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SZEGED INDEX OF SOME POLYCYCLIC BIPARTITE GRAPHS WITH CIRCUITS OF DIFFERENT SIZE

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Abstract

In this work we consider the Szeged index (Sz) of graphs belonging to the class $C(h, k_1, k_2, \ldots, k_h)$. This class consists of bipartite graphs with cyclomatic number h, possessing circuits of size $2k_i + 2$, $i = 1, 2, \ldots, h$, of which many are of chemical relevance. Some congruence relations for Sz are obtained. The findings presented in this article generalize results from a previous paper [A. A. Dobrynin, I. Gutman and G. Dömötör, *Appl. Math. Letters* **8**, 57 (1995)], in which the case $k_1 = k_2 = \cdots = k_h$ was studied.

Introduction

It is known for some time [1] that the Wiener indices of catacondensed benzenoid hydrocarbons with equal number of hexagons are congruent modulo 8. The extension of this result to a (below described) class of polycyclic bipartite graphs with circuits of arbitrary, but mutually equal size was also reported. [2] Recently it was discovered that also the Szeged indices of catacondensed benzenoid hydrocarbons with equal number of hexagons are congruent modulo 8 [3] and that also this result can be extended to the precisely same class of polycyclic bipartite graphs with circuits of arbitrary, but mutually equal size. [4] In this paper we go a step further and show that when the requirement of equal circuit size is abandoned, some of the previously noticed regularities for the Szeged index either remain valid or are pertinently modified.

In this article we use mathematical reasoning that is closely analogous to that in our previous paper [4]. Consequently, our notation and terminology also closely follow that of the paper [4] and are therefore explained here in a concise (yet complete) manner.

Let thus G denote a connected graph and $e = (u, v)$ be its edge. The distance $d(w, u)$ between two vertices w and u is the length of a shortest path connecting these vertices. The distance $d(v) = d(v|G)$ of a vertex v in a (connected) graph G is the sum of distances between the vertex v and all other vertices of G.

Denote by $n_u = n_u(e) = n_u(G)$ and $n_v = n_v(e) = n_v(G)$ the cardinalities of the vertex sets $B_u(e) = \{w \mid d(w,u) < d(w,v)\}$ and $B_v(e) = \{w \mid d(w,v) < d(w,u)\}$, respectively. We consider the graph invariant

$$Sz(G) = \sum_{(u,v)} n_u \, n_v \tag{1}$$

which is nowadays usually referred to as the *Szeged index* (of the graph G).

The Class of Cyclic Graphs Considered

In this section we define classes of (connected, bipartite) graphs characterized by a parameter h (the cyclomatic number, $h \geq 1$) and additional h parameters $k_1, k_2, \ldots, k_h$, associated with the size of the circuits.

Although not evident at the first glance, the below Definition has a direct chemical origin. The graphs determined by it are either molecular graphs of alternant catacondensed hydrocarbons or are closely related to them. In fact, the molecular graph of each of such catacondensed systems is contained in an appropriate class of the type $C(h, k_1, k_2, \ldots, k_h)$, but such classes include also graphs having no immediate chemical interpretation. In order to eliminate such "pathological" cases, one has to additionally require that the *two adjacent vertices* mentioned in the Definition be both of degree two. In other words: chemically relevant members of the class $C(h, k_1, k_2, \ldots, k_h)$ must not possess vertices of degree four or greater.

The example depicted in Fig. 1 and used throughout this paper was deliberately chosen so as to be "pathological". This was done in order to show that our results apply to a somewhat broader family of graphs than those usually encountered in mathematical chemistry. With a minimal effort, however, the chemical aspects of our investigations are easily recognized.

Definition. Let h and $k_1, k_2, \ldots, k_h$ be positive integers. If $h = 1$, then the class $C(1, k_1)$ consists of a single element - the circuit with $2k_1 + 2$ vertices. If $h > 1$, then every element of $C(h, k_1, k_2, \ldots, k_h)$ is a graph obtained by joining the endpoints of the path-graph P_n with $n = 2k_h$ vertices with two adjacent vertices of some graph from $C(h-1, k_1, k_2, \ldots, k_{h-1})$.

