MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **80** (2018) 215-226

ISSN 0340 - 6253

Equivalence of the Generalized Zhang–Zhang Polynomial and the Generalized Cube Polynomial

Petra Žigert Pleteršek

Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia

Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia

petra.zigert@um.si

(Received January 18, 2018)

Abstract

In this paper we study the resonance graphs of benzenoid systems, tubulenes, and fullerenes. We introduce the concept of the generalized Zhang-Zhang polynomial for these molecules. Instead of considering only interactions between 6-cycles (Clar covers), we also consider 10-cycles, which contribute to the resonance energy of a molecule as well. Therefore, we generalize the concepts of the Zhang-Zhang polynomial of the underlying molecular graphs and the cube polynomial of the corresponding resonance graph and prove the equality of these two polynomials.

1 Introduction

A benzenoid system is determined with all the hexagons lying inside cycle C of the hexagonal lattice. They represent molecules called benzenoid hydrocarbons. These graphs are also known as the hexagonal systems and form one of the most extensively studied family of chemical graphs. For fundamental properties of benzenoid systems see [9], while some recent results can be found in [11, 12, 19, 22]. If we embed benzenoid systems on a surface of a cylinder and join some edges we obtain structures called open-ended single-walled carbon nanotubes also called tubulenes. Carbon nanotubes are carbon compounds with a cylindrical structure and they were first observed in 1991 [10]. If we close a carbon

nanotube with two caps composed of pentagons and hexagons, we obtain a fullerene. More exactly, a fullerene is a molecule of carbon in the form of a hollow sphere, ellipsoid, tube, or many other shapes. The first fullerene molecule was discovered 30 years ago. In graph theory, a fullerene is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The overview of some results on fullerene graphs can be found in [1]. Papers [7, 18] present a sample of recent investigations.

The concept of the resonance graph appears quite naturally in the study of perfect matchings of molecular graphs of hydrocabons that represent Kekulé structures of corresponding hydrocarbon molecules. Therefore, it is not surprising that it has been independently introduced in the chemical [6, 8] as well as in the mathematical literature [21] (under the name Z-transformation graph) and then later rediscovered in [15, 16].

The equivalence of the Zhang-Zhang polynomial of the molecular graph and the cube polynomial of its resonance graph was established for benzenoid systems [23], tubulenes [2], and fullerenes [20]. The Zhang-Zhang polynomial counts Clar covers with given number of hexagons, i.e. conjugated 6-cycles and it was introduced in [24]. For some recent research on the Zhang-Zhang polynomial see [4, 5]. Cube polynomial of a graph H was introduced by Brešar et al. in [3] as a counting polynomial for the number of induced hypercubes in H of different dimensions.

The resonance energy is a theoretical quantity which is used for predicting the aromatic stability of conjugated systems. In the conjugated-circuit model, the resonance energy is determined with conjugated cycles of different lengths (see [14]), not only with 6-cycles. Among them, only 6-cycles and 10-cycles have uniquely determined structure. Therefore, we introduce the concept of the generalized Zhang-Zhang polynomial, which considers both of them. In this paper we prove the equivalence of the generalized Zhang-Zhang polynomial of a molecular graph and the generalized cube polynomial of the corresponding resonance graph.

2 Preliminaries

A *benzenoid system* consists of a cycle C of the infinite hexagonal lattice together with all hexagons inside C. A *benzenoid graph* is the underlying graph of a benzenoid system.

Next we formally define open-ended carbon nanotubes, also called *tubulenes* [17]. Choose any lattice point in the hexagonal lattice as the origin O. Let $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$ be the two basic

lattice vectors. Choose a vector $\overrightarrow{OA} = n\overrightarrow{a_1} + m\overrightarrow{a_2}$ such that n and m are two integers and $|n| + |m| > 1$, $nm \neq -1$. Draw two straight lines L_1 and L_2 passing through O and A perpendicular to OA, respectively. By rolling up the hexagonal strip between L_1 and L_2 and gluing L_1 and L_2 such that A and O superimpose, we can obtain a hexagonal tessellation $\mathcal{HT}$ of the cylinder. L_1 and L_2 indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *tubulene* T is defined to be the finite graph induced by all the hexagons of $\mathcal{H}T$ that lie between c_1 and c_2, where c_1 and c_2 are two vertex-disjoint cycles of $\mathcal{H}T$ encircling the axis of the cylinder. The vector $\overrightarrow{OA}$ is called the *chiral vector* of T and the cycles c_1 and c_2 are the two open-ends of T.

