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ON THE TERMINAL WIENER INDICES OF POLYCYCLIC AROMATIC HYDROCARBONS PAH$_s$

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Abstract: The Wiener index of a simple connected graph is defined as the sum of all distances between distinct vertices of the graph G, and the terminal wiener index is the sum of all distances between distinct pendent vertices of the graph G. Polycyclic Aromatic Hydrocarbons are important hydrocarbons, which are organic compounds containing only carbon and hydrogen. In this paper, we reformulate the terminal Wiener index with the help of orthogonal cuts and compute the terminal Wiener index of Polycyclic Aromatic Hydrocarbons.

AMS Subject Classification: 05C12, 05C90
Key Words: molecular graph, polycyclic aromatic hydrocarbons, Wiener index, hyper-Wiener index, terminal Wiener index, orthogonal cuts

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1. Introduction

Let $G(V, E)$ be a simple connected graph with vertex set V and edge set E. The number of elements in sets V and E are called the order and the size of the graph G. In a graph G, the distance between the vertices u and v is the length of the shortest path connecting them. It is denoted by $d_G(u, v)$ or $d(u, v)$ when graph G is obvious. In a graph G, the number of vertices attached to a vertex is called its degree. A vertex with degree one is called a pendent vertex.

A topological index is a number associated with a graph obtained from corresponding chemical structure. In mathematical chemistry, topological indices have been used in the study of Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR). The Wiener index [41] is the oldest topological and it is defined as the sum of all distances between distinct vertices, i.e.

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v)$$

In the last years, a numerous modification and extensions of the Wiener index was introduced and studied by mathematical chemists. In 1993, Milan Randić proposed the hyper-Wiener index [38]

$$WW(G) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} (d(u, v) + d(u, v)^2)$$

Recently, Gutman et. al. [33], [34] proposed another version of Wiener index named as terminal Wiener index. The terminal Wiener index is defined as the sum of the distances between all pairs of pendent vertices.

$$TW(G) = \sum_{\{u,v\}\subseteq V_P(G)} d(u, v)$$

where $V_P(G)$ is the set of pendent vertices of the graph G. In a molecular graph G, vertices are corresponding to the atoms and edges corresponding to the bonds. In this paper, we computed the terminal Wiener index of the molecular graph of Polycyclic Aromatic Hydrocarbons PAH_s. The Polycyclic Aromatic Hydrocarbons PAH_s is a family of hydro-carbon molecules, such that its structure is consisting of cycles with length six. The large polycyclic aromatic hydrocarbons (PAH_s) are ubiquitous combustion products. For further details, see [1],..., [32], [39], [40].

2. Discussion and Main Result

In this section, we compute the hyper-Wiener index and the terminal Wiener index of a molecular graph of Polycyclic Aromatic Hydrocarbons PAH_s. The graph representation of PAH_s has $6s^2+6s$ vertices and $9s^2+3s$ edges. The general graphical representation of the Polycyclic Aromatic Hydrocarbons PAH_s is shown in Figure 1.

From Figure 1, one can notice that there are $6s$ pendent vertices.

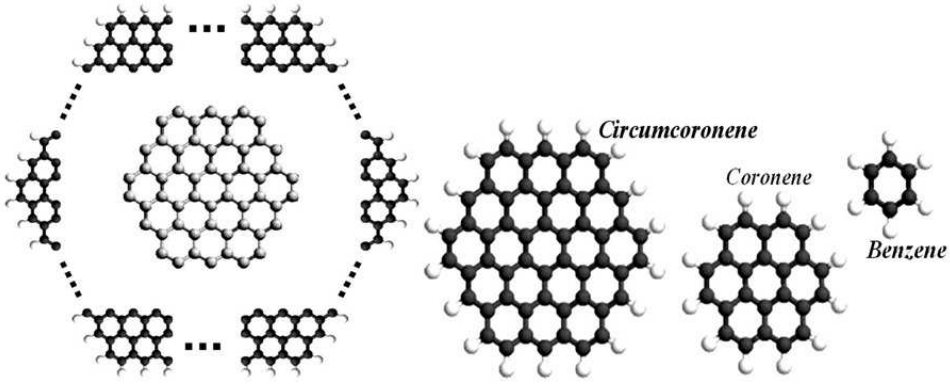

Figure 1. The general graphical representation of the Polycyclic Aromatic Hydrocarbons PAH_s

