ISSN 2321-807X

The Theta Polynomial Θ(G,x) and the Theta Index Θ(G) of Molecular Graph Polycyclic Aromatic Hydrocarbons PAH_k

Wei Gao[1] , Mohammad Reza Farahani[2*]

1.School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China.

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

ABSTRACT: The omega polynomial *Ω(G,x),* for counting *qoc* strips in molecular graph *G* was defined by *Diudea* as $\Omega(G,x)=\sum_c m(G,c)x^c$ with *m(G,c),* being the number of *qoc* strips of length *c*. The Theta polynomial *Θ(G,x)* and the Theta index *Θ(G)* of a molecular graph *G* were defined as *Θ(G,x)*= $\sum_c m(G,c).c.x^c$ and *Θ(G)*= $\sum_c m(G,c).c^2$, respectively.

In this paper, we compute the Theta polynomial *Θ(G,x)* and the Theta index *Θ(G)* of molecular graph *Polycyclic Aromatic Hydrocarbons* PAH_k, for all positive integer number *k*.

Keywords: Molecular graph, Polycyclic Aromatic Hydrocarbons, Omega polynomial, Theta polynomial, Theta index

Council for Innovative Research

Peer Review Research Publishing System

Journal: Journal of Advances in Chemistry

Vol. 12, No. 1

www.cirjac.com

editorjaconline@gmail.com, editor@cirjac.com

1. INTRODUCTION

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively.

A graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or by a single number (often called a topological index). A counting polynomial can be written as:

$$P(G, x)=\sum_{k} m(G,k)\, X^{k}$$

with the exponents showing the extent of partitions p(G), ∪p(G)=P(G) of a graph property P(G) while the coefficients m(G, k) are related to the number of partitions of extent k.

Let G(V,E) be a connected graph, two edges e=uv and f=xy of G are called co-distant: e co f, if and only if d(u,x)=d(v,y)=k and d(u,y)=d(v,x)=k+1 or vice versa, for a non-negative integer k.

If co is an equivalence relation: [1-3].

$$e \ co \ e$$

$$e \, co \, f \Leftrightarrow f \, co \, e$$

$$e \, co \, f \ \& \ f \, co \, h \Rightarrow e \, co \, h$$

Then, C(e):={f∈E(G)| f co e} is the set of edges in G, co-distant to the edge e∈E(G) and G is called a co-graph. Consequently, C(e) is called an orthogonal cut set ocs of G and E(G) is the union of disjoint orthogonal cuts:

$$E(G) = C_1 \cup C_2 \cup ... \cup C_{k-1} \cup C_k \text{ and } C_i \cap C_j = \varnothing,$$

for i≠j and i, j=1, 2, …, k. The relation ops is not necessarily transitive. Observe an ops is an ocs only in partial cubes.

Observe co is a θ relation, (Djokovic-Winkler relation) [4, 5] and G is a co-graph if and only if it is a partial cube, a result due to Klavžar [6]. In a plane bipartite graph, an edge e is in relation θ with any opposite edge f if the faces of the plane graph are isometric (which is the case of the most chemical graphs). Then an orthogonal cut oc with respect to a given edge is the smallest subset of edges closed under this operation and C(e) is precisely a θ-class of G.

The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by M.V. Diudea as [7]

$$\Omega(G,x)=\sum_{c} m(G,c)\, x^{c}$$

where *m*(*G*,*c*) is the number of opposite edge strips of length *c.*

If *ops* is an *ocs*, as in partial cubes, we can write the following counting polynomials [8-23]:

$$Sd(G,x)=\sum_{c} m(G,c)\, x^{|E(G)|-c}$$

$$\Theta(G,x)=\sum_{c} m(G,c).c.x^{c}$$

$$\Pi(G,x)=\sum_{c} m(G,c).c.x^{|E(G)|-c}$$

Ω(G,x)and Θ(G,x) count equidistant edges in G while Sd(G, X) and Π(G,x), count non-equidistant edges. The first two polynomials are counted once for a strip while the last two are counted for each edge, so that the coefficients are multiplied with k.

In this present study, we compute the Theta polynomial Θ(G,x) and the Theta index Θ(G) of molecular graph Polycyclic Aromatic Hydrocarbons PAH_k, for all positive integer number k.

