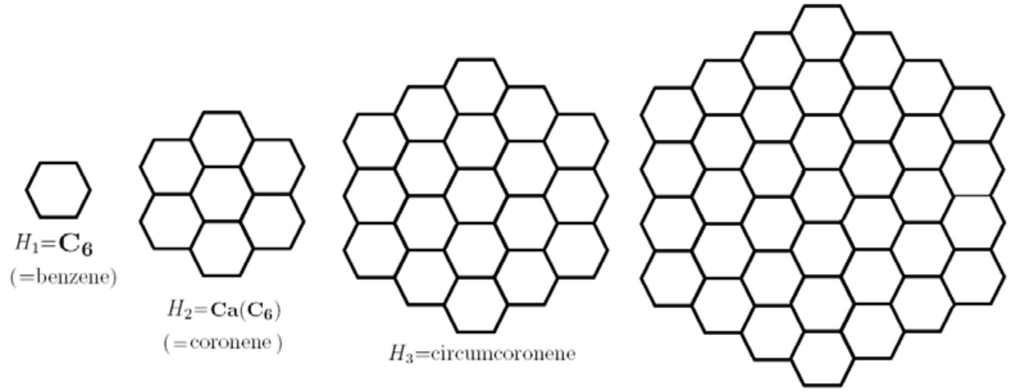

Figure 1: The first three graphs H_1, H_2, H_3 and H_4 from the circumcoronene series, such that H_1, H_2 are graphs $\mathbf{C_6}$ and the Capra of planer benzenoid $\mathbf{Ca}(\mathbf{C_6})$, respectively.

2 Main Result

In this paper, we focus on the structure of molecular graph *circumcoronene series of benzenoid* H_k *(*$k \geq 2$*)* and counting the eccentricity connectivity polynomial $ECP(H_k)$ and eccentricity connectivity index $\xi(H_k)$, by new method (called *Ring-cut Method*). In ring-cut method, we insert some vertices of G in a common ring-cut, such that these vertices have similar mathematical properties. For example, reader can see ring-cuts of circumcoronene series of benzenoid in Figure 3. Now, we compute eccentricity connectivity polynomial and its index in the following theorem. In continue, we proof this theorem by use of ring-cut method and present it for circumcoronene series of benzenoid.

Theorem 2.1. *Let* G *be the circumcoronene series,* H_k*,* $k \geq 2$*, of benzenoid. Then:*

- *Eccentricity connectivity polynomial of* H_k *is equal to*

$$ECP(H_k, x) = \sum_{i=1}^{k-1} 18i\left(x^{2(k+i)-1} + x^{2(k+i)}\right) + 12kx^{4k-1}$$

So Eccentricity connectivity index of H_k *is* $\xi(H_k) = 60k^3 - 24k^2 - 18k + 18$.

Proof. First we consider circumcoronene series of benzenoid $G = H_k$ ($k \geq 2$) as shown in Figure 2. Thus, this graph has $6k^2$ vertices and $9k^2 - 3k$ edges. Now, we name all vertices from center C_6 (or subgraph H_1) by $\gamma^1_{z,1}$ for all $z \in \mathbb{Z}_6$, respectively. We know $\mathbb{Z}_6$ is the cycle finite group of order 6 of branch Group theory from Algebra (or integer number of module 6 from Number theory). So, we name all $\gamma^1_{z,i}$'s adjacent vertices (without name) by $\beta^2_{z,i}$,