S. Klavžar [36], [37] and John [35] gave the general interpretation of the cut method and orthogonal cut, respectively. They also present its applications in chemical graph theory. An orthogonal cut $C(e)$, with respect to the edge e, is the set of all edges $f \in E(G)$ of the graph G which are strongly co-distant to f, i.e.

$$C(e) := \{f \in E(G) \mid f \ co \ e\}$$

where two edges $e = uv$ and $f = xy$ of the edge set $E(G)$ are co-distant, if and only if they obey the following relation

$$d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y)$$

Some edges of the graph G satisfied the following relations:

1. e co-distant e.
2. if e co-distant f, then f co-distant e.
3. if e co-distant f and f co-distant g, then e co-distant g.

which are reflexive, symmetric and transitive properties. In general, for a graph G co-distant is not transitive. If in a graph G, co-distant is transitive, then the graph is called co-graph and the cut $C(e)$ is called an orthogonal cut of G. In a co-graph, we can write

$$E(G) = \cup_{i=1}^{s} C(e_i) \text{ and } C(e_i) \cap C(e_j) = \emptyset, i \neq j$$

Now consider $C(e_i) = C_i$, thus for a co-graph G, let $C_1, \cdots, C_s$ be its classes and $n_1(C_i|G)$ and $n_2(C_i|G)$ $(i = 1, \cdots, s)$ be the number of vertices in the two connected components $G \setminus C_i$ [36]. So we have the following re-formula for the Wiener index of the co-graph G

$$W(G) = \sum_{i=1}^{s} n_1(C_i|G) \times n_2(C_i|G)$$

We refer the reader, to [30], [31], [32], [35], [36], [37], [42] for detailed study and application of cut and orthogonal cut methods.

Theorem 1. *The terminal Wiener index of the molecular graph of the Polycyclic Aromatic Hydro-carbons PAH$_s$ ($\forall s \geq 1$) is given as:*

$$TW(PAH_s) = 46s^3 + 15s^2 - 4s.$$

Proof. From the general graphical structure of the Polycyclic Aromatic Hydrocarbons PAH$_s$, we can notice that each edge cut in PAH$_s$ is an orthogonal cut this implies that the molecular graph of PAH$_s$ is a co-graph. For the i^th orthogonal cut $C_i = C(e_i)$ $(\forall i = 0, 1, \cdots, s)$, we have $|C_i = C(e_i)| = s + i$, and the number of pendent vertices in the two connected components of the graph of PAH$_s$ are

$$n_1(C_i) = s + 2i, \ n_2(C_i) = 5s - 2i, \ (\forall i = 0, 1, \cdots, s).$$

Now, from the re-formula of the terminal Wiener index for co-graph we can compute the terminal Wiener index of Polycyclic Aromatic Hydrocarbons PAH$_s$ as

$$\begin{aligned} TW(PAH_s) &= \sum_{i=0}^{s} n_1(C_i|G) \times n_2(C_i|G) \\ &= \sum_{i=0}^{s-1} n_1(C_i|G) \times n_2(C_i|G) + n_1(C_s|G) \times n_2(C_s|G) \end{aligned}$$

$$
\begin{aligned}
&=6\sum_{i=0}^{s-1}(s+2i)(5s-2i)+3(s+2s)(5s-2s)\\
&=6(5s^2\sum_{i=0}^{s-1}1+8s\sum_{i=0}^{s-1}i+4\sum_{i=0}^{s-1}i^2)+27s^2\\
&=6(5s^2(s)+8s\frac{(s-1)s}{2}-4\frac{(s-1)s(2s-1)}{6})+27s^2\\
&=46s^3+5s^2-4s,
\end{aligned}
$$

which is the required result. □

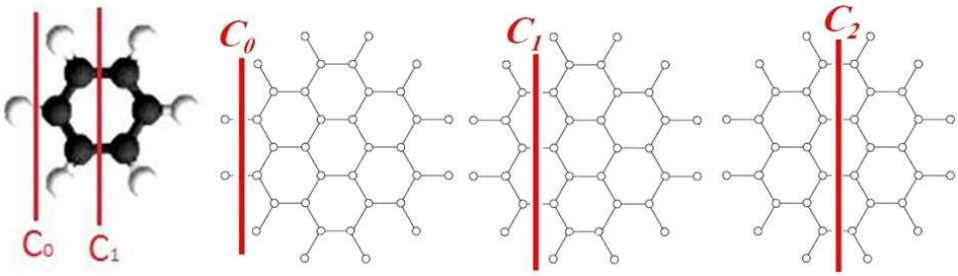

Figure 2. Representation of distinct orthogonal cuts of the Benzene PAH_1 and Coronene PAH_2

