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ON THE PI INDEX: PI-PARTITIONS AND CARTESIAN PRODUCT GRAPHS

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Abstract

PI index is an edge-additive topological index introduced as a counterpart to the vertex-multiplicative Szeged index. In this paper PI-partitions are introduced and used to simplify the computation of the PI-index on those graph that admit nontrivial PI-partitions. Partial Hamming graphs that in particular contain many important chemical graphs fall into this category. For several of them the PI index is obtained explicitly. PI index is also studied on Cartesian product graphs. In particular, a simple formula for the PI index of powers of bipartite graphs is obtained.

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1 Introduction

Molecular structure descriptors, frequently called *topological indices*, are used in theoretical chemistry for the design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities. The Wiener index [37] W is the most celebrated such index, see [9, 10, 19, 20] and references therein. The Szeged index [13, 25] is another such descriptor and is closely related to the Wiener index, in particular, the Wiener and the Szeged index coincide on trees. Also the latter index attracted considerable attention, see, for instance [5, 12, 15, 26, 29, 36, 39].

The Szeged index is a vertex-multiplicative type index that takes into account the way vertices of a given molecular graph G are distributed. Hence it seems natural to introduce an (additive) topological index that would consider a corresponding distribution of edges. This was indeed done in [24, 26] by introducing the PI index. Until now, this index has been studied from several points of view, [1, 2, 6, 7, 27, 28, 30] is just a selection of related references.

Applications of the PI index to QSRP/QSAR were studied in [27]. The index was mostly compared with the Wiener and the Szeged index. It turned out that the PI index has similar discriminating power as the other two indices and in many cases (for instance to model Δ_{max}, the so called difference in doublet of deformation mode, of unbranched cycloalkanes) it gives better result. Since on the other hand it is usually easier to compute than the Wiener and the Szeged index, PI is a topological index worth studying.

As we already mentioned, The Szeged index incorporates the distribution of vertices of a molecular graph, while the PI index does this job for the edges. Hence it seems that a combination of both could give good results in QSRP/QSAR studies. Indeed, the combination of the PI index and the Szeged index is the best for modeling polychlorinated biphenyls (PCBs) in environment among the three possible pairs of indices selected from the PI index, the Szeged index, and the Wiener index [27]. For the Wiener and the Szeged index such studied were previously done in [23, 35].

In this paper we introduce a general model for the computation of the PI index. More precisely, in Section 3 we introduce the so-called PI-partitions and express the PI index of a graph in terms of its PI-partition. Every graph admits a trivial PI-partition, but the computations makes sense when the graphs considered allow nontrivial PI-partitions. We note that graphs from a very wide class of graphs—partial Hamming graphs—naturally yield such partitions. Let us just mention that benzenoid systems, phenylenes, and many other molecular graphs are special examples of partial Hamming graphs. In the last section we consider the computation of the PI index on Cartesian product graphs. We obtain a general formula for the PI index of a product that involves the related invariants of the factors. In many cases, as for instance in the bipartite case, the formula significantly simplifies.

2 Preliminaries

All graph in this paper are supposed to be connected. Let $G = (V(G), E(G))$ be a graph. Then we will write $|G|$ and $\|G\|$ for the number of vertices and edges of G, respectively, that is, $|G| = |V(G)|$ and $\|G\| = |E(G)|$. Let G be a graph and $X \subseteq V(G)$. The subgraph of G induced by X will be denoted $\langle X \rangle$. Moreover, let ∂X stands for the set of edges of G with one end vertex in X and the other not in X.

The *Cartesian product* $G \,\Box\, H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $(g,h)(g',h') \in E(G \,\Box\, H)$ whenever either $gg' \in E(G)$ and $h = h'$, or $g = g'$ and $hh' \in E(H)$. The vertex set of the *n-cube* Q_n consists of all n-tuples $b_1 b_2 \ldots b_n$ with $b_i \in \{0, 1\}$, where two vertices are adjacent if the corresponding tuples differ in precisely one place. The vertices of Q_n can also be understood as characteristic vectors of subsets of an n-set.

A graph H is an isometric subgraph of G if $d_H(u,v) = d_G(u,v)$ for any vertices $u, v \in H$, where d_G denotes the usual shortest path distance in G. G is called a *partial Hamming graph* if G is an isometric subgraphs of some Cartesian product of complete graphs.