2. MAIN RESULTS AND DISCUSSION

The Polycyclic Aromatic Hydrocarbons PAH_k for all positive integer number k is ubiquitous combustion products. They have been implicated as carcinogens and play a role in graphitization of organic materials [24]. In addition, they are of interest as molecular analogues of graphite [25] as candidates for interstellar species [26] and as building blocks of functional materials for device applications [25-27]. Synthetic routes to Polycyclic Aromatic Hydrocarbons PAH_k are available [28] and a detailed knowledge of all these features would therefore be necessary for the tuning of molecular properties towards specific applications.

ISSN 2321-807X

Reader can see some first members of this family in Figure 1. In references [24-41] some properties and more historical details of this family of hydrocarbon molecules are studded.

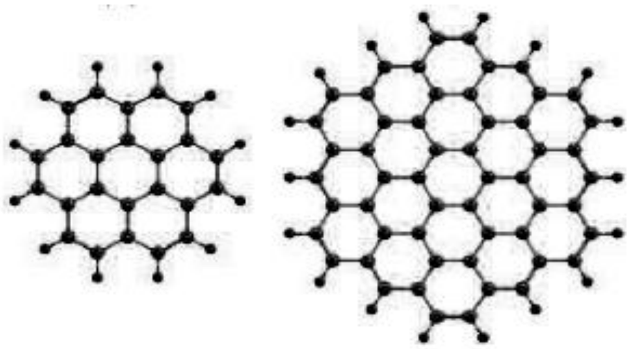

Figure 1. Two first members of the *Polycyclic Aromatic Hydrocarbons* PAH_k.

Theorem 1. The Theta polynomial $\Theta(G,x)$ and the Theta index $\Theta(G)$ $\forall k\geq 1$, are equal to

$$\Theta(PAH_k,x)=\sum_{i=0}^{k-1}6(k+i)x^{k+i}+(6k)x^{2k}$$

$$\Theta(PAH_k)=14k^3-3k^2+k.$$

Proof. Consider be the general representation of *Polycyclic Aromatic Hydrocarbons* PAH_k ($\forall k\geq 1$) with $6k^2+6k$ vertices/atoms and $9k^2+3k$ edge/chemical bonds.

Because, there are $6k^2$ Carbon atoms with degree 3 and $6k$ Hydrogen atoms with degree 1in vertex set $V(PAH_n)$, thus

$$|E(PAH_k)|=\frac{3\times 6k^2+1\times 6k}{2}=9k^2+3k$$

Now, we counting all opposite edge strips *ops* $m(PAH_k,c)$ of the general representation of *Polycyclic Aromatic Hydrocarbons* PAH_k, by using the Cut Method. The *Cut Method* and its general form studied by *S. Klavzar* [42].

By using the Cut Method, we see that the Polycyclic Aromatic Hydrocarbons is a co-graph and from Figure 2, one can see that there are $k+1$ distinct case of *qoc strips* for PAH_k such that the size of a *qoc strip* C_i for $\forall i=1,..,k-1$ is equal to $k+i$ ($=|C_i|=c_i$) and for $i=0$, $|C_0|=k$.

In other words,

- For $i=0$; $m(PAH_k,c_0)=6$ and $|C_k|=k$.
- For *all* $i=1,..,k-1$; $m(PAH_k,c_i)=6$ and $|C_i|=k+i$.
- For $i=k$; $m(PAH_k,c_k)=3$ and $|C_k|=2k$.

Thus the Theta polynomial of the Polycyclic Aromatic Hydrocarbons PAH_k ($\forall k\geq 1$) will be

$$\Theta(PAH_k,x)=\sum_c m(PAH_k,c).c.x^c$$

$$=\sum_{i=0}^{k} m(PAH_k,c_i).c_i.x^{c_i}$$

$$=m(PAH_k,c_0)|C_0|x^{|C_0|}+m(PAH_k,c_1)|C_1|x^{|C_1|}+\ldots$$

$$+m(PAH_k,c_{k-1})|C_{k-1}|x^{|C_{k-1}|}+m(PAH_k,c_k)|C_k|x^{|C_k|}$$

$$=6|C_0|x^{|C_0|}+6|C_1|x^{|C_1|}+\ldots+6|C_{k-1}|x^{|C_{k-1}|}+3|C_k|x^{|C_k|}$$