Example 1. First member of Polycyclic Aromatic Hydrocarbons PAH_s is Benzene PAH_1. It has 12 vertices in which 6 are pendent. Benzene has two distinct orthogonal cuts C_0 and C_1, where $n_1(C_0) = 1$, $n_2(C_0) = 5$, $n_1(C_1) = 3$ and $n_2(C_1) = 3$. So the terminal Wiener index of Benzene is

$$TW(PAH_1) = 6(1 \times 5) + 3(3 \times 3) = 57.$$

Example 2. Second member of Polycyclic Aromatic Hydrocarbons PAH_s is Coronene PAH_2. It has 36 vertices in which 12 are pendent. Coronene has three distinct orthogonal cuts C_0, C_1 and C_2, where $n_1(C_0) = 2, n_2(C_0) = 10, n_1(C_1) = 4, n_2(C_1) = 8, n_1(C_2) = 6$ and $n_2(C_2) = 6$. So the terminal Wiener index of Coronene is

$$TW(PAH_2) = 6(2 \times 10) + 6(4 \times 8) + 3(6 \times 6) = 420.$$

Example 3. Third member of Polycyclic Aromatic Hydrocarbons PAH_s is Circumcoronene PAH_3. It has 54 vertices in which 18 are pendent. Coronene

has four distinct orthogonal cuts C_0, C_1, C_2 and C_3, where $n_1(C_0) = 3$, $n_2(C_0) = 15, n_1(C_1) = 5, n_2(C_1) = 13, n_1(C_2) = 7, n_2(C_2) = 11, n_1(C_3) = 9$ and $n_2(C_3) = 9$. So the terminal Wiener index of Circumcoronene is

$$TW(PAH_3) = 6(3 \times 15) + 6(5 \times 13) + 6(7 \times 11) + 3(9 \times 9) = 1365.$$

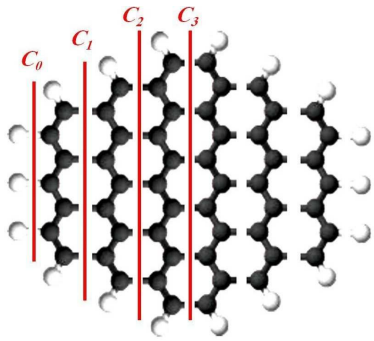

Figure 3. Representation of distinct orthogonal cuts of the Circumcoronene PAH_3

References

[1] M. Alaeyan, M.R. Farahani, M.K. Jamil. Computation of the fifth Geometric-Arithmetic Index for Polycyclic Aromatic Hydrocarbons PAH_k, *Applied Mathematics and Nonlinear Sciences*, **1** No. 1 (2016) 283-290. doi:10.21042/AMNS.2016.1.00023

[2] C.W. Bauschlicher, E.L.O. Bakes, Infrared spectra of polycyclic aromatic hydrocarbons (PAH_s), *Chemical Physics*, **262** (2002), 285-291, doi: 10.1016/S0301-0104(00)00310-4.

[3] A.J. Berresheim, M. Müller, K. Mullen, Polyphenylene Nanostructures, *Chemical Reviews*, **99** No. 7 (1999), 1747-1785, doi: 10.1021/cr970073.

[4] F. Dietz, N. Tyutyulkov, G. Madjarova, K. Mllen. (2000), Is 2-D graphite an ultimate large hydrocarbon II. Structure and energy spectra of polycyclic aromatic hydrocarbons with defects, *J. Phys. Chem. B*, **104** No. 8, 1746-1761. Doi 10.1021/jp9928659

[5] A. Soncini, E. Steiner, P.W. Fowler, R.W.A. Havenith. (2003), Perimeter effects on ring currents in polycyclic aromatic hydrocarbons: Circumcoronene and two hexabenzocoronenes, *Chemistry European Journal*, **9** No. 13, 2974-2981. doi 10.1002/chem.200204183

[6] K. Jug, T. Bredow. (2004), Models for the treatment of crystalline solids and surfaces, *Journal of Computational Chemistry*, **25** No. 3, 1551-1567. doi 10.1002/jcc.20080

[7] M.K. Jamil, M.R. Farahani, M.R.R. Kanna. Fourth geometric-arithmetic index of polycyclic aromatic hydrocarbons (PAH_k), *The Pharmaceutical and Chemical Journal*, **, 3** No. 1, (2016), 94-99

[8] M.R. Farahani. (2013), Some connectivity indices of polycyclic aromatic hydrocarbons PAH_s, *Advances in Materials and Corrosion*, **1**, 65-69.