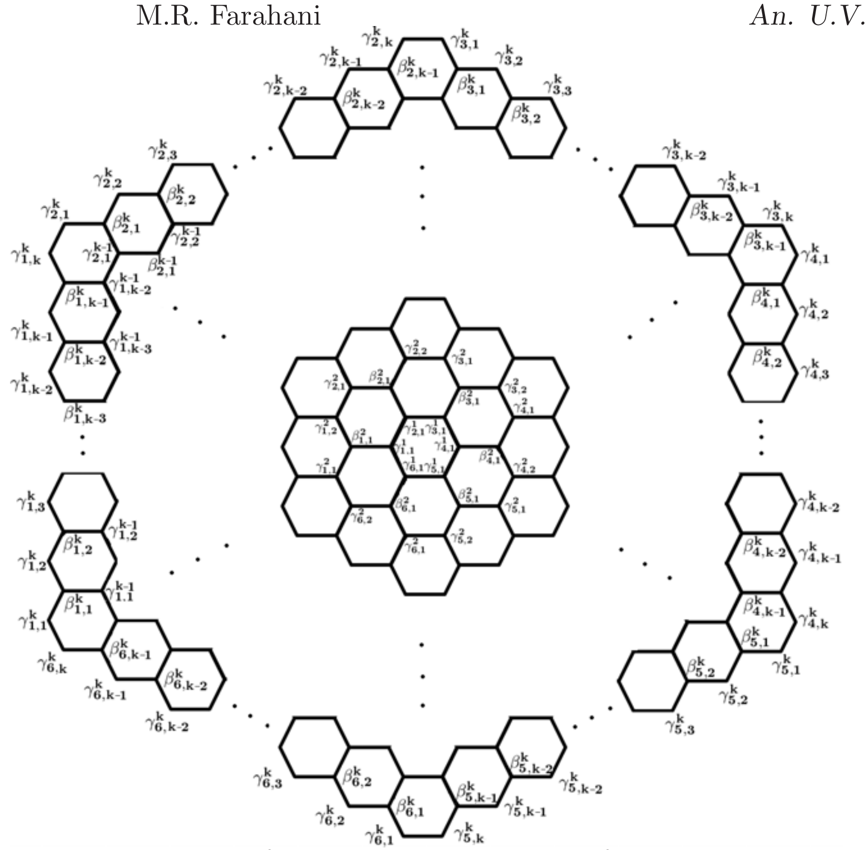

Figure 2: The general view of circumcoronene series of benzenoid H_k, $k \geq 2$.

$(\forall z \in \mathbb{Z}_6, i = 1)$ and name adjacent vertices with $\beta^2_{z,i}$ by $\gamma^2_{z,i}$ and $\gamma^2_{z,i+1}, z \in \mathbb{Z}_6, i = 1$, such that edges $\beta^2_{z,i}\gamma^2_{z,i}$ and $\beta^2_{z,i}\gamma^2_{z,i+1}$ are in $E(H_k)$. By repeat this work, we notation all vertices and obtain desirable ring-cuts, see Figure 2 and Figure 3. Therefore, the vertex set and edge set of circumcoronene series of benzenoid H_k will be

$$V(H_k) = \{\gamma^i_{z,j}, \beta^i_{z,l} | i = 1, ..., k,\ j \in \mathbb{Z}_i,\ l \in \mathbb{Z}_{i-1}\ and\ z \in \mathbb{Z}_6\}.$$

$$E(H_k) = \{\beta^i_{z,j}\gamma^i_{z,j}, \beta^i_{z,j}\gamma^i_{z,j+1}, \beta^i_{z,j}\gamma^{i-1}_{z,j}\ and\ \gamma^i_{z,i}\gamma^i_{z+1,1} | i \in \mathbb{Z}_k\ j \in \mathbb{Z}_i, z \in \mathbb{Z}_6\}.$$