For an edge $e = uv$ of a graph G set

$$G_1(e) = \{x \in V(G) \mid d_G(x,u) < d_G(x,v)\}$$

and

$$G_2(e) = \{x \in V(G) \mid d_G(x,u) < d_G(x,v)\}\,,$$

that is, $G_1(e)$ is the set of vertices closer to u than to v while $G_2(e)$ consists of those vertices that are closer to v. Note that the roles of $G_1(e)$ and $G_1(e)$ would be interchanged if the edge e would be considered as $e = vu$. Since these two sets will always be considered in pairs, this imprecision in the definition will cause no problem. We did, however, selected the present notation in order to simplify the presentation.

Observe that if G is bipartite then for any edge e of G, $G_1(e)$ and $G_2(e)$ form a partition of $V(G)$. We also note that in metric graph theory these sets are usually denoted W_{uv} and W_{vu}, respectively. (The latter notation however does not reflect the graph G in question.)

For an edge $e = uv$ of a graph G let $n_1(G,e)$ (resp., $n_2(G,e)$) be the number of edges in the subgraph of G induced by $G_1(e)$ (resp., $G_2(e)$). Again, the roles of $n_1(G,e)$ and $n_2(G,e)$ could be interchanged, but since only the sum $n_1(G,e)+n_2(G,e)$ will be considered, such a definition suffices. Now, the *PI index* of G is defined as

$$PI(G) = \sum_{e\in E(G)} \Big(n_1(G,e) + n_2(G,e)\Big)\,.$$

As we already mentioned, the PI index is the edge-additive counterpart of the Szeged index. Indeed, the Szeged index of G is defined as $\sum_{e\in E(G)} |G_1(e)|\cdot|G_2(e)|$.

3 PI index and PI-partitions

Let G be a graph. Then we say that a partition $E_1,\dots,E_k$ of $E(G)$ is a *PI-partition* of G if for any i, $1\le i\le k$, and for any $e,f\in E_i$ we have $G_1(e) = G_1(f)$ and $G_2(e) = G_2(f)$.

Let $e = uv$ be an edge a graph G. In addition to the sets $G_1(e)$ and $G_2(e)$ introduced earlier, let $G_3(e)$ be the set of all vertices that are at equal distance from u and v. Then $V(G) = G_1(e)\cup G_2(e)\cup G_3(e)$.

Theorem 3.1 *Let $E_1,\dots,E_k$ be a PI-partition of a graph G. Then*

$$PI(G) = \|G\|^2 - \sum_{i=1}^{k} |E_i|\cdot\Big(|E_i| + \|\langle G_3(e)\rangle\| + |\partial G_3(e)|\Big)\,.$$

Proof. Compute as follows:

$$\begin{aligned}
PI(G) &= \sum_{e\in E(G)} \Big(n_1(G,e)+n_2(G,e)\Big)\\
&= \sum_{i=1}^{k}\sum_{e\in E_i} \Big(n_1(G,e)+n_2(G,e)\Big)\\
&= \sum_{i=1}^{k}\sum_{e\in E_i} \Big(\|G\| - |E_i| - \|\langle G_3(e)\rangle\| - |\partial G_3(e)|\Big)\\
&= \sum_{i=1}^{k}\sum_{e\in E_i} \|G\| - \sum_{i=1}^{k}\sum_{e\in E_i} \Big(|E_i| + \|\langle G_3(e)\rangle\| + |\partial G_3(e)|\Big)\\
&= \|G\|^2 - \sum_{i=1}^{k} |E_i|\Big(|E_i| + \|\langle G_3(e)\rangle\| + |\partial G_3(e)|\Big)
\end{aligned}$$

which is the claimed expression. □

If G is bipartite then $G_3(e) = \emptyset$ and consequently $\partial G_3(e) = \emptyset$. In such a case Theorem 3.1 reduces to a very simple form.

Corollary 3.2 *Let $E_1, \ldots, E_k$ be a PI-partition of a bipartite graph G. Then*

$$PI(G) = \|G\|^2 - \sum_{i=1}^{k} |E_i|^2 .$$

Consider the n-cube Q_n. For an edge uv of Q_n we say that it is of *color i* if u and v differ in the ith coordinate. Then we have n colors and this coloring forms a PI-partition of Q_n. Consequently,

$$PI(Q_n) = (n2^{n-1})^2 - n \cdot (2^{n-1})^2 = n \cdot (n-1) \cdot 2^{2n-2} = \binom{n}{2} \cdot 2^{2n-1} .$$

Let G be a graph with edges $e_1, \ldots, e_m$. Then the partition $E_1 = \{e_1\}, \ldots, E_m = \{e_m\}$ of $E(G)$ is a *PI-partition*, let us call it the *trivial partition*. Of course, for an application of Theorem 3.1 we wish to find some nontrivial partition of G. This is not always possible, for instance, odd cycles admit only trivial partitions. On the other hand, there exist important classes of graphs (containing important molecular graphs) that allows natural nontrivial PI-partitions. One such class is the class of partial Hamming graphs. Let us explain this in more detail.