$$=6(k)x^k+6(k+1)x^{k+1}+\ldots+6(^{2k-1})x^{2k-1}+3(2k)x^{2k}$$

$$=\sum_{i=0}^{k-1}6(k+i)x^{k+i}+(6k)x^{2k}$$

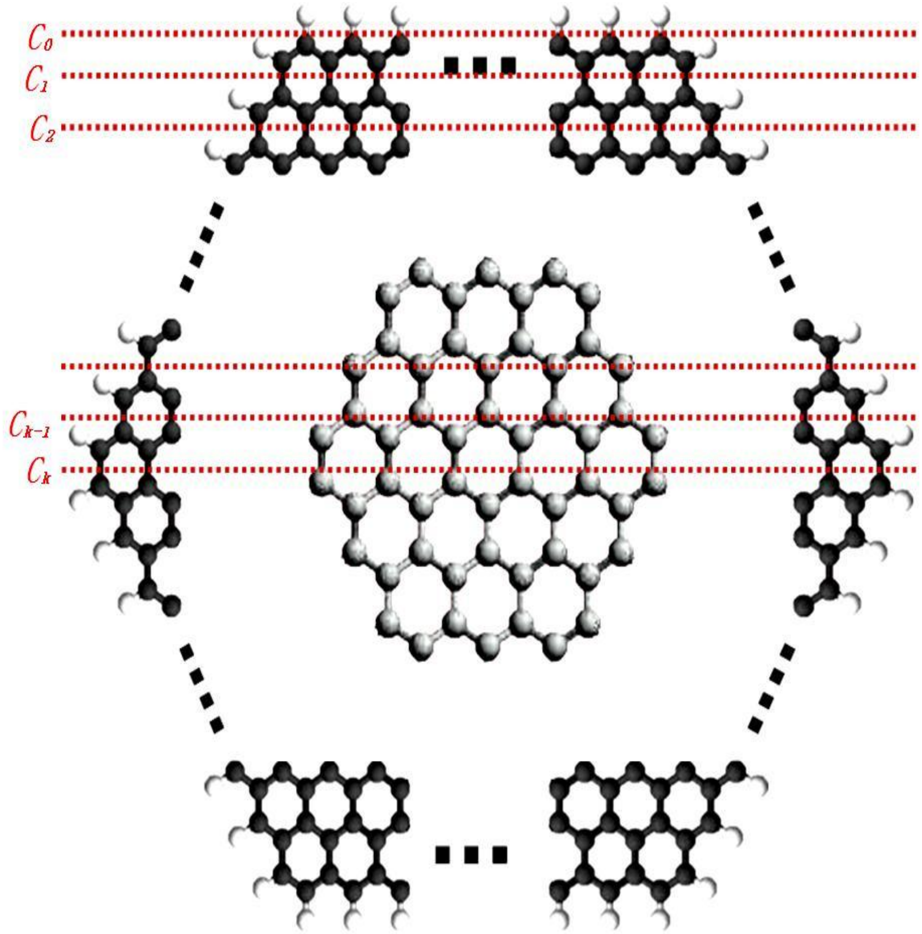

Figure 2. The presentation of quasi-orthogonal cuts qoc strips of Circumcoronene PAH_3.

$$\Theta(PAH_k)=\frac{\partial\Theta(PAH_k,x)}{\partial x}\bigg|_{x=1}$$

$$=\frac{\partial}{\partial x}\left(6(k)x^k+6(k+1)x^{k+1}+\ldots+6(2k-1)x^{2k-1}+3(2k)x^{2k}\right)_{x=1}$$

$$=\left(6(k)^2x^{k-1}+6(k+1)^2x^k+\ldots+6(2k-1)^2x^{2k-2}+3(2k)^2x^{2k-1}\right)_{x=1}$$

$$=\left(\sum_{i=0}^{k-1}6\left(k+i\right)^2\mathrm{x}^{k+i-1}+12k^2x^{2k-1}\right)_{x=1}$$

$$=\sum_{i=1}^{k-1}6\left(k+i\right)^2+12k^2$$

$$=6k^2\left(k-1\right)+12k\left(\frac{k^2}{2}-\frac{k}{2}\right)+6\left(\frac{k^3}{3}-\frac{k^2}{2}+\frac{k}{6}\right)+12k^2$$

$$=14k^3-3k^2+k$$

Here the proof of theorem is completed.■

ACKNOWLEDGMENTS

We thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by NSFC (no. 11401519).

REFERENCES

[1] P.E. John, P.V. Khadikar, and J. Singh. A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts, J. Math. Chem., 42 (1) (2007), 27-45.

[2] P.E. John, A.E. Vizitiu, S. Cigher, and M.V. Diudea, CI index in tubular nanostructures, MATCH Commun. Math. Comput. Chem., 57 (2007), 479–484.