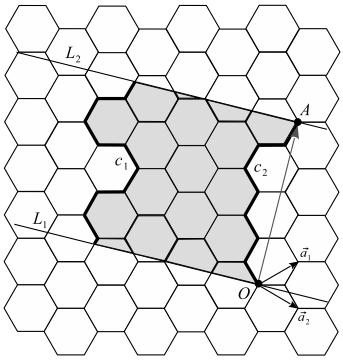

Figure 1. Illustration of a $(4, -3)$-type tubulene.

For any tubulene T, if its chiral vector is $n\overrightarrow{a_1} + m\overrightarrow{a_2}$, T will be called an (n, m)-type tubulene, see Figure 1.

A *fullerene* G is a 3-connected 3-regular plane graph such that every face is bounded by either a pentagon or a hexagon. By Euler's formula, it follows that the number of pentagonal faces of a fullerene is exactly 12.

A *1-factor* of a graph G is a spanning subgraph of G such that every vertex has degree one. The edge set of a 1-factor is called a *perfect matching* of G, which is a set of independent edges covering all vertices of G. In chemical literature, perfect matchings are known as Kekulé structures (see [9] for more details). Petersen's theorem states that every bridgeless 3-regular graph always has a perfect matching [13]. Therefore, a fullerene always has at least one perfect matching. A hexagon of G with exactly 3 edges in a perfect matching

M of G is called a *sextet*.

Let G be a benzenoid system, a tubulene or a fullerene with a perfect matching. The *resonance graph* $R(G)$ is the graph whose vertices are the perfect matchings of G, and two perfect matchings are adjacent whenever their symmetric difference forms a hexagon of G.

The *hypercube* Q_n of dimension n is defined in the following way: all vertices of Q_n are presented as n-tuples $(x_1, x_2, \ldots, x_n)$ where $x_i \in \{0, 1\}$ for each $1 \leq i \leq n$ and two vertices of Q_n are adjacent if the corresponding n-tuples differ in precisely one coordinate.

A *convex subgraph* H of a graph G is a subgraph of G such that every shortest path between two vertices of H is contained in H.

3 The generalized polynomials

Let G be a benzenoid system, a tubulene or a fullerene. A *Clar cover* is a spanning subgraph of G such that every component of it is either C_6 or K_2. The *Zhang-Zhang polynomial* of G is defined in the following way:

$$ZZ(G, x) = \sum_{k \geq 0} z(G, k) x^k,$$

where $z(G, k)$ is the number of Clar covers of G with k hexagons.

A *generalized Clar cover* is a spanning subgraph of G such that every component of it is either C_6, C_{10} or K_2. See Figure 2 for an example.

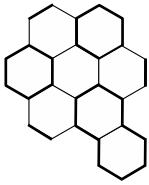

Figure 2. A generalized Clar cover of a benzenoid system G.

The *generalized Zhang-Zhang polynomial* of G is defined in the following way:

$$GZZ(G, x, y) = \sum_{k \geq 0, l \geq 0} gz(G, k, l) x^k y^l,$$

where $gz(G,k,l)$ is the number of generalized Clar covers of G with k cycles C_6 and l cycles C_{10}. Note that for a graph G number $gz(G,0,0)$ equals the number of vertices of $R(G)$ and $gz(G,1,0)$ equals the number of edges of $R(G)$. Furthermore, number $gz(G,k,0)$ represents the number of Clar covers with k hexagons.

Let H be a graph. The *Cube polynomial* of H is defined as follows:

$$C(H,x) = \sum_{k\geq 0} \alpha_k(H) x^k,$$

where $\alpha_k(H)$ denotes the number of induced subgraphs of H that are isomorphic to the k-dimensional hypercube.

