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The Harmonic Polynomial and Harmonic Index of Certain Carbon Nanotubes

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ABSTRACT. In the study of QSPR/QSAR, we used topological indices to predict or estimate the bioactivity of chemical compounds. The harmonic index is an useful tool in predicting the heats of vaporizations, critical temperatures and melting points. In this paper, we compute the harmonic index of certain carbon nanotubes $TUC_4C_8[m,n]$ and $TUC_4[m,n]$, respectively.

1 Introduction

Let $G(V,E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The number of vertices in $V(G)$ is called the order and the number of edges in $E(G)$ is called the size of the graph G. The number of adjacent vertices to the vertex v is called its degree and denoted as $d(v)$. For notation and concepts not defined here we refer to [20].

The quantitative structure-property relationship (QSPR) makes a connection between the structure and the properties of molecules. In 1975, Randiċ proposed the first degree based structural descriptor [25] named the Randiċ index, which is defined as

$$R(G) = \sum_{uv\in E(G)} \left(d(u)d(v)\right)^{-\frac{1}{2}}.$$

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Later on, Bollobàs et al. replaced the exponent $-\frac{1}{2}$ by any real number α and defined the general Randiĉ index as

$$R_\alpha(G) = \sum_{uv\in E(G)} \Big(d(u)d(v)\Big)^\alpha.$$

Zhou [29] extended this concept to the general sum-connectivity index as

$$\chi_\alpha(G) = \sum_{uv\in E(G)} \Big(d(u)+d(v)\Big)^\alpha,$$

where α is any real number.

In 1980, Fajtlowicz defined an invariant of the Randiĉ index called the harmonic index, as

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

He examined the possible relations between countless graph invariants. With single exception $H(G)$ did not attract anybody's attention, especially not chemists. Recently, Hosmani et al. [22] explored the chemical applications of the harmonic index. They revealed that harmonic index is also an useful tool in predicting the heats of vaporizations and critical temperatures of alkanes.

Iranmanesh et. al [23] were the first to introduced the harmonic polynomial of a caterpillar graph G of diameter 4 as follows:

$$H(G,x) = 2\sum_{uv\in E(G)} x^{d(u)+d(v)-1},$$

where $\int_0^1 H(G,x)dx = H(G)$. For further details on the above mentioned degree based topological indices see [6, 7, 18, 21, 23, 24, 28].

Carbon nanotubes form an interesting class of carbon nanomaterials. These can be imagined as rolled sheets of graphite about different axes. Armchair, chiral and zigzag are three types of well known nanotube structures. Moreover, nanotubes can be categorized as single-walled and multi-walled nanotubes. Diudea considered the problem of computing topological indices of nanostructures, referred to [2, 3, 4, 5]. Nowadays, computing topological indices of nanostructures have been the subject of many papers. In this paper, we continue this program and compute the harmonic index of the graphs corresponding to the $TUC_4(S)$ and $TUC_4C_8(S)$ nanotubes.

2 Main results and discussions

In this section, we compute the exact formulas for the harmonic polynomial and the harmonic index for $TUC_4[m,n]$ and $TUC_4[m,n]$ carbon nanotubes. For further results see [19, 26].

First of all, we compute the harmonic polynomial and harmonic index of carbon nanotubes $TUC_4C_8[m,n]$, where m and n are any natural numbers. The corresponding nanotube is a trivalent decoration having plane tiling of C_4 and C_8 and this type of tiling can either cover a cylinder or a torus. In the structure of $TUC_4C_8[m,n]$ nanotube, m is the number of octagons in any row and n is the number of octagons in any column. Also, the size and the order of carbon nanotubes TUC_4C_8 is $4m(2n+1)$ and $4m(3n+1)$, respectively. For instance, Fig. 1 depicts the molecular structure of carbon nanotubes $TUC_4C_8[m,n]$. For further study and results see [1], [8],..., [17].