[9] M.R. Farahani. (2013), Zagreb indices and Zagreb polynomials of polycyclic aromatic hydrocarbons, *Journal of Chemica Acta*, **2**, 70-72.

[10] M.R. Farahani. (2013), Hosoya, Schultz, modified Schultz polynomials and their topological indices of benzene molecules: first members of polycyclic aromatic hydrocarbons (PAH_s), *Int. Journal of Theoretical Chemistry*, **1** No. 2, 09-16.

[11] M.R. Farahani. (2014), Schultz and modified Schultz polynomials of Coronene polycyclic aromatic hydrocarbons, *Int. Letters of Chemistry, Physics and Astronomy*, **13** No. 1-10.

[12] W. Gao, M.R. Farahani (2015), Degree-based indices computation for special chemical molecular structures using edge dividing method, *Applied Mathematics and Nonlinear Sciences*, **1** No. 1, 94-117. doi 10.21042/AMNS.2016.1.00009

[13] M.R. Farahani. (2015), Exact formulas for the first Zagreb eccentricity index of polycyclic aromatic hydrocarbons (PAH_s), *Journal of Applied Physical Science International*, **4** No, 185-190.

[14] M.R. Farahani. (2015), The second Zagreb eccentricity index of polycyclic aromatic hydrocarbons PAH_k, *Journal of Computational Methods in Molecular Design*, **5** No. 2, 115-120.

[15] M.R. Farahani, W. Gao, M.R.R. Kanna. (2015), On the Omega polynomial of a family of hydrocarbon molecules polycyclic aromatic hydrocarbons PAH_k, *Asian Academic Research Journal of Multidisciplinary*, **2** No. 7, 263-268.

[16] M.R. Farahani, W. Gao. (2015), On multiple Zagreb indices of polycyclic aromatic hydrocarbons PAH, *Journal of Chemical and Pharmaceutical Research*, **7** No. 10, 535-539.

[17] M.R. Farahani, W. Gao. (2015), Theta polynomial W(G;x) and Theta index W(G) of polycyclic aromatic hydrocarbons PAH_k, *Journal of Advances in Chemistry*, **12** No. 1, 3934-3939.

[18] M.R. Farahani, M.R.R. Kanna. (2015), The PI polynomial and the PI index of a family hydrocarbons molecules, *Journal of Chemical and Pharmaceutical Research*, **7** No. 11, 253-257.

[19] M.R. Farahani, W. Gao, M.R.R. Kanna. (2015), The edge-Szeged index of the polycyclic aromatic hydrocarbons PAH_k, *Asian Academic Research Journal of Multidisciplinary*, **2** No. 7, 136-142.

[20] M.R. Farahani, M.R.R. Kanna. (2015), The edge-PI index of the polycyclic aromatic hydrocarbons PAH_k, *Indian Journal of Fundamental and Applied Life Sciences*, **5** No. S4, 614-617.

[21] M.K. Jamil, H.M. Rehman, M.R. Farahani, D.W. Lee. (2016), Vertex PI index of polycyclic aromatic hydrocarbons PAH_k, *The Pharmaceutical and Chemical Journal, 3* No. 1, 138-141.

[22] M.R. Farahani, M.K. Jamil, M.R.R. Kanna. (2016), Fourth geometric arithmetic index of polycyclic aromatic hydrocarbons (PAH_k), *The Pharmaceutical and Chemical Journal*, **3** No. 1, 1-6.

[23] M.R. Farahani, M.K. Jamil, M.R.R. Kanna, P.R. Kumar. (2016), The second Zagreb eccentricity index of polycyclic aromatic hydrocarbons PAH_k, *Journal of Chemical and Pharmaceutical Research*, **8** No. 4, 80-83.

[24] M.R. Farahani, M.K. Jamil, M.R.R. Kanna, P.R. Kumar. (2016), Computation on the fourth Zagreb index of polycyclic aromatic hydrocarbons (PAH_k), *Journal of Chemical and Pharmaceutical*, **8** No. 4, 41-45.

[25] D.W. Lee, M.K. Jamil, M.R. Farahani, H.M. Rehman. (2016), The ediz eccentric connectivity index of polycyclic aromatic hydrocarbons PAH_k, *Scholars Journal of Engineering and Technology*, **4** No. 3, 148-152.