Let G be a graph and $i \geq 1$ an integer. Then by G^i we denote the Cartesian product of i copies of G, i.e. $G^i = G\Box\cdots\Box G$. Also, $G^0 = K_1$. Furthermore, for any $k,l \geq 0$ we define $Q_{k,l} = P_2^k \Box P_3^l$, where P_2 and P_3 are paths on 2 and 3 vertices, respectively. Obviously, $Q_{k,0}$ is the k-dimensional hypercube. Moreover, if $k+l > 0$, vertices of the graph $Q_{k,l}$ can be presented as $(k+l)$-tuples $(b_1,\ldots,b_k,b_{k+1},\ldots,b_{k+l})$, where $b_i \in \{0,1\}$ if $i \in \{1,\ldots,k\}$ and $b_i \in \{0,1,2\}$ if $i \in \{k+1,\ldots,k+l\}$. In such representation two vertices $(b_1,\ldots,b_k,b_{k+1},\ldots,b_{k+l})$ and $(b'_1,\ldots,b'_k,b'_{k+1},\ldots,b'_{k+l})$ are adjacent if and only if there is $i \in \{1,\ldots,k+l\}$ such that $|b_i - b'_i| = 1$ and $b_j = b'_j$ for any $j \neq i$.

Let H be a graph. The *generalized Cube polynomial* of H is defined as follows:

$$GC(H,x,y) = \sum_{k\geq 0, l\geq 0} \alpha_{k,l}(H) x^k y^l,$$

where $\alpha_{k,l}(H)$ denotes the number of induced convex subgraphs of H that are isomorphic to the graph $Q_{k,l}$.

4 The main result

In this section we prove that the generalized Zhang-Zhang polynomial of every benzenoid system, tubulene or fullerene equals the generalized cube polynomial of its resonance graph.

Theorem 4.1 *Let G be a benzenoid system, a tubulene or a fullerene with a perfect matching. Then the generalized Zhang-Zhang polynomial of G equals the generalized cube polynomial of its resonance graph $R(G)$, i.e.*

$$GZZ(G,x,y) = GC(R(G),x,y)\,.$$

Proof. Let k and l be nonnegative integers. For the graph G we denote by $\mathbb{GZ}(G,k,l)$ the set of all generalized Clar covers of G with exactly k cycles C_6 and l cycles C_{10}. On the other hand, consider a graph H; the set of induced convex subgraphs of H that are isomorphic to a graph $Q_{k,l}$ is denoted by $\mathbb{GQ}_{k,l}(H)$. For this graph G let us define a mapping $f_{k,l} : \mathbb{GZ}(G,k,l) \longrightarrow \mathbb{GQ}_{k,l}(R(G))$ as follows: for a generalized Clar cover $C \in \mathbb{GZ}(G,k,l)$ consider all perfect matchings M_1, M_2, ..., M_i, $i = 2^k3^l$, of G such that:

- if cycle C_6 is in C, then $|M_j \cap E(C_6)| = 3$ for all $j = 1, 2, \ldots, i$,
- if cycle C_{10} of C is the boundary of two adjacent hexagons h_1 and h_2, then $|M_j \cap (E(h_1) \cup E(h_2))| = 5$ for all $j = 1, 2, \ldots, i$,
- each isolated edge of C is in M_j for all $j = 1, 2, \ldots, i$.

Finally, assign $f_{k,l}(C)$ as an induced subgraph of $R(G)$ with vertices M_1, M_2,..., M_i.

Note first that in case when $k = 0$ and $l = 0$ generalized Clar covers are the perfect matchings of G and if C is such a generalized Clar cover then $f_{k,l}(C)$ is a vertex of the resonance graph and the mapping is obviously bijective. So from now on at least one of k and l will be positive. We first show that $f_{k,l}$ is a well-defined function.