It is obvious that $n_k = |V(H_k)| = 6\sum_{i=1}^{k} i + 6\sum_{i=0}^{k-1} i = 6k^2$ and $e_k = |E(H_k)| = 6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i + 6k = 9k^2 - 3k$.
Now, we divide all vertices in some partitions (we call ring-cuts r_i), such that a ith ring-cut consist of vertices $\gamma^i_{z,j}$ and $\beta^i_{z,l}$ $(\forall j \in \mathbb{Z}_i,\ l \in \mathbb{Z}_{i-1})$ and the size of this ring-cut is equal to $6i + 6(i-1)$. Also, one common properties of members of a ring-cut is their farthest vertices. And another properties of them is $d(\gamma^i_{z,j}, \gamma^k_{z,j}) = d(\beta^i_{z,l}, \beta^k_{z,l}) = 2(k-i)$, in other words the distance of these vertices are equal to two times of difference between order of their ring-cuts (See Figure 4 and Figure 5). Therefore, by use above notations

and properties, we can calculate eccentricity of every vertex v. Of curse, it is important for me that "Where v' ring-cut is?".

On the other hands, the farthest distance between two vertices of H_k is equal to $4k-1$, obviously. Thus, the diameter $d(H_k)$ of circumcoronene series of benzenoid is $4k-1$, (by simple induction on $d(H_k+1) = d(H_k)+4$ and its first terms are $d(H_1 = C_6) = 3$, $d(H_2) = 7$, $d(H_3) = 11$,...).

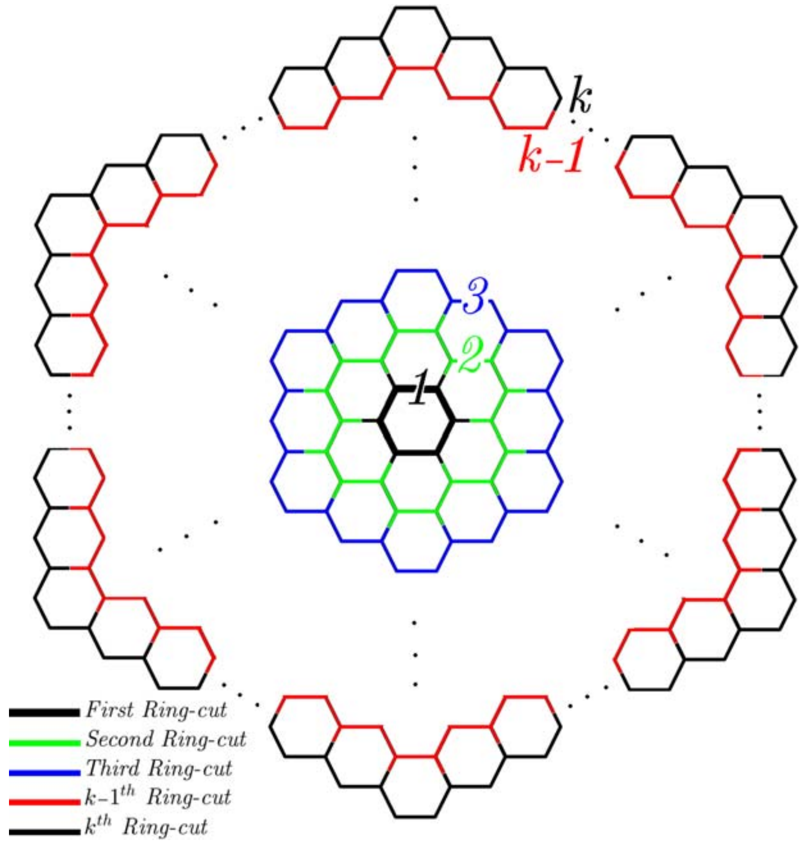

Figure 3: The length of blue path and red path are equal to eccentricity $ecc(\gamma^{i'}_{z',j'})$ and $ecc(\beta^{i}_{z,j})$ of H_4, respectively.