[3] M.V. Diudea, S. Cigher, and P.E. John. Omega and related counting polynomials, MATCH Commun. Math. Comput. Chem, 60 (2008), 237–250.

[4] D. Ž. Djokovic, Distance-preserving subgraphs of hypercubes, J. Combin. Theory Ser. B, 1973, 14, 263–267.

[5] P. M. Winkler, Isometric embedding in products of complete graphs, Discrete Appl. Math.,1984, 7, 221-225.

[6] S. Klavžar, Some comments on CO graphs and CI index, MATCH Commun. Math. Comput. Chem., 2008, 59, 217-222.

[7] M.V. Diudea, Omega polynomial, Carpath. J. Math. 22 (2006), 43–47.

[8] M.V. Diudea, S. Cigher, A.E. Vizitiu, O. Ursu, and P.E. John. Omega polynomial in tubular nanostructures, Croat. Chem. Acta, 79 (2006), 445-448.

[9] A.E. Vizitiu, S. Cigher, M.V. Diudea, and M.S. Florescu, Omega polynomial in ((4,8)3) tubular nanostructures, MATCH Commun. Math. Comput. Chem., 57 (2007), 457-462.

[10] M.V. Diudea, S. Cigher, A.E. Vizitiu, M.S. Florescu, and P.E. John, Omega polynomial and its use in nanostructure description, J. Math. Chem. 45 (2009) 316–329.

[11] M.V. Diudea, A.E. Vizitiu, and S. Cigher, Omega and related polynomials in crystal-like structures, MATCH Commun. Math. Comput. Chem., 65 (2011) 131-142.

[12] M. Ghorbani and M. Ghazi, Computing Omega and PI polynomials of graphs, Digest Journal of Nanomaterials and Biostructures, 5 (4) (2010), 843-849.

[13] M.R. Farahani, K. Kato, and M.P. Vlad. Omega polynomials and Cluj-Ilmenau index of circumcoronene series of benzenoid, Studia Univ. Babes-Bolyai, 57(3) (2012), 177-182.

[14] M.R. Farahani, Computing the Omega and theta polynomials and their indices of an armchair polyhex nanotubes, Journal of Applied Physical Science International, 4(3) (2015), 160-164.

[15] M.R. Farahani, On the SD- polynomial and SD- index of an infinite class of "Armchair Polyhex Nanotubes", International Letters of Chemistry, Physics and Astronomy, 12 (2014), 63-68.

[16] M.R. Farahani, Omega and Sadhana polynomials of circumcoronene series of benzenoid, World Applied Sciences Journal, 20(9) (2012) 1248-1251.

[17] M.R. Farahanii, Π(G,x) polynomials of armchair polyhex nanotubes $TUAC_6[m,n]$, Int. Letters of Chemistry, Physics and Astronomy, 17(2) (2014), 201-206.

[18] M.R. Farahani, Computing Theta polynomial and Theta index of V-phenylenic planar, nanotubes and nanotoris, International Journal of Theoretical Chemistry, 1(1) (2013), 1-9.

[19] M.R. Farahani, Θ(G,X) polynomial and Θ(G) index of V-phenylenic planar, nanotubes and nanotori, World Journal of Science and Technology Research, 1(7) (2013), 135-143.

[20] M.R. Farahani, Computing the Omega polynomial of an infinite family of the linear parallelogram P(*n,m*), Journal of Advances in Chemistry, 1 (2013) 106-109.

[21] M.R. Farahani, On Sadhana polynomial of the linear parallelogram P(*n,m*) of benzenoid graph, Journal of Chemica Acta, 2(2) (2013), 95-97.

[22] M.R. Farahani, Computing a Counting polynomial of an infinite family of linear polycene parallelogram benzenoid graph P(a,b), Journal of Advances in Physics, 3(1) (2013), 186-190.

[23] M.R. Farahani, The Theta Θ(G,x) polynomial of an infinite family of the linear parallelogram P(*n,m*), Journal of Applied Physical Science International, 4(4) 2015, 206-209.

[24] U.E. Wiersum, L. W. Jenneskens in Gas Phase Reactions in Organic Synthesis, (Ed.: Y. Valle. e), Gordon and Breach Science Publishers, Amsterdam, The Netherlands, 1997, 143–194.

[25] J. Berresheim, M. Müller, and K. Müllen, Polyphenylene nanostructures, Chem. Rev., 99 (7) (1999), 1747–1786.