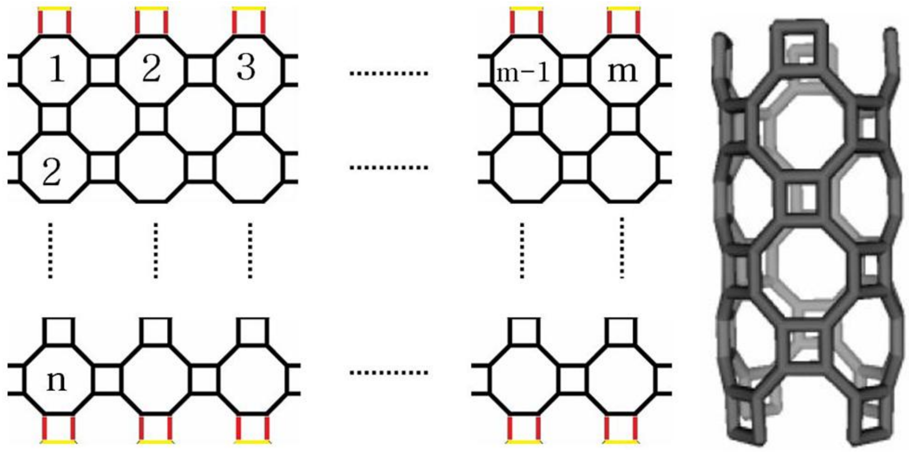

Figure 1: Molecular structure of carbon nanotubes $TUC_4C_8[m,n]$.

Theorem 2.1. *Let $TUC_4C_8[m,n]$ be the graph of carbon nanotubes, where $m,n \in \mathbb{N}$. Then the harmonic polynomial and the harmonic index of $TUC_4C_8[m,n]$ are equal to*

$$H(TUC_4C_8,x) = 4mx^3 + 8mx^4 + 4m(6n-1)x^5,$$
$$H(TUC_4C_8) = m + \frac{8m}{5} + \frac{2m(6n-1)}{3}.$$

Proof. The graph of the carbon nanotube $TUC_4C_8[m,n]$ contains $4m(2n+1)$ vertices and $4m(3n+1)$ edges. From Fig.1, we notice that there are three types of edges based on degree of their end vertices, namely:

$$E_4 = \{uv \in E(TUC_4C_8[m,n]) | d(u) = d(v) = 2\},$$
$$E_5 = \{uv \in E(TUC_4C_8[m,n]) | d(u) = 2, d(v) = 3\},$$
$$E_6 = \{uv \in E(TUC_4C_8[m,n]) | d(u) = d(v) = 3\}.$$

The number of edges in E_4, E_5 and E_6 are $2m, 4m$ and $12mn - 2m$. We are now able to find the harmonic polynomial.

$$\begin{aligned} H(TUC_4C_8,x) &= 2\sum_{uv\in E(TUC_4C_8)} x^{d(u)+d(v)-1} \\ &= 2\sum_{uv\in E_4} x^{d(u)+d(v)-1} + 2\sum_{uv\in E_5} x^{d(u)+d(v)-1} + 2\sum_{uv\in E_6} x^{d(u)+d(v)-1} \\ &= 2m \times 2x^{2+2-1} + 4m \times 2x^{3+2-1} + (12mn-2m) \times 2x^{3+3-1} \\ &= 4mx^3 + 8mx^4 + 4m(6n-1)x^5. \end{aligned}$$

Since

$$\begin{aligned} H(TUC_4C_8) &= \int_0^1 H(TUC_4C_8, x)dx \\ &= \int_0^1 4mx^3 + 8mx^4 + 4m(6n-1)x^5 \\ &= mx^4 + \frac{8mx^5}{5} + \frac{2m(6n-1)x^6}{3}\Big|_0^1 \\ &= m + \frac{8m}{5} + \frac{2m(6n-1)}{3}. \end{aligned}$$

This completes the proof. □

Next we compute the harmonic polynomial and harmonic index of the graph of carbon nanotube $TUC_4[m,n]$, where m and n are the natural numbers. The graphical structure of TUC_4 is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. In the graph of $TUC_4[m,n]$, m is the number of squares in any row and n is the number of squares in any column as shown in Figure 2. The molecular graph of $TUC_4[m,n]$ nanotube have $2m(n+1)$ atoms and $2m(2n+1)$ bonds.