Now, by according to the vertices of an arbitrary ring-cut R_i, we have two part of eccentricity $ecc(v)$, as follow:

1- If $v = \beta^i_{z,j}$, $\forall i = 1, ..., k, j \in \mathbb{Z}_{i-1} \& z \in \mathbb{Z}_6$ (see Figure 4):

$$\mathbf{ecc}(\beta^{\mathbf{i}}_{\mathbf{z,j}}) = \underbrace{\mathbf{d}(\beta^{\mathbf{i}}_{\mathbf{z,j}}, \beta^{\mathbf{i}}_{\mathbf{z+3,j}})}_{4i-3} + \underbrace{\mathbf{d}(\beta^{\mathbf{i}}_{\mathbf{z+3,j}}, \gamma^{\mathbf{k}}_{\mathbf{z+3,j}})}_{\underbrace{\mathbf{d}(\beta^{\mathbf{i}}_{\mathbf{z+3,j}}, \beta^{\mathbf{k}}_{\mathbf{z+3,j}})}_{2(k-i)}+1} = \mathbf{2(k+i-1)}$$

2- If $v = \gamma^i_{z,j}$, $\forall i = 1, ..., k, j \in \mathbb{Z}_i \& z \in \mathbb{Z}_6$ (see Figure 5):

$$\mathbf{ecc}(\gamma^{\mathbf{i}}_{\mathbf{z,j}}) = \underbrace{\mathbf{d}(\gamma^{\mathbf{i}}_{\mathbf{z,j}}, \gamma^{\mathbf{i}}_{\mathbf{z+3,j}})}_{4i-1} + \underbrace{\mathbf{d}(\gamma^{\mathbf{i}}_{\mathbf{z+3,j}}, \gamma^{\mathbf{k}}_{\mathbf{z+3,j}})}_{2(k-i)} = \mathbf{2(k+i)-1}$$

Upshot, we are ready to computing eccentricity connectivity polynomial and eccentricity connectivity index of circumcoronene series of benzenoid. By according to definition of ring-cut, we will have

$$\begin{aligned}
ECP(H_k, x) &= \sum_{v\in V} d_v x^{ecc(v)} \\
&= \sum_{i=1}^{k}\sum_{v\in R_i} d_v x^{ecc(v)} \\
&= \sum_{i=2}^{k}\sum_{\beta^i_{z,j}\in R_i} d_{\beta^i_{z,j}} x^{ecc(\beta^i_{z,j})} + \sum_{i=1}^{k}\sum_{\gamma^i_{z,j}\in R_i} d_{\gamma^i_{z,j}} x^{ecc(\gamma^i_{z,j})} \\
&= \sum_{i=1}^{k}\left(\sum_{j=1}^{i}\sum_{z=1}^{6} d_{\gamma^i_{z,j}} x^{ecc(\gamma^i_{z,j})} + \sum_{j=1}^{i-1}\sum_{z=1}^{6} d_{\beta^i_{z,j}} x^{ecc(\beta^i_{z,j})}\right) \\
&= \sum_{z=1}^{6}\left(\sum_{i=1}^{k}(\sum_{j=1}^{i} d_{\gamma^i_{z,j}} x^{ecc(\gamma^i_{z,j})}) + \sum_{i=2}^{k}(\sum_{j=1}^{i-1} d_{\beta^i_{z,j}} x^{ecc(\beta^i_{z,j})})\right) \\
&= 6\left((\sum_{j=1}^{k} 2x^{2(k+k)-1}) + \sum_{i=1}^{k-1}(\sum_{j=1}^{i} 3x^{2(k+i)-1})\right) \\
&\qquad +6\left(\sum_{i=2}^{k}(\sum_{j=1}^{i-1} 3x^{2(k+i-1)})\right) \\
&= 6\left((k\times 2x^{4k-1}) + \sum_{i=1}^{k-1}(i\times 3x^{2(k+i)-1})\right) \\
&\qquad +6\left(+\sum_{i=2}^{k}((i-1)\times 3x^{2(k+i-1)})\right) \\
&= 18\sum_{i=2}^{k}\left((i-1)x^{2(k+i-1)} + (i-1)x^{2(k+i-1)-1}\right) \\
&\qquad +12kx^{4k-1} \qquad (2.1)
\end{aligned}$$