Lemma 4.2 *For each generalized Clar cover $C \in \mathbb{GZ}(G,k,l)$ the image $f_{k,l}(C)$ is in $\mathbb{Q}_{k,l}(R(G))$.*

Proof. First we show that $f_{k,l}(C)$ is isomorphic to the graph $Q_{k,l}$. Let c_1, c_2,...,c_k be the hexagons of C and let $c_{k+1}, \ldots, c_{k+l}$ be cycles C_{10} that are in C. Obviously, every hexagon of C has two possible perfect matchings. Let us call these "possibility 0" and "possibility 1". Moreover, for every cycle C_{10} in C we obtain tree possible perfect matchings of graph $\langle V(C_{10})\rangle$, which will be denoted as "possibility 0", "possibility 1", and "possibility 2". Also, if cycle C_{10} is the boundary of adjacent hexagons h_1 and h_2, "possibility 1" denotes the perfect matching containing the common edge of h_1 and h_2.

For any vertex M of $f_{k,l}(C)$ let $b(M) = (b_1, b_2, \ldots, b_k, b_{k+1}, \ldots, b_{k+l})$, where $b_j = i$ if on c_j possibility i is selected. It is obvious that $b : V(f_{k,l}(C)) \to V(Q_{k,l})$ is a bijection. Let $b(M') = (b'_1, b'_2, \ldots, b'_k, b'_{k+1}, \ldots, b'_{k+l})$ for $M' \in V(f_{k,l}(C))$. If M and M' are adjacent in $f_{k,l}(C)$, then $M \oplus M' = E(h)$ for a hexagon h of some c_i, where

$1 \leq i \leq k+l$. Therefore, $b_j = b'_j$ for each $j \neq i$ and $|b_i - b'_i| = 1$, which implies that $b(M)$ and $b(M')$ are adjacent in $Q_{k,l}$. Conversely, if $(b_1, b_2, \ldots, b_k, b_{k+1}, \ldots, b_{k+l})$ and $(b'_1, b'_2, \ldots, b'_k, b'_{k+1}, \ldots, b'_{k+l})$ are adjacent in $Q_{k,l}$, it follows that M and M' are adjacent in $f_{k,l}(C)$. Hence b is an isomorphism between $f_{k,l}(C)$ and $Q_{k,l}$.

To complete the proof we have to show that $f_{k,l}(C)$ is a convex subgraph of $R(G)$. Therefore, let M and M' be two vertices of $f_{k,l}(C)$. Obviously, perfect matchings M and M' can differ only in the edges of hexagons that belong to cycles of C. Therefore, any shortest path between M and M' in $R(G)$ contains perfect matchings that are vertices of $f_{k,l}(C)$. It follows that $f_{k,l}(C)$ is convex in $R(G)$.
The following lemma shows that $f_{k,l}$ is injective.

Lemma 4.3 *The mapping $f_{k,l} : \mathbb{GZ}(G,k,l) \longrightarrow \mathbb{Q}_{k,l}(R(G))$ is injective for any integers k, l.*

Proof. Let C and C' be distinct generalized Clar covers in $\mathbb{GZ}(G,k,l)$. If C and C' contain the same set of cycles, then the isolated edges of C and C' are distinct. Therefore, $f_{k,l}(C)$ and $f_{k,l}(C')$ are disjoint induced subgraphs of $R(G)$ and thus $f_{k,l}(C) \neq f_{k,l}(C')$. Therefore, suppose that C and C' contain different sets of cycles. Without loss of generality we can assume that there is hexagon h such that h has at least five edges in C and h has at most three edges in C'. Hence at least one edge e of h does not belong to C'. From the definition of the function $f_{k,l}$, e is thus unsaturated by those perfect matchings that correspond to the vertices in $f_{k,l}(C')$. However, there obviously exists perfect matching $M \in V(f_{k,l}(C))$ such that $e \in M$. As a result, $M \notin V(f_{k,l}(C'))$ and $f(C) \neq f(C')$.
The next lemma was proved in [23] for benzenoid systems. The same proof can be applied in the case of tubulenes or fullerenes.