Let G be a graph and $e = uv$ and $f = xy$ edges of G. Then we say that e is in the *Djoković relation* $\sim$ with f if $x \in G_1(u)$ and $y \in G_2(v)$. Then it is well known, see [3, 38], that $\sim$ is an equivalence relation on the edge set of a partial Hamming graph G. Moreover, if $e \sim f$ then $G_1(e) = G_1(f)$ and $G_2(e) = G_2(f)$. Consequently, the partition of $E(G)$ induced by the Djoković relation $\sim$ is a PI-partition of G.

In the bipartite case, partial Hamming graphs reduce to partial cubes, that is, isometric subgraphs of hypercubes [8, 22]. Already here one finds important examples of molecular graphs. For instance, every benzenoid system is a partial cube [32] as well as is every phenylene [11, 17].

In the case of benzenoid systems and phenylenes, the Djoković relation $\sim$ partitions the edge set of a given graph into the so-called orthogonal cuts. This was first implicitly observed in [32] and later elaborated and applied in several papers to obtain many appealing properties of the Wiener index, Szeged index, as well as the hyper-Wiener index, see [4, 16, 33, 34].

let G_h be a catacondensed benzenoid system with h hexagons. Then $\|G\| = 5h+1$, therefore Corollary 3.2 implies the following result that is a reformulation of [6, Theorem 1]:

Corollary 3.3 *Let G be a catacondensed benzenoid system with h hexagons and let $E_1, \ldots, E_k$ be the PI-partition of G consisting of orthogonal cuts of G. Then*

$$PI(G) = 25h^2 + 10h + 1 - \sum_{i=1}^{k} |E_i|^2 \,.$$

In the rest of the section we demonstrate the introduced method on several important classes of molecular graphs.

Example 1. Linear chains L_h, $h \geq 1$ (see Fig. 1).

Figure 1: The linear chain L_h

Clearly, L_h has one cut containing $h+1$ edges and $2h$ cuts containing 2 edges. Therefore, applying Corollary 3.3,

$$PI(L_h) = 25h^2 + 10h + 1 - (h+1)^2 - (2h) \cdot 2^2 = 24h^2 \,.$$

Example 2. Linear phenylenes P_h, $h \geq 1$ (see Fig. 2).

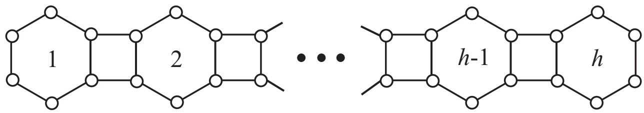

Figure 2: The linear phenylene P_h

Clearly, $\|P_h\| = 8h-2$. The horizontal cut of P_h contains $2h$ edges, while any of the remaining $(h-1)+2h$ cuts contains 2 edges. Therefore from Corollary 3.2 we immediately get:

$$PI(P_h) = (8h-2)^2 - (2h)^2 - (3h-1) \cdot 2^2 = 60h^2 - 44h + 8 \,.$$

We note that this expression has been previously computed in [28] but it is evident that the present method further simplifies computations.

Example 3. Fibonacenes.

Fibonacenes are unbranched catacondensed benzenoid hydrocarbons in which all non-terminal hexagons are angularly annelated. See Fig. 3 for an example of a fibonacene and [18] for an overview of the chemical graph theory of this class of molecular graphs.

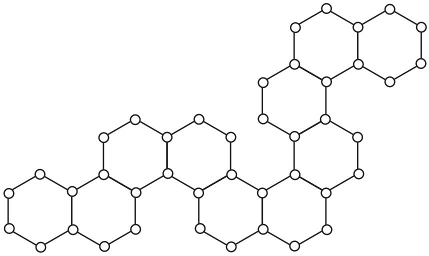

Figure 3: A fibonacene with $h = 10$

A fibonacene F_h with h hexagons contains $h-1$ cuts with 3 edges and $h+2$ cuts with 2 edges. Therefore, using Corollary 3.3,

$$PI(F_h) = 25h^2 + 10h + 1 - 9(h-1) - 4(h+2) = 25h^2 - 3h + 2\,.$$

Example 4. Parallelograms $P(n,k)$, $1 \leq k \leq n$ (see Fig. 4).