Hence, eccentricity connectivity polynomial of circumcoronene series of benzenoid is equal to $ECP(H_k, x) = \sum_{i=1}^{k-1} 18i\left(x^{2(k+i)-1} + x^{2(k+i)}\right) + 12kx^{4k-1}$. On other hands, eccentricity connectivity index H_k is

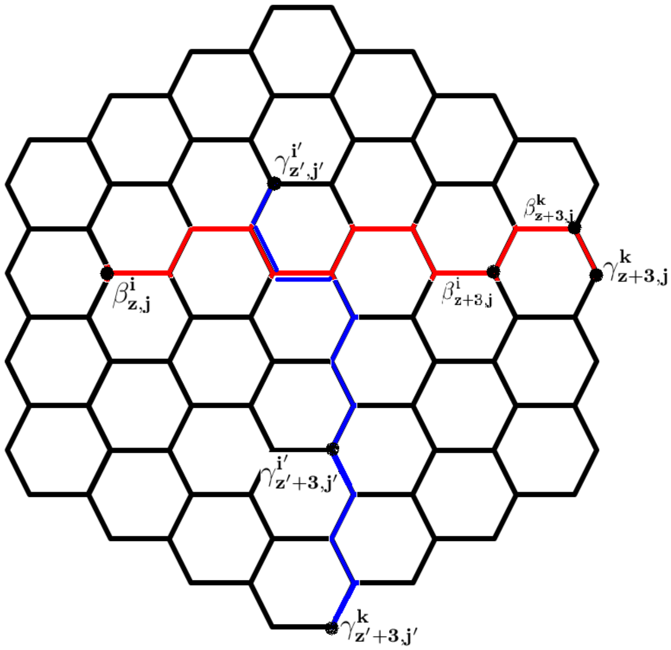

Figure 4: The length of blue path and red path are equal to eccentricity $ecc(\gamma^{i'}_{z',j'})$ and $ecc(\beta^{i}_{z,j})$ of H_4, respectively.

$$
\begin{aligned}
\xi(H_k) &= \frac{\partial ECP(H_k,x)}{\partial x}|_{x=1} = \sum_{v\in V} d_G(v)\times ecc(v) \\
&= \sum_{i=1}^{k-1} 18(i)\times(4k+4i-1) + 12k\times(4k-1) \\
&= 18\sum_{i=1}^{k-1} 4i^2 + 18\sum_{i=1}^{k-1} 4ki - (k-1) + (48k^2-12k) \\
&= 12k(k-1)(2k-1) + 36k^2(k-1) - 18(k-1) + (48k^2-12k) \\
&= 24k^3 - 36k^2 + 12k + 36k^3 - 36k^2 - 18k + 18 + 48k^2 - 12k \\
&= \mathbf{60k^3 - 24k^2 - 18k + 18} \qquad (2.2)
\end{aligned}
$$

Obviously, the radius number of circumcoronene series of benzenoid H_k is $r(H_k) = 2k+1$. Here, we complete the proof of the theorem.□

3 Conclusion

In Theoretical Chemistry, the topological indices and molecular structure descriptors are used for modeling physico-chemical, toxicologic, biological and other properties of chemical compounds and nano steucture analizing. A family of Benzenoid built solely from Benzene CR6 R(or hexagons), Circumcoronene Series of Benzenoid H_k $(k \geq 1)$, have been studied here and its Eccentric connectivity polynomial have been counted.