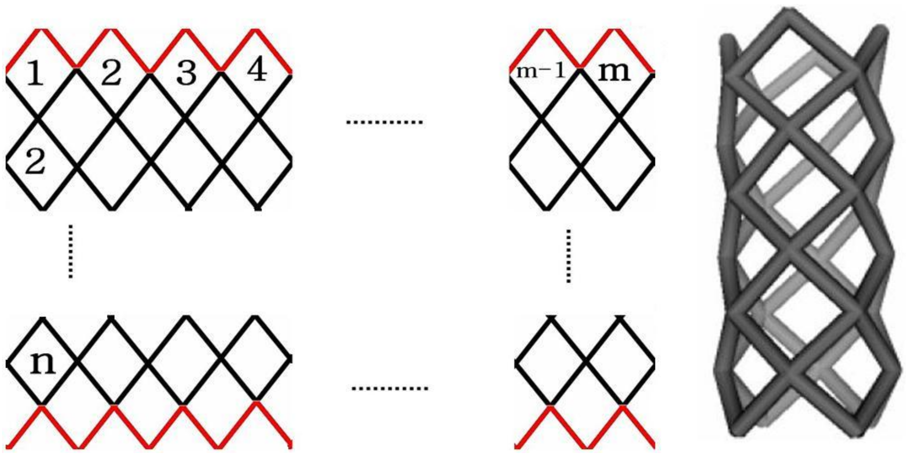

Figure 2: The graphical structure of $TUC_4[m,n]$ carbon nanotube.

Theorem 2.2. *Let $TUC_4[m,n]$ be the graph of carbon nanotubes, where $m,n \in N$. Then the harmonic polynomial and the harmonic index of $TUC_4[m,n]$ are equal to*

$$H(TUC_4, x) = 8mx^5 + 4m(n+1)x^7,$$

$$H(TUC_4) = \frac{4m}{3} + \frac{m(n+1)}{2}.$$

Proof. The molecular graph of the carbon nanotubes $TUC_4[m,n]$ contains $2m(n+1)$ vertices and $2m(2n+1)$ edges. From Fig. 2, we see that there are two types of edges based on degree of their end vertices, namely:

$$E_6 = \{uv \in E(TUC_4[m,n]) | d(u) = 2, d(v) = 4\},$$

$$E_8 = \{uv \in E(TUC_4[m,n]) | d(u) = d(v) = 4\}.$$

The numbers of edges in E_6 and E_8 are $4m$ and $4mn-2m$. We can find the harmonic polynomial.

$$\begin{aligned} H(TUC_4,x) &= 2\sum_{uv\in E(TUC_4)} x^{d(u)+d(v)-1} \\ &= 2\sum_{uv\in E_6} x^{d(u)+d(v)-1} + 2\sum_{uv\in E_8} x^{d(u)+d(v)-1} \\ &= 4m\times 2x^{4+2-1} + 2m(n+1)\times 2x^{4+4-1} \\ &= 8mx^5 + 4m(n+1)x^7. \end{aligned}$$

Since

$$\begin{aligned} H(TUC_4) &= \int_0^1 H(TUC_4,x)dx \\ &= \int_0^1 8mx^5 + 4m(n+1)x^7 \\ &= \frac{4mx^6}{3} + \frac{m(n+1)x^8}{2}\Big|_0^1 \\ &= \frac{4m}{3} + \frac{m(n+1)}{2}, \end{aligned}$$

which completes the proof. □

References

[1] M. Alaeiyan, A. Bahrami, M.R. Farahani. Cyclically Domination Polynomial of Molecular Graph of Some Nanotubes, *Digest Journal of Nanomaterials and Biostructures.* **6**(1), 143-147 (2011).

[2] M.V. Diudea, Graphenes from 4-valent tori, *Bull. Chem. Soc. Jpn.*, **75** (2002) 487-492.

[3] M.V. Diudea, Hosoya polynomial in tori, *MATCH Commun. Math. Comput. Chem.*, **45** (2002) 109-122.

[4] M.V. Diudea, A. Graovac, Generation and graph theoretical properties of C_4-tori, *MATCH Commun. Math. Comput. Chem.*, **44** (2001) 93-102.

[5] M.V. Diudea, I. Silaghi-Dumitrescu, B. Parv, Toranes versus torenes, *MATCH Commun. Math. Comput. Chem.*, **44** (2001) 117-133.

[6] Z. Du, B. Zhou, N. Trinajstic̀, On the general sum-connectivity index of trees, *Appl. Math. Lett.*, **24** (2011) 402-405.

