Communications in Mathematics and Applications
Vol. 9, No. 1, pp. 99–105, 2017
ISSN 0975-8607 (online); 0976-5905 (print)
Published by RGN Publications

http://www.rgnpublications.com

Research Article

Four Vertex-Degree-Based Topological Indices of $VC_5C_7[p;q]$ Nanotubes

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Abstract. Recently, I. Gutman et.al. presented four vertex-degree based graph invariants, that earlier have been considered in the chemical and/or mathematical literature, but, that evaded the attention of most mathematical chemists. These are the reciprocal Randić index (RR), the reduced reciprocal Randić index (RRR), the reduced second Zagreb index (RM_2) and the forgotten index (F). In this article, we compute these indices of $VC_5C_7[p;q]$ Nanotubes.

Keywords. Reciprocal Randić index; Reduced reciprocal Randić index; Reduced second Zagreb index; Forgotten index; $VC_5C_7[p;q]$ nanotube

MSC. 05A15; 05C05; 05C12; 05C50

Received: December 18, 2016 **Accepted:** March 14, 2017

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of elements in $V(G)$ is called the order of G, denoted as $|V(G)|$, and the number of elements in $E(G)$ is called the size of G, denoted as $|E(G)|$. For a vertex $u \in V(G)$, the degree of u is the number of first neighbors of u in the underlying graph.

A topological index is a numerical descriptor of a molecular structure derived from the corresponding molecular graph. In chemical graph theory, several vertex-degree based topological indices have been and are currently considered and applied in $QSPR = QSAR$ studies. Among them first Zagreb index M_1, the second Zagreb index M_2 and the Randić index R are the oldest and most thoroughly investigated. Following are there definitions:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2,$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v),$$

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

In addition, we mention some other vertex-degree based topological indices widely used in chemical literature. The sum-connectivity index, is obtained from Randić index by replacing $d(u)d(v)$ by $d(u)+d(v)$,

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}.$$

Randić index has another variant, called harmonic index, defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}.$$

For further details of degree-based topological indices we refer [4–6, 19, 24, 28, 32, 33, 35–40]. Recently, Gutman et al. [26, 27] re-introduced the neglected topological indices and succeeds to demonstrate that these indices also have very promising applicative potential. The new/old topological indices studied by Gutman et al. are the following: The reciprocal Randić index is defined as

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}.$$

It is, of course, a special case of general Randić index $\sum_{uv \in E(G)} (d(u)d(v))^{\alpha}$, where α is any real number. The reduced reciprocal Randić index is defined as

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)(d(v)-1)}.$$

The reduced second Zagreb index is defined as

$$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1).$$

In a study on the structure-dependency of the total π-electron energy, beside the first Zagreb index, it was indicated that another term on which this energy depends is of the form

$$F(G) = \sum_{v \in V(G)} d(v)^3 = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2).$$

Recently, this sum was named forgotten index, or shortly the F index. Carbon nanotubes are types of nanostructure which are allotropes of carbon and having a cylindrical shape. A nanostructure is an object of intermediate size between molecular and microscopic structures. Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, architecture, optics and materials science. Carbon nanotubes provide a certain potential for metal-free catalysis of inorganic and organic reactions.

2. Main Results

In this section, we will compute the reciprocal Randić, reduced reciprocal Randić, reduced second Zagreb and forgotten indices of VC_5C_7 nanotubes. For further study reader can see [1, 2, 7–23, 30, 31, 34] In order to compute certain topological indices of thee nanotubes, we will partition the edge set based on degrees of end vertices of each edge of the graph.

2.1 Nanotube $VC_5C_7[p,q]$, $(p,q > 1)$

VC_5C_7[p;q] nanotube is a C_5C_7 net and constructed by alternating C_5 and C_7 following the trivalent decoration as shown in Figure 1. In VC_5C_7[p;q], p represents the number of pentagons in one row and q is the number of periods in whole graph, a period contain four rows in Figure **??** an mth period is shown. One period contains 16p vertices and $3p$ vertices which are joined at the end of the graph of these nanotubes, so $|V(VC_5C_7[p;q])| = 16pq + 3p$. Similarly, there are $24p$ edges in one period and 3p extra edges which are joined to the end of the graph in these nanotubes, so $|E(VC_5C_7[p;q])| = 24pq - 3p$. This type of tiling can cover a either a torus or a cylinder.