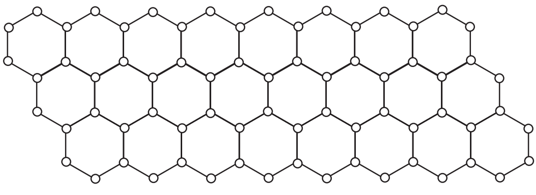

Figure 4: The parallelogram P(8,3)

The Wiener index of $P(n,k)$ has been computed in [33]. We will now apply Corollary 3.2 to obtain the PI index of $P(n,k)$. The followings facts are straightforward to derive:

- $\|P(n,k)\| = n(3k+2)+2k-1$;
- There are k horizontal cuts each having $n+1$ edges;
- There are n cuts in the direction "\" each having $k+1$ edges;
- There are $n-k+1$ cuts in the direction "/" each having $k+1$ edges; and
- For any $j = 2,\ldots,k$ there are 2 cuts in the direction "/" having j edges.

By the above and Corollary 3.2 we conclude that

$$\begin{aligned} PI(P(n,k)) &= (n(3k+2)+2k-1)^2 - k(n+1)^2 - (2n-k+1)(k+1)^2 - 2\cdot\sum_{j=2}^{k} j^2 \\ &= \frac{k^3}{3} + 9k^2n^2 + 10k^2n + 4k^2 + 11kn^2 - 4kn - \frac{19k}{3} + 4n^2 - 6n + 2\,. \end{aligned}$$

In the particular case when $k = n$ the result reduces to

$$PI(P(n,n)) = 9n^4 + \frac{64n^3}{3} + 4n^2 - \frac{37n}{3} + 2\,,$$

while for $k = 1$ we get

$$PI(P(n,1)) = 24n^2\,,$$

the result reported in Example 1.

4 PI index of Cartesian products

For the results in this chapter, the following well-known result (see [22]) is crucial.

Lemma 4.1 [Distance Lemma] *Let G and H be graphs, and $(g,h),(g',h')$ be vertices of $G\Box H$. Then*

$$d_{G\Box H}((g,h),(g',h')) = d_G(g,g') + d_H(h,h')\,.$$

The PI index of a Cartesian product graph can be expressed in terms of the related invariants of the factors as follows.

Theorem 4.2 *For any graphs G and H,*

$$\begin{aligned} PI(G\Box H) &= PI(G)\cdot|H|^2 + PI(H)\cdot|G|^2 + |H|\cdot\|H\|\cdot\sum_{e\in E(G)}\Big(|G_1(e)|+|G_2(e)|\Big) \\ &\quad +|G|\cdot\|G\|\cdot\sum_{e\in E(H)}\Big(|H_1(e)|+|H_2(e)|\Big)\,. \end{aligned}$$

Proof. The edges of $G \,\square\, H$ naturally partition into two classes, the edges $(g,h)(g',h')$ with $h = h'$ and the edges $(a,x)(b,y)$ with $g = g'$. In other words, the first edges project onto the edges of G and the other onto the edges of H. Therefore, let us denote these two subsets of edges of $G \,\square\, H$ with E_G and E_H, respectively. Clearly, $E(G \,\square\, H) = E_G \cup E_H$. For an edge e of E_G let $p_G(e)$ be the edge of G onto which e is projected and let similarly $p_H(f)$ be the edge of H onto which an edge $f \in E_H$ is projected.

Let $e = (g,h)(g',h) \in E(G \,\square\, H)$, so that $e \in E_G$. Then Distance Lemma implies that

$$\{(G \,\square\, H)_1(e), (G \,\square\, H)_2(e)\} = \{G_1(p_G(e)) \times V(H), G_2(p_G(e)) \times V(H)\}\,. \qquad (1)$$

The fact (1) is illustrated in Fig. 5, where $p_G(e)$ is denoted with e'.