Lemma 4.4 *[23] Let G be a benzenoid systems, a tubulene, or a fullerene with a perfect matching. If the resonance graph $R(G)$ contains a 4-cycle $M_1M_2M_3M_4$, then $h = M_1 \oplus M_2$ and $h' = M_1 \oplus M_4$ are disjoint hexagons. Also, we have $h = M_3 \oplus M_4$ and $h' = M_2 \oplus M_3$.*
The following lemma shows that $f_{k,l}$ is surjective.

Lemma 4.5 *The mapping $f_{k,l} : \mathbb{GZ}(G,k,l) \longrightarrow \mathbb{Q}_{k,l}(R(G))$ is surjective for any integers k, l.*

Proof. Let k, l be integers and $Q \in \mathbb{Q}_{k,l}(R(G))$. Then the vertices of Q can be identified with strings $(b_1, \ldots, b_k, b_{k+1}, \ldots, b_{k+l})$, where $b_i \in \{0,1\}$ if $i \in \{1, \ldots, k\}$ or $b_i \in \{0,1,2\}$ if $i \in \{k+1, \ldots, k+l\}$, so that two vertices of Q are adjacent in Q if and only if their strings b and b' differ in precisely one position i, such that $|b_i - b'_i| = 1$.

Let $M = (0,0,0,\ldots,0)$, $N^1 = (1,0,0,\ldots,0)$, $N^2 = (0,1,0,\ldots,0)$, ..., $N^{k+l} = (0,0,0,\ldots,1)$ be the vertices of Q. It is obvious that MN^i is an edge of $R(G)$ for every $i, 1 \leq i \leq k+l$. By definition of $R(G)$, the symmetric difference of perfect matchings M and N^i is the edge set of a hexagon of G. We denote this hexagon by h_i and we obtain the set of hexagons $\{h_1, \ldots, h_{k+l}\}$ of graph G. If two of these hexagons were the same, for example if $h_i = h_j$ for $i, j \in \{1, \ldots, k+l\}$ and $i \neq j$, then $N^i = N^j$ - a contradiction. Hence, we have the set of $k+l$ distinct hexagons. In the next claim we show that these hexagons are pairwise disjoint.

Claim 4.6 *The hexagons h_i, $1 \leq i \leq k+l$, are pairwise disjoint.*

Proof. Let $i, j \in \{1, \ldots, k+l\}$ and $i \neq j$. Let W be a vertex of Q having exactly two 1's (and these are in the ith and jth position) and 0 at every other position. Obviously, MN^iWN^j is a 4-cycle and therefore, by Lemma 4.4, h_i and h_j are disjoint hexagons.

Next, we consider the vertices O^i, $i \in \{k+1, \ldots, k+l\}$, such that O^i has 2 in the ith position and 0 in every other position. Obviously, N^iO^i is the edge of $R(G)$ for any $i \in \{k+1, \ldots, k+l\}$. Let h'_i be the hexagon of G corresponding to the edge N^iO^i.

Claim 4.7 *If $i \in \{k+1, \ldots, k+l\}$, the hexagon h'_i has exactly one common edge with h_i.*

Proof. It is easy to see that $h_i \neq h'_i$ (otherwise $M = O^i$). Therefore, suppose that h_i and h'_i are disjoint. Since they are both sextets in the perfect matching N^i, there is a vertex X of $R(G)$, $X \neq N^i$, which is adjacent to M and O^i. If $X \in V(Q)$, the string of X must differ from M for 1 in exactly one position and must differ from O^i for 1 in exactly one position, which means $X = N^i$ - a contradiction. Therefore, X is not in Q. Since MXO^i is a shortest path between M and O^i, Q is not convex subgraph of $R(G)$, which is a contradiction. Hence, h_i and h'_i have exactly one common edge.

Claim 4.8 *Let $i \in \{k+1, \ldots, k+l\}$. Then the hexagon h'_i is disjoint with every h_j, $j \in \{1, \ldots, k+l\} \setminus \{i\}$.*

Proof. Let X be a vertex in Q with 2 in the ith position, 1 in the jth position and 0 in every other position. Furthermore, let Y be a vertex in Q with 1 in the ith position, 1 in the jth position and 0 in every other position. Obviously, $h'_i \neq h_j$ (otherwise $O^i = Y$, which is a contradiction). Since N^iO^iXY is a 4-cycle such that h'_i corresponds to the edge N^iO^i and h_j corresponds to the edge N^iY, it follows from Lemma 4.4 that hexagons h'_i and h_j are disjoint.