[7] Z. Du, B. Zhou, N. Trinajstic̀, Minimum general sum-connectivity index of unicyclic graphs, *J. Math. Chem.*, **48** (2010) 697-703.

[8] M.R. Farahani, M. Imran, M.K. Siddiqui, M.H. Afzal. Siddiqui, Sh. Baby. The Second and Second-Sum-connectivity indices of $TUC_4C_8(S)$ Nanotubes, *Journal of Optoelectronic and Biomedical Materials.* **8**(2), 2016, 107-111.

[9] M.R. Farahani. On Domination Polynomial of $TUC_4C_8(S)$ Nanotube, *Pacific Journal of Applied Mathematics.* **7**(2), 2015, 75-86.

[10] M.R. Farahani. Domination polynomial of Nanotorus by Using the 2-variables Generating Function, *Pacific Journal of Applied Mathematics.* **6**(1), 2014, 79-95.

[11] M.R. Farahani. Computing some connectivity indices of Nanotubes, *Adv. Mater. Corrosion.* **1**, (2012), 57-60.

[12] M.R. Farahani. The Hyper-Zagreb Index of $TUSC_4C_8(S)$ Nanotubes, *International Journal of Engineering and Technology Research.* **3**(1), 2015, 1-6.

[13] M.R. Farahani. Fifth Geometric-Arithmetic Index of $TURC_4C_8(S)$ Nanotubes, *Journal of Chemica Acta.* **2**(1), (2013), 62-64.

[14] M.R. Farahani. New Version of Atom-Bond Connectivity Index of $TURC_4C_8(S)$, *International Journal of Chemical Modeling.* **4**(4), 527-521, (2012).

[15] M.R. Farahani. Zagreb indices of $TUHRC_4(S)$ and $USC_4C_8(S)$ Nanotubes, *Journal of Advance in Mathematical Science.* **2**(1), 2015, 98-105.

[16] M.R. Farahani. On the Higher Randic Indices of Nanotubes, *Journal of Computational Methods in Molecular Design.* **5**(3), 2015, 10-15

[17] M.R. Farahani. Multiplicative Versions of Zagreb indices of $TUSC_4C_8(S)$, *Journal of Chemistry and Materials Research.* **2**(2), 2015, 67-70.

[18] M.R. Farahani, W. Gao, M.R.R. Kanna, P.R. Kumar, J.B. Liu. General Randic, Sum-Connectivity, Hyper-Zagreb and Harmonic Indices, and Harmonic Polynomial of Molecular Graphs, *Advances in Physical Chemistry.* **2016**, Article ID 2315949, 6 pages, 2016. doi:10.1155/2016/2315949.

[19] M. Ghojavand, A. R. Ashrafi, Computing bipartite edge frustration of some nanotubes, *Digest Journal of Nanomaterials and Biostructures*, **4** (2008) 209-214.

[20] F. Harary, Graph Theory, *Addison-Wesley, Reading MA*, **1969**.

[21] Y. Hu, X. Li, Y. Yuan, Trees with maximum general Randiȅ index, *MATCH Commun. Math. Comput. Chem.*, **52** (2004) 129-146.

[22] S.M. Hosamani, D. M. Perigidad, S. Y. Jamagoud, Y. B. Maled, S. Gavade, QSPR analysis of certain degree based topological indices, *in press*.

[23] M.A. Iranmanesh, M. Saheli, On the harmonic index and harmonic polynomial of catepillars with diameter four, *Iranian J. Math. Chem* **5 (2)** (2014) 35-43.

[24] J. Li, W.C. Shiu, The harmonic index of a graph, *Rocky Mountain J. Math.*, **44** (2014) 1607-1620.

[25] M. Randiȅ, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609-6615.

[26] B. Rajan, A. William, C. Grigorious, S. Stephen, On certain topological indices of silicate, honeycomb and hexagonal networks, *J. Comp. Math. Sci.*, **3 (5)** (2012) 530-535.

[27] I. Tomescu, M.K. Jamil, Maximum general sum-connectivity index for trees with given independence number, *MATCH Commun. Math. Comput. Chem.*, **72** (2014) 715-722.

[28] L. Zhong, The harmonic index for graphs, *Appl. Math. Lett.*, **25** (2012) 561-566.

[29] B. Zhou, N. Trinajstiȅ, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210-218.