An illustration of the above Definition is provided in Fig. 1

If $k_1 = k_2 = \cdots = k_h$, then the elements of the class $C(h, k_1, k_2, \ldots, k_h)$ are precisely the same as the graphs whose Wiener and Szeged indices were previously studied. [2, 4] In other words, the results obtained in this paper represent straightforward generalizations of our previous findings. [4]

From the above Definition it immediately follows that if G is a graph from $C(h, k_1, k_2, \ldots, k_h)$, then G is connected, bipartite and its cyclomatic number is equal to h. Indeed, by joining the endpoints of the path graph P_n to adjacent vertices of a graph from $C(h-1, k_1, k_2, \ldots, k_{h-1})$ we close an $(n+2)$-membered circuit, increasing thus the cyclomatic number by one. Since n is assumed to be even ($n = 2k_h$), the size of the newly formed circuit is even. Bearing in mind that the the construction starts with the (unique) element of $C(1, k_1)$, which evidently is connected, bipartite and has cyclomatic number equal to one, we reach the above conclusion by mathematical induction.

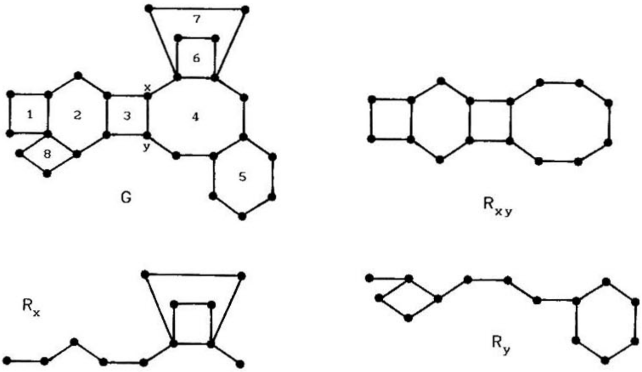

Fig. 1. A graph G belonging to the class $C(8,1,2,1,3,2,1,1,1)$ and the subgraphs R_{xy}, R_x and R_y, corresponding to the edge (x,y)

Further, the number of vertices and edges of $G \in C(h,k_1,k_2,\ldots,k_h)$ are given by

$$p(G) = 2 + 2\sum_{i=1}^{h} k_i = 2K_G + 2$$

and

$$q(G) = h + 1 + 2\sum_{i=1}^{h} k_i = 2K_G + h + 1$$

respectively, where the quantity K_G is defined via

$$K_G = \sum_{i=1}^{h} k_i \ . \tag{2}$$

Some Auxiliary Subgraphs and Their Properties

As before [4], we associate with an edge $e = (x,y)$ of $G \in C(h,k_1,k_2,\ldots,k_h)$ three subgraphs: R_x, R_y and R_{xy}.

Denote by $E_1(e) = E_1(e|G)$ the subset of the edge set of G, containing the edges (u,v) of G for which $u \in B_x(e)$ and $v \in B_y(e)$. [Recall that the sets $B_x(e)$ and $B_y(e)$

were defined in connection with Eq. (1).] In the example given in Fig. 1, the elements of the set $E_1(e|G)$ are the five vertical edges, belonging to the circuits 1,2,3 and 4.

Then R_{xy} is spanned by those $(2k_i+2)$-membered circuits which contain the edges from $E_1(e)$. Consequently, R_{xy} is also a graph of the kind studied in this paper; it belongs to the class $C(h_{xy}, k_1, k_2, \ldots, k_{h_{xy}})$, where $h_{xy} = |E_1(e)| - 1$.

In the example depicted in Fig. 1, $|E_1(e)| = 5$, implying that $h_{xy} = 4$. Here the graph R_{xy} belongs to the class $C(4,1,2,1,3)$.

The subgraph R_x is spanned by those vertices of G that lie closer to x than to y. Analogously, R_y is spanned by the vertices of G whose distance to y is smaller than the distance to x. Note that the vertex sets of R_{xy} and R_x, as well as of R_{xy} and R_y have non-empty intersections. Observe also that R_x and R_y may be disconnected. [4] An example illustrating the construction of R_x and R_y is found in Fig. 1.