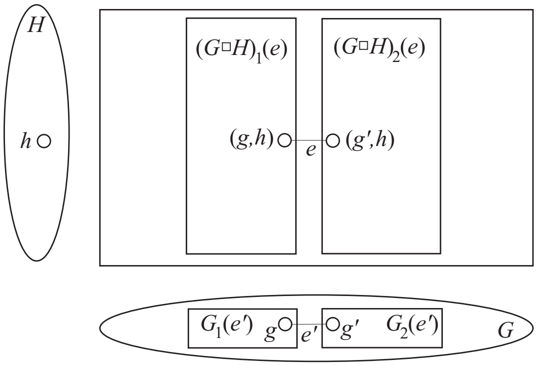

Figure 5: Illustration of (1)

Since $E(G \,\square\, H) = E_G \cup E_H$, $PI(G \,\square\, H) = \sum_{e \in E(G \,\square\, H)} \Big(n_1(G \,\square\, H, e) + n_2(G \,\square\, H, e)\Big)$ can be decomposed as

$$\sum_{e \in E_G} \Big(n_1(G \,\square\, H, e) + n_2(G \,\square\, H, e)\Big) + \sum_{e \in E_H} \Big(n_1(G \,\square\, H, e) + n_2(G \,\square\, H, e)\Big)\,. \qquad (2)$$

Consider the first term of (2). Using (1) it can be written as

$$\sum_{e \in E_G} \Big(\| \langle G_1(p_G e) \times V(H) \rangle \| + \| \langle G_2(p_G e) \times V(H) \rangle \|\Big)\,,$$

which is in turn equal to

$$\sum_{e \in E_G} \Big(\|H\| \cdot |G_1(p_G e)| + |H| \cdot n_1(G, p_G e) + \|H\| \cdot |G_2(p_G e)| + |H| \cdot n_2(G, p_G e)\Big)\,. \qquad (3)$$

Under the projection map, $e \in E(G)$ is the image of precisely $|H|$ edges of $G \Box H$. Therefore, the expression (3) can be further written as

$$|H| \cdot \sum_{e \in E(G)} \Big(\|H\| \cdot |G_1(e)| + |H| \cdot n_1(G,e) + \|H\| \cdot |G_2(e)| + |H| \cdot n_2(G,e) \Big) . \tag{4}$$

Now rewrite (4) as

$$|H|^2 \cdot \sum_{e \in E(G)} \Big(n_1(G,e) + n_2(G,e) \Big) + |H| \cdot \|H\| \cdot \sum_{e \in E(G)} \Big(|G_1(e)| + |G_2(e)| \Big)$$

which gives

$$PI(G) \cdot |H|^2 + |H| \cdot \|H\| \cdot \sum_{e \in E(G)} \Big(|G_1(e)| + |G_2(e)| \Big) . \tag{5}$$

By the commutativity of the Cartesian product, the second term of (2) is equal to

$$PI(H) \cdot |G|^2 + |G| \cdot \|G\| \cdot \sum_{e \in E(H)} \Big(|H_1(e)| + |H_2(e)| \Big) . \tag{6}$$

Combining (5) and (6) the result follows. □

As we already mentioned, for a bipartite graph G and its edge e, $V(G) = G_1(e) \cup G_2(e)$. Therefore:

Corollary 4.3 *For any bipartite graphs G and H,*

$$PI(G \Box H) = PI(G) \cdot |H|^2 + PI(H) \cdot |G|^2 + 2 \cdot |G| \cdot |H| \cdot \|G\| \cdot \|H\| .$$

As a simple example consider the grid graphs, that is, Cartesian products of paths $P_m \Box P_n$; see Fig. 6 for $P_7 \Box P_4$.

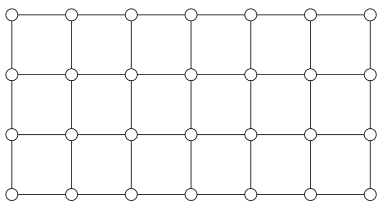

Figure 6: $P_7 \Box P_4$

Let T be a tree on n vertices. Then clearly $PI(T) = (n-1)(n-2)$. Hence Corollary 4.3 gives:

$$\begin{aligned} PI(P_m \,\Box\, P_n) &= (m-1)(m-2)n^2 + (n-1)(n-2)m^2 + 2mn(m-1)(n-1) \\ &= 4m^2n^2 - 5mn(m+n) + 2(m+mn+n)\,. \end{aligned}$$

The situation further simplifies if we consider the Cartesian product of a graph by itself. In the bipartite case we have:

Corollary 4.4 *For any bipartite graph G,*

$$PI(G \,\Box\, G) = 2 \cdot |G|^2 \cdot (PI(G) + \|G\|^2)\,.$$

The Cartesian product is associative, hence the product of several factors is well-defined. Let us denote the Cartesian product of n copies of a graph G with G^n.