Claim 4.9 *Let $i \in \{k+1, \ldots, k+l\}$. Then the hexagon h'_i is disjoint with every h'_j, $j \in \{k+1, \ldots, k+l\} \setminus \{i\}$.*

Proof. Define the following vertices in Q:

- X_1 has 1 in the ith position, 1 in the jth position and 0 in every other position,
- X_2 has 1 in the ith position, 2 in the jth position and 0 in every other position,
- X_3 has 2 in the ith position, 1 in the jth position and 0 in every other position,
- X_4 has 2 in the ith position, 2 in the jth position and 0 in every other position.

Using Lemma 4.4 we can easily see that hexagon h'_j corresponds to the edge X_1X_2 and hexagon h'_i corresponds to the edge X_1X_3. Since $X_1X_2X_4X_3$ is a 4-cycle in the resonance graph, Lemma 4.4 again implies that h'_i and h'_j are disjoint and the proof is complete.

Let C_i, $i \in \{k+1, \ldots, k+l\}$ be a 10-cycle formed by h_i and h'_i. Moreover, let C be a spanning subgraph of G such that $E(C) = M \cup E(h_1) \cup \ldots \cup E(h_k) \cup E(C_{k+1}) \cup \ldots E(C_{k+l})$. Therefore, C is a generalized Clar cover with k hexagons and l 10-cycles. It is obvious that every edge in Q corresponds to some hexagon h_i, $i \in \{1, \ldots, k+l\}$ or h'_i, $i \in \{k+1, \ldots, k+l\}$. Therefore, $V(f_{k,l}(C)) = V(Q)$. Since both Q and $f_{k,l}(C)$ are induced subgraphs of the resonance graph, it follows $f_{k,l}(C) = Q$.

We have proved that $f_{k,l}$ is bijective function and hence, $|\mathbb{GZ}(G,k,l)| = |\mathbb{GQ}_{k,l}(R(G))|$. Therefore, the proof is complete.

5 An example

In this final section we give an example of a benzenoid system G and calculate the generalized Zhang-Zhang polynomial of G, i.e. the generalized cube polynomial of the resonance graph of G. See Figures 3 and 4.

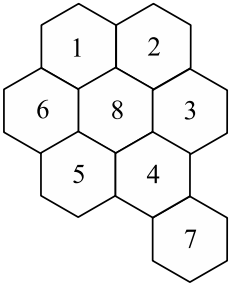

Figure 3. Benzenoid system G.

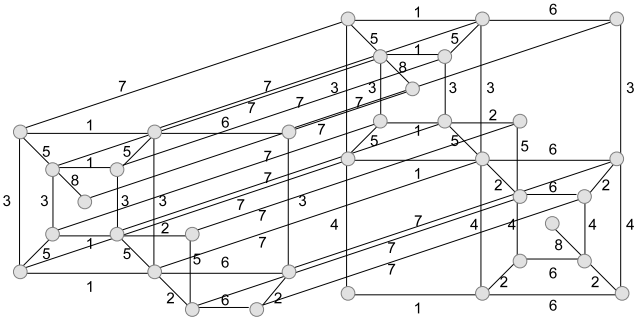

Figure 4. Resonance graph $R(G)$.

The polynomials are

$$GZZ(G,x,y) = GC(R(G),x,y) =$$

$$= 34 + 53x + 35x^2 + 12x^3 + x^4 + 48y + 7y^2 + 37xy + xy^2 + 3x^2y\,.$$

For example, the coefficient in front of x^2y is 3, since there are 3 generalized Clar covers in G with two C_6 and one C_{10}. On the other hand, this coefficient counts the number of induced convex subgraphs of $R(G)$ isomorphic to the graph $P_2^2 \Box P_3$.