We denote by p_x, p_y and p_{xy} the number of vertices of the subgraphs R_x, R_y and R_{xy}, respectively. Let h_x and h_y be the number of the $(2k_i+2)$-circuits in R_x and R_y, respectively. Then $h_x + h_y + h_{xy} = h$. [In the example depicted in Fig. 1, $h_x = h_y = 2$ and $h_{xy} = 4$.]

The subgraphs R_x, R_y and R_{xy} are the same for any choice of an edge from $E_1(e)$. Thus, for arbitrary edges $(x_1,y_1),(x_2,y_2) \in E_1(e)$ we have $R_{x_1} = R_{x_2} = R_x$, $R_{y_1} = R_{y_2} = R_y$ and $R_{x_1y_1} = R_{x_2y_2} = R_{xy}$.

Denote by $k'_1, k'_2, \ldots, k'_{h_{xy}}$ the parameters k_i, corresponding to the circuits belonging to the subgraph R_{xy}. Further, let $k''_1, k''_2, \ldots, k''_{h_x}$ and $k'''_1, k'''_2, \ldots, k'''_{h_y}$ be the analogous parameters pertaining to the subgraphs R_x and R_y, respectively. Then we define

$$K_{xy} = \sum_{i=1}^{h_{xy}} k'_i \quad ; \quad K_x = \sum_{i=1}^{h_x} k''_i \quad ; \quad K_y = \sum_{i=1}^{h_y} k'''_i \, . \tag{3}$$

It is clear that $\{k'_1, k'_2, \ldots, k'_{h_{xy}}\}$, $\{k''_1, k''_2, \ldots, k''_{h_x}\}$ and $\{k'''_1, k'''_2, \ldots, k'''_{h_y}\}$ are disjoint sets and that their union is equal to $\{k_1, k_2, \ldots, k_h\}$. As a consequence of this,

$$K_x + K_y + K_{xy} = K_G \, .$$

In the sense of Eq. (2), $K_{xy} \equiv K_{R_{xy}}$.

In the example given in Fig. 1,

$$K_{xy} = k_1 + k_2 + k_3 + k_4 = 1 + 2 + 1 + 3 = 7$$

$$K_x = k_6 + k_7 = 1 + 1 = 2 \quad ; \quad K_y = k_5 + k_8 = 2 + 1 = 3 \ .$$

Change of the Szeged Index upon Addition of a Circuit

In this section we show how to calculate the invariant Sz when a new circuit is attached to a graph from $C(h-1, k_1, k_2, \ldots, k_{h-1})$. We first need the following two simple lemmas.

Lemma 1. Let G be a connected bipartite graph and u and v be its adjacent vertices. Then

$$d(u|G) - d(v|G) = n_v - n_u \qquad \text{and} \qquad n_v + n_u = p(G) \ .$$

Further, if $G \in C(h, k_1, k_2, \ldots, k_h)$, then

$$d(u|G) - d(v|G) = 2(K_v - K_u)$$

where K_v and K_u are defined via Eq. (3).

Recall that the quantities n_u and n_v were defined in connection with Eq. (1).

Proof. Let $e = (u,v) \in E(G)$, where $E(G)$ is the edge set of G. Then we have

$$\begin{aligned} d(u|G) &= \sum_{w \in B_u(e)} d(w,u) + \sum_{w \in B_v(e)} d(w,u) \\ &= \sum_{w \in B_u(e)} [d(w,v) - 1] + \sum_{w \in B_v(e)} [d(w,v) + 1] = d(v|G) - n_u + n_v \ . \end{aligned}$$

Since G has no circuits of odd length, $n_v + n_u = p(G)$. If, in addition, the graph G belongs to $C(h, k_1, k_2, \ldots, k_h)$, then

$$\begin{aligned} d(u|G) - d(v|G) &= n_v - n_u = \left(2\sum_{i=1}^{h_v} k_i'' + \frac{1}{2}\, p_{uv}\right) - \left(2\sum_{i=1}^{h_u} k_i''' + \frac{1}{2} p_{uv}\right) \\ &= 2(K_v - K_u) \ . \ \Box \end{aligned}$$

Lemma 2. Let G be a connected bipartite graph. Then

$$Sz(G) = (K_G + 1)^2 \, (2K_G + h + 1) \ - \sum_{(u,v) \in E(G)} [d(u|G) - d(v|G)]^2 \ . \qquad (4)$$