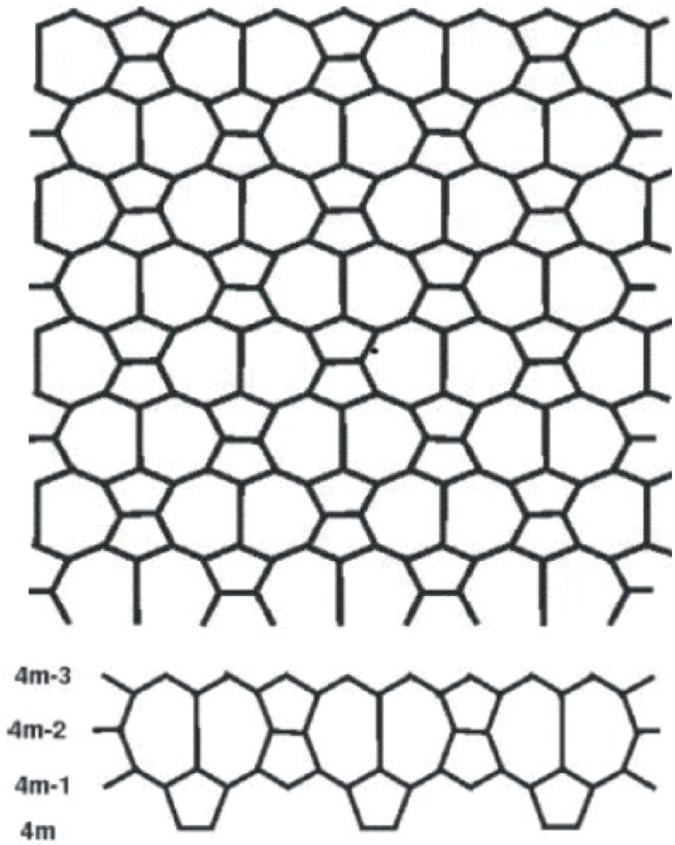

Figure 1. The graph of VC_5C_7[p;q] nanotube with $p = 3$ and $q = 4$ and mth period of VC_5C_7

Theorem 2.1. *Consider the graph of VC_5C_7[p;q] nanotube, then*

$$RR(VC_5C_7[p,q]) = (36q + 5\sqrt{6} - 20)2p\,, \tag{2.1}$$

$$RRR(VC_5C_7[p,q]) = (48q + 10\sqrt{2} - 27)p\,, \tag{2.2}$$

$$RM_2(VC_5C_7[p,q]) = (96q - 35)p\,, \tag{2.3}$$

$$F(VC_5C_7[p,q]) = (72q - 19)6p\,. \tag{2.4}$$

Proof. Consider the nanotube G=VC_5C_7[p;q], where p is the number of pentagons in one row and q is the number of periods in whole lattice. To obtain the final results we partition the edge set based on degrees of end vertices of G. There are three partitions of edge set correspond to their degrees of end vertices which are

$$E_1 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 2\}$$

$$E_2 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 3\}$$

$$E_3 = \{uv \in E(G) | d(u) = 3 \text{ and } d(v) = 3\}$$

The number of edges in E_1; E_2 and E_3 are p; $10p$ and $24pq - 14p$. Now, we are able to apply the formula of RR; RRR; RM_2 and F to compute these indices for G. Since,

$$\begin{aligned} RR(G) &= \sum_{uv\in E(G)} \sqrt{d(u)d(v)} \\ &= \sum_{uv\in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv\in E_2(G)} \sqrt{d(u)d(v)} + \sum_{uv\in E_3(G)} \sqrt{d(u)d(v)} \\ &= p\sqrt{2\cdot 2} + 10p\sqrt{2\cdot 3} + (24pq - 14p)\sqrt{3\cdot 3} = (36q + 5\sqrt{6} - 20)2p \end{aligned}$$

which is the required (2.1) result.

$$\begin{aligned} RRR(G) &= \sum_{uv\in E(G)} \sqrt{(d(u)-1)(d(v)-1)} \\ &= \sum_{uv\in E_1(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv\in E_2(G)} \sqrt{(d(u)-1)(d(v)-1)} \\ &\quad + \sum_{uv\in E_3(G)} \sqrt{(d(u)-1)(d(v)-1)} \\ &= p\sqrt{(2-1)(2-1)} + 10p\sqrt{(2-1)(3-1)} + (24pq - 14p)\sqrt{(3-1)(3-1)} \\ &= (48q + 10\sqrt{2} - 27)p \end{aligned}$$

which is the required (2.2) result.

$$\begin{aligned} RM_2(G) &= \sum_{uv\in E(G)} (d(u)-1)(d(v)-1) \\ &= \sum_{uv\in E_1(G)} (d(u)-1)(d(v)-1) + \sum_{uv\in E_2(G)} (d(u)-1)(d(v)-1) \\ &\quad + \sum_{uv\in E_3(G)} (d(u)-1)(d(v)-1) \\ &= p(2-1)(2-1) + 10p(2-1)(3-1) + (24pq - 14p)(3-1)(3-1) = (96q - 35)p \end{aligned}$$

which is the required (2.3) result.