We will conclude with the open problem. It would be interesting to express the generalized Zhang-Zhang polynomial of considered molecular graphs in the term of recurrence relations.

Acknowledgment: The author acknowledge the financial support from the Slovenian Research Agency (research core funding No. P1-0297).

References

[1] V. Andova, F. Kardoš, R. Škrekovski, Mathematical aspects of fullerenes, *Ars Math. Contemp.* **11** (2016) 353–379.

[2] M. Berlič, N. Tratnik, P. Žigert Pleteršek, Equivalence of Zhang–Zhang polynomial and cube polynomial for spherical benzenoid systems, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 443–456.

[3] B. Brešar, S. Klavžar, R. Škrekovski, The cube polynomial and its derivatives: the case of median graphs, *El. J. Comb.* **10** (2003) #R3.

[4] C. P. Chou, J. S. Kang, H. A. Witek, Closed–form formulas for the Zhang–Zhang polynomials of benzenoid structures: Prolate rectangles and their generalizations, *Discr. Appl. Math.* **198** (2016) 101–108.

[5] C. P. Chou, H. A. Witek, ZZDecomposer: a graphical toolkit for analyzing the Zhang-Zhang polynomials of benzenoid structures, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 741–764.

[6] S. El–Basil, Generation of lattice graphs. An equivalence relation on Kekulé counts of catacondensed benzenoid hydrocarbons, *J. Mol. Struct. (Theochem)* **288** (1993) 67–84.

[7] M. Faghani, T. Došlić, On two Graffiti conjectures about fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 723–730.

[8] W. Gründler, Signifikante Elektronenstrukturen fur benzenoide Kohlenwasserstoffe, *Wiss. Z. Univ. Halle* **31** (1982) 97–116.

[9] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, 1989.

[10] S. Iijima, Helical microtubules of graphitic carbon, *Nature* **354** (1991) 56–58.

[11] A. Kelenc, S. Klavžar, N. Tratnik, The edge–Wiener index of benzenoid systems in linear time, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 521–532.

[12] J. Kovič, T. Pisanski, A. T. Balaban, P. W. Fowler, On symmetries of benzenoid systems, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 3–26.

[13] J. Petersen, Die Theorie der regulären Graphen, *Acta Math.* **15** (1891) 193–220.

[14] D. Plavšić, S. Nikolić, N. Trinajstić, The conjugated–circuit model: application to nonalternant hydrocarbons and a comparison with some other theoretical models of aromaticity, *J. Mol. Struct. (Theochem)* **277** (1992) 213–237.

[15] M. Randić, Resonance in catacondensed benzenoid hydrocarbons, *Int. J. Quantum Chem.* **63** (1997) 585–600.

[16] M. Randić, D. J. Klein, S. El–Basil, P. Calkins, Resonance in large benzenoid hydrocarbons, *Croat. Chem. Acta* **69** (1996) 1639–1660.

[17] H. Sachs, P. Hansen, M. Zheng, Kekulé count in tubular hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **33** (1996) 169–241.

[18] L. Shi, H. Zhang, Forcing and anti–forcing numbers of $(3, 6)$-fullerenes, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 597–614.

[19] N. Tratnik, The edge–Szeged index and the PI index of benzenoid systems in linear time, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 393–406.

[20] N. Tratnik, P. Žigert Pleteršek, Resonance graphs of fullerenes, *Ars Math. Contemp.* **11** (2016) 425–435.

[21] F. Zhang, X. Guo, R. Chen, Z-transformation graphs of perfect matchings of hexagonal systems, *Discr. Math.* **72** (1988) 405–415.

[22] H. Zhang, J. Cai, On the global forcing number of hexagonal systems, *Discr. Appl. Math.* **162** (2014) 334–347.

[23] H. Zhang, W. C. Shiu, P. K. Sun, A relation between Clar covering polynomial and cube polynomial, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 477–492.

[24] H. Zhang, F. Zhang, The Clar covering polynomial of hexagonal systems I, *Discr. Appl. Math.* **69** (1996) 147–167.