Proof. From Lemma 1, we have $n_u = [p(G) + d(v|G) - d(u|G)]/2$ and $n_v = [p(G) - d(v|G) + d(u|G)]/2$. Formula (4) is obtained by combining the above relations with the definition of Sz and expressions for $p(G)$. $\square$

Suppose that the graph $G \in C(h, k_1, k_2, \ldots, k_h)$ has been obtained from the graph $H \in C(h-1, k_1, k_2, \ldots, k_{h-1})$ by attaching to it a new $(2k_h + 2)$-membered circuit. Then the change of the invariant Sz may be described by a polynomial depending only on the number of circuits of certain subgraphs of H, as well as on the size of these circuits.

Theorem 3. Let $G \in C(h, k_1, k_2, \ldots, k_h)$ be obtained by joining the endpoints of a path-graph with $2k_h$ vertices, with the endpoints of the edge $e = (x, y)$ of the graph $H \in C(h-1, k_1, k_2, \ldots, k_{h-1})$. Then

$$Sz(G) = Sz(H) \; - \; 2k_h \sum_{(u,v)\in E_2(e|H)} (K_v - K_u) \; - \; f(k_h, x, y) \; + \; g(h, k_1, k_2, \ldots, k_h)$$

where $E_2(e|H) = E(H) \setminus E_1(e|H)$,

$$f(k_h, x, y) = k_h^2 \; (h_x + h_y) + (K_y - K_x)^2$$

and

$$g(h, k_1, k_2, \ldots, k_h) =$$

$$-2k_h \; K_H \; (K_H - k_h) - (K_G + 1)^2 \; (2K_G + h + 1) + (K_H + 1)^2 \; (2K_H + h) \; .$$

Proof. The edge set of the graph G may be partitioned as

$$\begin{aligned} E(G) &= E(H) \cup E(P_{2k_h}) \cup \{e_x, e_y\} \\ &= E_1(e|H) \cup E_2(e|H) \cup E(P_{2k_h}) \cup \{e_x, e_y\} \end{aligned}$$

where e_x and e_y are the edges connecting H with P_{2k_h}. Using Lemma 1 we calculate the difference between vertex distances for the edges from each of the above given subsets.

(a) Let $(u,v) \in E_1(e|H)$. Then

$$\begin{aligned} d(u|G) - d(v|G) &= n_v(G) - n_u(G) = [n_v(H) + p(P_{2k_h})/2] - [n_u(H) + p(P_{2k_h})/2] \\ &= d(u|H) - d(v|H) \ . \end{aligned} \tag{5}$$

(b) Let $(u,v) \in E_2(e|H)$. Then

$$d(u|G) - d(v|G) = [n_v(H) + p(P_{2k_h})] - n_u(H) = d(u|H) - d(v|H) + 2k_h \ . \tag{6}$$

(c) For the unique edge $e^* = (u,v) \in E(P_{2k_h}) \cap E_1(e|G)$,

$$\begin{aligned} d(u|G) - d(v|G) &= [p(P_{2k_h})/2 + n_y(H)] - [p(P_{2k_h})/2 + n_x(H)] \\ &= d(x|H) - d(y|H) \ . \end{aligned} \tag{7}$$

(d) If $(u,v) \in (E(P_{2k_h}) - e^*) \cup \{e_x, e_y\}$, then

$$\begin{aligned} d(u|G) - d(v|G) &= [[p(P_{2k_h}) + 2]/2 + p(H) - 2] - [p(P_{2k_h}) + 2]/2 \\ &= 2\sum_{i=1}^{h-1} k_i \ . \end{aligned} \tag{8}$$

Substituting Eqs. (5)–(8) back into Eq. (4), we obtain

$$\begin{aligned} 4Sz(G) &= (K_G+1)^2(2K_G+h+1) - \sum_{(u,v)\in E(H)} [d(u|H) - d(v|H)]^2 \\ &- 4k_h \sum_{(u,v)\in E_2(e|H)} [d(u|H) - d(v|H)] - 4k_h^2 \ |E_2(e|H)| \\ &- 4\left(\sum_{i=1}^{h-1} k_i\right)^2 [|E(P_{2k})| + 1] - [d(x|H) - d(y|H)]^2 \ . \end{aligned}$$