References

[1] **V. Sharma, R. Goswami, and A. K. Madan**, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies., *J. Chem. Inf. Comput. Sci.*, **37**, (1997), 273

[2] **A.R. Ashrafi, M. Ghorbani, and M. Hemmasi**, Eccentric connectivity polynomial of C12n+2 fullerenes, *Digest Journal of Nanomaterials and Biostructures*, **4** (3), (2009), 483-486

[3] **S. Alikhani and M.A. Iranmanesh**, Eccentric connectivity polynomial of an infinite family of Dendrimer, *Digest Journal of Nanomaterials and Biostructures*, **6** (1), (2011), 253-257

[4] **I. Gutman and O.E. Polansky**, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, New York, 1986

[5] **M.A. Johnson and G.M. Maggiora**, *Concepts and Applications of Molecular Similarity*, Wiley Interscience, New York, 1990

[6] **J. Brunvoll, B.N. Cyvin, and S.J. Cyvin**, Enumeration and Classification of Benzenoid Hydrocarbons. Symmetry and Regular Hexagonal Benzenoids, *J. Chem. If. Comput. Sci.*, **27**, (1987), 171-177

[7] **V. Chepoi and S. Klavžar**, Distances in benzenoid systems: Further developments, *Discrete Mathematics*, **192**, (1998), 27-39

[8] **I. Gutman and S. Klavžar**, A method for calculationg Wiener numbers of benzenoid hydrocarbons and phenylenes, *ACH Models Chem.*, **133**, (1996), 389-399

[9] **A. Ilic, S. Klavžar, and D. Stevanovic**, Calculating The Degree Distance of Partial Hamming Graphs, *Manuscript*

[10] **S. Klavžar and I. Gutman**, Bounds for The Schultz Molecular Topological index of benzenoid Systems in Terms of Wiener index, *J. Chem. Inf. Comput. Sci.*, **37** (4), (1997), 741-744

[11] **S. Klavžar**, A Bird's Eye View of The Cut Method And A Survey of Its Applications In Chemical Graph Theory, *Commun. Math. Comput. Chem. (MATCH)*, **60**, (2008), 255-274

[12] **S. Klavžar, I. Gutman, and B. Mohar**, Labeling of Benzenoid Systems which Reflects the Vertex-Distance Relations, *J. Chem. Int Comput. Sci.*, **35**, (1995), 590-593

[13] **S. Klavžar and I. Gutman**, A Comparison of the Schultz Molecular Topological index with the Wiener index, *J. Chem. Inf. Comput. Sci.*, **36**, (1996), 1001-1003

[14] **A. Soncini, E. Steiner, P.W. Fowler, R.W.A. Havenith, and L.W. Jenneskens**, Perimeter Effects on Ring Currents in Polycyclic Aromatic Hydrocarbons: Circumcoronene and Two Hexabenzocoronenes, *Chem. Eur. J.*, **9**, (2003), 2974-2981

[15] **P. Zigert, S. Klavžar, and I. Gutman**, Calculating the hyper-Wiener index of benzenoid hydrocarbons, *ACH Models Chem.*, **137**, (2000), 83-94

[16] **J.R. Dias**, From benzenoid hydrocarbons to fullerene carbons, *Commun. Math. Comput. Chem. (MATCH)*, **4**, (1996), 57-85

[17] **M.V. Diudea**, Capra-leapfrog related operation on maps, *Studia Univ. Babes-Bolyai*, **4**, (2003), 3-21

[18] **A. Dress and G. Brinkmann**, Commun. Math. Comput. Chem. (MATCH), **33**, (1996), 87-100

[19] **M. Goldberg**, A class of multisymmetric polyhedra, *Tohoku Math. J.*, **43**, (1937), 104-108

[20] **M.V. Diudea, M. Stefu, P. E. John, and A. Graovac**, Generalized operations on maps, *Croat. Chem. Acta*, **79**, (2006), 355-362

[21] **M.V. Diudea**, Nano porous carbon allotropes by septupling map operations, *J. Chem. Inf. Model*, **45**, (2005), 1002-1009

[22] **W.C. Shiu and P.C.B. Lam**, The Wiener number of a hexagonal net, *Discrete Appl. Math.*, **73**, (1997), 101-111

Mohammad Reza Farahani

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

E-mail: MR_Farahani@mathdep.iust.ac.ir & MRFarahani88@gmail.com

Received: 22.05.2013

Accepted: 3.11.2013