$$\begin{aligned}
F(G) &= \sum_{uv\in E(G)} (d(u)^2+d(v)^2)\\
&= \sum_{uv\in E_1(G)} (d(u)^2+d(v)^2) + \sum_{uv\in E_2(G)} (d(u)^2+d(v)^2) + \sum_{uv\in E_3(G)} (d(u)^2+d(v)^2)\\
&= p(2^2+2^2)+10p(2^2+3^2)+(24pq-14p)(3^2+3^2)\\
&= (72q-19)6p
\end{aligned}$$

which is the required (2.4) result, and the proof is complete. □

3. Conclusion

In this study we have calculated the reciprocal Randić index (RR), the reduced reciprocal Randić index (RRR), the reduced second Zagreb index (RM_2) and the forgotten index (F) of $VC_5C_7[p;q]$ nanotubes.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

References

[1] A.R. Ashrafi, B. Bazigaran and M. Sadati, Some experimental conjectures on energy and Estrada index of VC_5C_7 $[4p,8]$ nanotubes, *Optoelectronics and Advanced Materials-Rapid Communications* **3** (10) (2009), 1080 – 1082.

[2] A.R. Ashrafi, H. Saati and M. Ghorbani, On distance-based topological indices of $HC_5C_7[4p,8]$ nanotubes, *Digest Journal of Nanomaterials and Biostructures* **3** (2008), 227 – 236.

[3] A. Bahrami and J. Yazdani, Padmakar-Ivan index of H-phenylinic nanotubes and nanotore, *Digest Journal of Nanomaterials and Biostructures* **3** (2008), 265 – 267.

[4] K.C. Das, I. Gutman and B. Furtula, Survey on geometric-arithmetic in-dices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595 – 644.

[5] K.C. Das and I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004), 103 – 112.

[6] T. Doslic, B. Furtula, A. Graovac, I. Gutman, S. Moradi and Z. Yarah-Madi, On vertex-degree-based molecular structure descriptors, *MATCH Commun. Math. Comput Chem.* **66** (2011), 613 – 626.

[7] M.R. Farahani, Atom bond connectivity and geometric-arithmetic indices Of HAC_5C_7[p,q] nanotube, *International Journal of Chemical Modeling* **5** (1) (2013), 127 – 132.

[8] M.R. Farahani, Computing the geometric-arithmetic and atom bond connectivity indices for some nanotubes, *Polymers Research Journal* **7** (3) (2013), 1 – 6.

[9] M.R. Farahani, Connectivity indices of pent-heptagonal nanotubes $VAC_5C_7[p,q]$, *Advances in Materials and Corrosion* **2** (2013), 33 – 35.

[10] M.R. Farahani, First and second Zagreb polynomials of VC_5C_7[p,q] and HC_5C_7[p,q] nanotubes, *International Letters of Chemistry, Physics and Astronomy* **12** (2) (2014), 56 – 62, doi:10.18052/www.scipress.com/ILCPA.31.56.

[11] M.R. Farahani, On the geometric-arithmetic and atom bond connectivity index of $HAC_5C_6C_7$[p,q] nanotube, *Chemical Physics Research Journal* **6** (1) (2013), 21 – 26.

[12] M.R. Farahani, On the Randić and sum-connectivity index of nanotubes, *Annals of West University of Timisoara-Mathematics and Computer Science* **51** (2) (2013), 39 – 46, doi:10.2478/awutm-2013-0013.

[13] M.R. Farahani, On the Randić and sum-connectivity index of some graphs, *Algebras, Goups and Geometries* **29** (4) (2012), 415 – 422.

[14] M.R. Farahani, The atom bond connectivity ABC and geometric-arithmetic GA indices of pent-heptagonal nanotube, *PJAM-Pacific Journal of Applied Mathematics* **7** (1) (2015), in press.

[15] M.R. Farahani, The first and second Zagreb indices, first and second Zagreb polynomials of $HAC_5C_6C_7$[p,q] And HAC_5C_7[p,q] nanotubes, *Int. J. Nanosci. Nanotechnol.* **8** (3) (September 2012), 175 – 180

[16] M.R. Farahani, Zagreb indices and Zagreb polynomials of pent-heptagon nanotube VAC_5C_7(S), *Chemical Physics Research Journal* **6** (1) (2013), 35 – 40.