It is easy to see that

$$\begin{aligned} |E_2(e|H)| &= |E(H)| - |E_1(e|H)| = 2\sum_{i=1}^{h-1} k_i + (h-1) + 1 - (h_{xy}+1) \\ &= 2\sum_{i=1}^{h-1} k_i + h_x + h_y = 2K_H + h_x + h_y \end{aligned}$$

and

$$|E(P_{2k_h})| + 1 = 2k_h \ .$$

Bearing in mind the form of the expression for $Sz(H)$, obtained from Lemma 2, and applying Lemma 1, we obtain

$$\begin{aligned} Sz(G) &= Sz(H) - 2k_h \sum_{(u,v)\in E_2(e|H)} (K_v - K_u) - k_h^2\ (h_x + h_y) \\ &- (K_y - K_x)^2 - 2k_h\ K_H^2 - 2k_h^2\ K_H \\ &- \left[(K_G+1)^2\ (2K_G+h+1) - (K_H+1)^2\ (2K_H+h)\right] \ . \end{aligned}$$

Theorem 3 follows now by direct calculation. □

Corollaries

Suppose that the graphs $G_j \in C(h, k_1, k_2, \ldots, k_h)$ are obtained from the graphs $H_j \in C(h-1, k_1, k_2, \ldots, k_{h-1})$ by means of the previously described construction, $j = 1, 2$. Let $e_j = (x_j, y_j) \in E(H_j)$ be the edge, to the endpoints of which the path–graph P_{2k_h} is attached, $j = 1, 2$.

By Theorem 3 we have

$$\begin{aligned} Sz(G_1) - Sz(G_2) &= Sz(H_1) - Sz(H_2) \\ &+ 2k_h \sum_{(u,v)\in E_2(e|H_2)} (K_v - K_u) - 2k_h \sum_{(u,v)\in E_2(e|H_1)} (K_v - K_u) \\ &+ k_h^2\,(h_{x_2} + h_{y_2}) + (K_{y_2} - K_{x_2})^2 - k_h^2\,(h_{x_1} + h_{y_1}) - (K_{y_1} - K_{x_1})^2 \\ &= Sz(H_1) - Sz(H_2) \\ &+ 2k_h \sum_{(u,v)\in E_2(e|H_2)} (K_v - K_u) - 2k_h \sum_{(u,v)\in E_2(e|H_1)} (K_v - K_u) \\ &+ k_h^2\,(h_{x_1y_1} - h_{x_2y_2}) + (K_{y_2} - K_{x_2})^2 - (K_{y_1} - K_{x_1})^2 . \end{aligned} \tag{9}$$

The previous result [4] is now immediately deduced:

Corollary 3.1. [4] Let $G_1, G_2 \in C(h, k_1, k_2, \ldots, k_h)$ and $k_i = k$ for all $i = 1, 2, \ldots, h$. Then

$$Sz(G_1) \equiv Sz(G_2) \pmod{2k^2} .$$

Proof. Indeed, in this case

$$f(k, x, y) = k^2\,(h_x + h_y) + k^2\,(h_y - h_x)^2 = k^2\,[h_x(h_x + 1) + h_y(h_y + 1) - 2h_x\,h_y]$$

and the factor in square brackets is necessarily an even number. □

If G is the molecular graph of a catacondensed benzenoid hydrocarbon, then all $(2k_i + 2)$-membered circuits are of size six, i.e., $k_1 = k_2 = \cdots = k_h = 2$. Then as a special case of Corollary 3.1 we arrive at

Corollary 3.2. [3] Let G_1 and G_2 be molecular graphs of isomeric catacondensed benzenoid hydrocarbons (which necessarily possess equal number of hexagons). Then

$$Sz(G_1) \equiv Sz(G_2) \pmod 8 .$$

In a more general case we have the following weaker version of Corollary 3.1.

Corollary 3.3. Let $G_1, G_2 \in C(h, k_1, k_2, \ldots, k_h)$ and $k_i = \kappa c_i$ for all $i = 1, 2, \ldots, h$. [In other words, κ is a common divisor of the numbers $k_1, k_2, \ldots, k_h$.] Then

$$Sz(G_1) \equiv Sz(G_2) \pmod{\kappa^2} .$$

Corollary 3.4. Let G_1 and G_2 be molecular graphs of isomeric catacondensed hydrocarbons, all rings of which are even-membered, but not divisible by 4. [In other words, such hydrocarbons are composed of 6- and/or 10- and/or 14- ... -membered rings.] Then the congruence relation stated in Corollary 3.3 applies with $\kappa = 2$.