[26] M.R.R. Kanna, R. Pradeep Kumar, M.K. Jamil, M. R. Farahani. Omega and Clu-Ilmenau Indices of Hydrocarbon Molecules "Polycyclic Aromatic Hydrocarbons PAH_k", *Computational Chemistry*, **4**, 91-96. http://dx.doi.org/10.4236/cc.2016.44009

[27] L. Yan, Y. Li, M.R. Farahani, M. Imran, M.R.R. Kanna. (2016), Computing the Szeged, revised Szeged and Normalized revised Szeged indices of the polycyclic aromatic hydrocarbons PAH_k, *Journal of Computational and Theoretical Nanoscience*, In press.

[28] M. Jamil, M.R. Farahani, M. Ali Malik, M. Imran. (2016), Computing the eccentric version of second Zagreb index of polycyclic aromatic hydrocarbons (PAH_k), *Applied Mathematics and Nonlinear Sciences*, **1** No. 1, 247-251. doi10.21042/AMNS.2016.1.00019

[29] M.R. Farahani. (2013), Computing eccentricity connectivity polynomial of Circumcoronene series of Benzenoid H_k by ring-cut method, *Annals of West University of Timisoara-Mathematics and Computer Science*, **51** No. 2, 29-37. Doi 10.2478/awutm-2013-0013

[30] M.R. Farahani, The application of cut method to computing the edge version of Szeged index of molecular graphs, *Pacific Journal of Applied Mathematics*, **6** No. 4 (2014), 249-258.

[31] M.R. Farahani, M.K. Jamil, M.R.R. Kanna, R.P. Kumar, Computing Edge Co-Padmakar-Ivan Index of Titania Nanotubes $TiO_2(m;n)$, *Journal of Environmental Science, Computer Science and Engineering & Technoology, Sec. C*, **5** No. 3 (2016), 326-334.

[32] M.R. Farahani, H.M. Rehman, M.K. Jamil, D. W. Lee, Vertex version of PI index of Polycyclic aromatic hydrocarbons PAH_k, *The Pharmaceutical and Chemical Journal*, **3** No. 1 (2016), 138-141.

[33] I. Gutman, B. Furtula, M. Petrovic, Terminal Wiener index, *Journal of Mathematical Chemistry*, **46** (2009), 522-531, doi: 10.1007/s10910-008-9476-2.

[34] I. Gutman, B. Furtula, A survey on terminal Wiener index, in: I. Gutman, B. Furtula (Eds.) Novel Molecular Structure Descriptors-Theory and Applications I, *Univ. Kragujevac, Kragujevac*, (2010), 173-190.

[35] P.E. John, P.V. Khadikar, J. Singh, A method of computing the PI index of Benzenoid hydrocarbons using orthogonal cuts, *Journal of Mathematical Chemistry*, **42** No. 1 (2007), 27-45, doi: 10.1007/s10910-006-9100-2.

[36] S. Klavžar, A bird's eye view of the cut method and a survey of its applications in chemical graph theory, *MATCH Communications in Mathematical and in Computer Chemistry*, **60** (2008), 255-274.

[37] S. Klavžar, M.J. Nadjafi-Arani, Cut method; update on recent developments and equivalence of independent approaches, *Current Organic Chemistry*, **19** No. 4 (2015), 348-358, doi: 10.2174/1385272819666141216232659.

[38] M. Randić. Novel molecular descriptor for structure-property studies, *Chemical Physics Letters*, **211** (1993), 478-483, doi: 10.1016/0009-2614(93)87094-J.

[39] U.E. Wiersum, L.W. Jenneskens. In gas phase reactions in organic synthesis, (Ed.: Y. Valle), *Gordon and Breach Science Publisher*, Amsterdam, The Netherlands, (1997), 143-194.

[40] F. Morgenroth, C. Kübel, M. Müller, U.M. Wiesler, A.J. Berresheim, M. Wagner, K. Mllen, From three-dimensional polyphenylene dendrimers to large graphite subunits, *Carbon*, **36** (1998), 833-837, doi: 10.1016/S0008-6223(98)00018-9.

[41] H. Wiener, Structural determination of paraffin boiling points, *Journal of the American Chemical Society*, **1** No. 69 (1947), 17-20, doi: 10.1021/ja01193a005.

[42] L. Yan, Y. Li, M.R. Farahani, M.K. Jamil, S. Zafar, Vertex version of co-PI index of the polycyclic aromatic hydrocarbons systems PAH_k, *Int. Journal of Biology, Pharmacy and Allied Sciences*, **5** No. 6 (2016), 1244-1253.