[17] W. Gao, M.K. Siddiqui, M. Imran, M.K. Jamil and M.R. Farahani, Forgotten topological index of chemical structure in drugs, *Saudi Pharmaceutical Journal* **24** (3) (2016), 258 – 264, doi:10.1016/j.jsps.2016.04.012.

[18] W. Gao and M.R. Farahani, Computing the reverse eccentric connectivity index for certain family of nanocone and fullerene structures, *Journal of Nanotechnology*, ID 3129561, **2016**, doi:10.1155/2016/3129561.

[19] W. Gao, M.R. Farahani, S.H. Wang and M.N. Husin, On the edge-version atom-bond connectivity and geometric arithmetic indices of certain graph operations, *Applied Mathematics and Computation* **308** (2017), 11 – 17, doi:10.1016/j.amc.2017.02.046

[20] W. Gao, W.F. Wang and M.R. Farahani, Topological indices study of molecular structure in anti-cancer drugs, *Journal of Chemistry* ID 3216327, **2016**, doi:10.1155/2016/3216327.

[21] W. Gao and W.F. Wang, The eccentric connectivity polynomial of two classes of nanotubes, *Chaos, Solitons and Fractals* **89** (2016), 290 – 294.

[22] W. Gao and W.F. Wang, The fifth geometric arithmetic index of bridge graph and carbon nanocones, *Journal of Difference Equations and Applications* **2016**, doi:10.1080/10236198.2016.1197214.

[23] M. Ghojavand and, A.R. Ashrafi, Computing the bipartite edge frustration of some nanotubes, *Digest J. Nanomaterials and Biostructures* **3** (2008), 209 – 214.

[24] I. Gutman and B. Furtula (Eds.), *Novel Molecular Structure Descriptors Theory and Applications I*, Univ. Kragujevac, Kragujevac (2010).

[25] I. Gutman and B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[26] I. Gutman, B. Furtula and C. Elphick, Three new/old vertex-degree based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014), 617 – 632.

[27] I. Gutman, D. Dimitrov and H. Abdo, *On extremal trees with respect to the F-index*, arXive:1509303574v1.

[28] I. Gutman and K.C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem* **50** (2004), 83 – 92.

[29] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1971), 535 – 538, doi:10.1016/0009-2614(72)85099-1.

[30] S. Hayat and M. Imran, Computation of certain topological indices of Nanotubes covered by C_5 and C_7, *J. Comput. Theor. Nanosci.* **12** (2015), 533 – 541, doi:10.1166/jctn.2015.3761.

[31] A. Iranmanesh, Y. Alizadeh and B. Taherkhani, Computing the Szeged and PI indices of VC_5C_7[p,q] and HC_5C_7[p,q] nanotubes, *Int. J. Mol. Sci.* **9** (2) (2008), 131 – 144.

[32] M.K. Jamil, I. Tomescu and N. Akhter, Extremal degree-product indices of graphs with fixed number of pendant vertices and cyclomatic number, *International Letters of Chemistry, Physics and Astronomy* **59** (2015), 53 – 61, doi:10.18052/www.scipress.com/ILCPA.59.53.

[33] R. Lang, T. Li, D. Mo and Y. Shi, A novel method for analyzing inverse problem of topological indices of graphs using competitive agglomeration, *Appl. Math. Comput.* **291** (2016), 115 – 121, doi:10.1016/j.amc.2016.06.048.

[34] Y. Li, L. Yan, M.K. Jamil, M.R. Farahani, W. Gao and J.B. Liu, Four new/old vertex-degree-based topological indices of HAC_5C_7[p,q] and $HAC_5C_6C_7$[p,q] nanotubes, *J. Comput. Theor. Nanosci.* **14** (1) (2017), 796 – 799, doi:10.1166/jctn.2017.6275.

[35] S. Nikolic, G. Kovacevic, A. Milicevic and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003), 113 – 124.

[36] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, *MATCH Commun. Math. Comput. Chem.* **59** (2008), 5124.

[37] M. Randić, The connectivity index 25 years after, *Journal of Molecular Graphics and Modelling* **20** (2001), 19 – 35, doi:10.1016/S1093-3263(01)00098-5.

[38] Y. Shi, Note on two generalizations of the Randić index, *Appl. Math. Comput.* **265** (2015), 1019 – 1025, doi:10.1016/j.amc.2015.06.019.

[39] S. Wang and B. Wei, Multiplicative Zagreb indices of cacti, *Discrete Math. Algorithm. Appl.* **8**, 1650040 (2016) [15 pages], doi:10.1142/S1793830916500403.

[40] S. Wang and B. Wei, Multiplicative Zagreb indices of k-trees, *Discrete Appl. Math.* **180** (2015), 168 – 175.