For some subclasses of $C(h, k_1, k_2, \ldots, k_h)$ the result of Corollary 3.3 can be strengthened:

Corollary 3.5. Let $G_j \in C(h, k_1, k_2, \ldots, k_h)$ be obtained by attaching a new $(2k_h + 2)$-membered circuit to the graph $H_j \in C(h-1, k_1, k_2, \ldots, k_{h-1})$, $j = 1, 2$, and let $k_i = \kappa c_i$ for all $i = 1, 2, \ldots, h$. Suppose that for every edge (x, y) of H_1 and H_2, h_{xy} is odd. [In other words, we assume that every "linear" segment R_{xy} (corresponding to H_1 or H_2) consists of an odd number of circuits.] Suppose, further, that k_i is odd for all i. Then

$$Sz(G_1) \equiv Sz(G_2) \pmod{2\kappa^2} .$$

Proof. First notice that because k_i , $i = 1, 2, \ldots, h$ are odd numbers, κ must be odd too. From Eq. (3) follows then that the parameters K_x, K_y and K_{xy} are all divisible by κ. Since $K_x + K_y + K_{xy} = K_H$, we have

$$K_{y_2} - K_{x_2} = 2K_{y_2} + K_{x_2y_2} - K_{H_2}$$

and

$$K_{y_1} - K_{x_1} = 2K_{y_1} + K_{x_1y_1} - K_{H_1} .$$

Then

$$\begin{aligned}(K_{y_2} - K_{x_2})^2 - (K_{y_1} - K_{x_1})^2 &= (2K_{y_2} + 2K_{y_1} - 2K_{H_1} + K_{x_2y_2} + K_{x_1y_1}) \times \\ &\times \; (2K_{y_2} - 2K_{y_1} + K_{x_2y_2} - K_{x_1y_1}) .\end{aligned}$$

If h_{xy} is odd for every R_{xy}, then $h(H)$ is also odd and $h_x + h_y$ must be even. Therefore, h_x, h_y are either both odd or both even. This implies that both $K_{x_2y_2} + K_{x_1y_1}$ and $K_{x_2y_2} - K_{x_1y_1}$ are always even.

Then the expression $(K_{y_2} - K_{x_2})^2 - (K_{y_1} - K_{x_1})^2$ occurring on the right-hand side of Eq. (9) is divisible by $4\kappa^2$. It is easy to see that the terms

$$2k_h \sum_{(u,v)\in E_2(e|H_2)} (K_v - K_u) \qquad \text{and} \qquad 2k_h \sum_{(u,v)\in E_2(e|H_1)} (K_v - K_u)$$

in the same equation are divisible by $2\kappa^2$. Because both $h_{x_1y_1}$ and $h_{x_2y_2}$ are assumed to be odd-valued, also $k_h^2\,(h_{x_1y_1} - h_{x_2y_2})$ is divisible by $2\kappa^2$. Corollary 3.5 follows now by induction on the cyclomatic number h. □

The Szeged indices of the (molecular) graphs examined in this paper frequently coincide. Below we show how catacondensed systems with equal Szeged indices can be designed in a systematic manner.

Corollary 3.6. Let the graphs $G_1, G_2 \in C(h, k_1, k_2, \ldots, k_h)$ be obtained from the same graph $H \in C(h-1, k_1, k_2, \ldots, k_{h-1})$. By $e_1 = (x_1, y_1) \in E(H)$ we denote the edge the endpoints of which are connected to the path P_{2k_h} within the construction $H \to G_1$. The edge $e_2 = (x_2, y_2)$ has the same meaning with regard to $H \to G_2$. Let $E_1(e_1|H) = E_1(e_2|H)$. Suppose (for simplicity) that $R_{x_1y_1}$ consists of linearly connected circuits between e_1 and e_2, i.e., that these circuits separate two subgraphs of G. If the numbers of vertices of these subgraphs coincide, then

$$Sz(G_1) = Sz(G_2) \ .$$

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