[26] C.W. Bauschlicher, and Jr, E. L.O. Bakes, Infrared spectra of polycyclic aromatic hydrocarbons (PAHs), Chem. Phys., 2000, 262, 285-291.

[27] J.D Brand,.; Y. Geerts,; K. Mullen , A.M. Craats and J.M. Warman, Rapid charge transport along self-assembling graphitic nano-wires. Adv. Mater. 1998, 10, 36-38.

[28] F. Morgenroth, C. Kübel, M. Müller, U.M. Wiesler, A.J. Berresheim, M. Wagner, and K. Müllen, From three-dimensional polyphenylene dendrimers to large graphite subunits, Carbon, 36 (5-6) (1998), 833-837.

[29] F. Dtz, J. D. Brand, S. Ito, L. Ghergel, and K. Müllen, Synthesis of large polycyclic aromatic hydrocarbons: variation of size and periphery, J. Am. Chem. Soc., 122(32) (2000), 7707-7717.

[30] K. Yoshimura, L. Przybilla, S. Ito, J. D. Brand, M. Wehmeir, H. J.Rder, and K. Müllen, Macromol. Chem. Phys., 202 (2001), 215-222.

[31] S. E. Stein, and R. L. Brown, .pi.-Electron properties of large condensed polyaromatic hydrocarbons, J. Am. Chem. Soc.,109(12) (1987), 3721-3729.

[32] F. Dietz, N. Tyutyulkov, G.Madjarova, and K. Müllen, Is 2-D graphite an ultimate large hydrocarbon? II. structure and energy spectra of polycyclic aromatic hydrocarbons with defects, J. Phys. Chem. B, 104(8) (2000), 1746-1761.

[33] S.E. Huber, A. Mauracher, and M.Probst. Permeation of low-Z atoms through carbon sheets: density functional theory study on energy barriers and deformation effects, Chem. Eur. J., 9 (2003), 2974-2981.

[34] K. Jug and T. Bredow, Models for the treatment of crystalline solids and surfaces, Journal of Computational Chemistry, 25 (2004) 1551-1567.

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

[36] M.R. Farahani, Zagreb indices and Zagreb polynomials of polycyclic aromatic hydrocarbons, J. Chem. Acta, 2 (2013), 70-72.

[37] M.R. Farahani, Schultz and Modified Schultz Polynomials of Coronene Polycyclic Aromatic Hydrocarbons. Int. Letters of Chemistry, Physics and Astronomy. 13(1), (2014), 1-10.

[38] M.R. Farahani, Exact Formulas for the First Zagreb Eccentricity Index of Polycyclic Aromatic Hydrocarbons (PAHs). Journal of Applied Physical Science International. 4(3), 2015, 185-190.

[39] M.R. Farahani, The Second Zagreb Eccentricity Index of Polycyclic Aromatic Hydrocarbons PAHk. Journal of Computational Methods in Molecular Design. 5(2),2015,115-120.

[40] M.R. Farahani, Hosoya, Schultz, Modified Schultz Polynomials and Their Topological Indices of Benzene Molecules: First Members of Polycyclic Aromatic Hydrocarbons (PAHs). International Journal of Theoretical Chemistry. 1(2), (2013),09-16.

[41] M.R. Farahani and W. Gao. On Multiple Zagreb indices of Polycyclic Aromatic Hydrocarbons PAH. Journal of Chemical and Pharmaceutical Research. 7(10), (2015), 535-539.

[42] S. Klavzar. A bird's eye view of the cut method and a survey of its applications In chemical graph theory, MATCH Commun. Math. Comput. Chem., 60 (2008), 255-274.

Author' biography with Photo

Wei Gao, male, was born in the city of Shaoxing, Zhejiang Province, China on Feb.13, 1981. He got two bachelor degrees on computer science from Zhejiang industrial university in 2004 and mathematics education from College of Zhejiang education in 2006. Then, he was enrolled in department of computer science and information technology, Yunnan normal university, and got Master degree there in 2009. In 2012, he got PhD degree in department of Mathematics, Soochow University, China.

He acted as lecturer in the department of information, Yunnan Normal University from July 2012 to November 2015. Now, he acts as associate professor in the department of information, Yunnan Normal University. As a researcher in computer science and mathematics, his interests are covering two disciplines: Graph theory, Statistical learning theory, Information retrieval, and Artificial Intelligence.