Theorem 4.5 *For any bipartite graph G and any $n \geq 1$,*

$$PI(G^n) = n \cdot |G|^{2n-2} \cdot (PI(G) + (n-1) \cdot \|G\|^2)\,.$$

Proof. The result clearly holds for $n = 1$. If holds for $n = 2$ by Corollary 4.4.

For the induction step we first note that by a simple induction we infer that for any $n \geq 1$ and any graph G,

$$\|G^n\| = n \cdot |G|^{n-1} \cdot \|G\|\,. \tag{7}$$

Suppose now that the result holds for $n \geq 2$ and consider $PI(G^{n+1})$. Using Corollary 4.3 and (7) we have:

$$\begin{aligned} PI(G^{n+1}) &= PI(G^n \,\Box\, G) \\ &= \left(n \cdot |G|^{2n-2} \cdot (PI(G) + (n-1) \cdot \|G\|^2\right) \cdot |G|^2 \\ &\quad + PI(G) \cdot |G^n|^2 + 2 \cdot |G^n| \cdot |G| \cdot (n \cdot |G|^{n-1} \cdot \|G\|) \cdot \|G\| \\ &= (n+1) \cdot |G|^{2n} \cdot (PI(G) + n \cdot \|G\|^2)\,. \end{aligned}$$

$\square$

An equivalent description of the n-cube Q_n is that it is the nth power of K_2 with respect to the Cartesian product, that is, $Q_n = K_2^n$. Since $PI(K_2) = 0$, Theorem 4.5 immediately gives $PI(Q^n) = n \cdot 2^{2n-2} \cdot (n-1) \cdot 1^2 = n \cdot (n-1) \cdot 2^{2n-2}$.

References

[1] A. R. Ashrafi and A. Loghman, PI index of armchair polyhex nanotubes, Ars Combin. 80 (2006) 193–199.

[2] A. R. Ashrafi and A. Loghman, PI index of zig-zag polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 55 (2006) 447–452.

[3] B. Brešar, Partial Hamming graphs and expansion procedures, Discrete Math. 237 (2001) 13–27.

[4] V. Chepoi, M. Deza and V. Grishukhin, Clin d'oeil on L_1-embeddable planar graphs, Discrete Appl. Math. 80 (1997) 3–19.

[5] V. Chepoi and S. Klavžar, The Wiener index and the Szeged index of benzenoid systems in linear time, J. Chem. Inf. Comput. Sci. 37 (1997) 752–755.

[6] H. Deng, Extremal catacondensed hexagonal systems with respect to the PI index, MATCH Commun. Math. Comput. Chem. 55 (2006) 453–460.

[7] H. Deng, The PI index of $TUVC_6[2p, q]$, MATCH Commun. Math. Comput. Chem. 55 (2006) 461–476.

[8] M. Deza and M. Laurent, *Geometry of Cuts and Metrics*, Springer-Verlag, Berlin, 1997.

[9] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.

[10] A. A. Dobrynin, I. Gutman, S. Klavžar and P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.

[11] B. Furtula, I. Gutman, Ž. Tomović, A. Vesel and I. Pesek, Wiener-type topological indices of phenylenes, Indian J. Chem. 41A (2002) 1767–1772.

[12] A. Graovac, M. Juvan, M. Petkovšek, A. Vesel, J. Žerovnik, The Szeged index of fasciagraphs, MATCH Commun. Math. Comput. Chem. 49 (2003) 47–66.

[13] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes N. Y. 27 (1994) 9–15.

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

[15] I Gutman and A. A. Dobrynin, The Szeged index—a success story, Graph Theory Notes N. Y. 34 (1998) 37–44.

[16] I. Gutman and S. Klavžar, A method for calculationg Wiener numbers of benzenoid hydrocarbons and phenylenes, ACH Models Chem. 133 (1996) 389–399.

[17] I. Gutman and S. Klavžar, Relations between Wiener numbers of benzenoid hydrocarbons and phenylenes, ACH Models Chem. 135 (1998) 45–55.

[18] I. Gutman and S. Klavžar, Chemical graph theory of fibonacenes, MATCH Commun. Math. Comput. Chem. 55 (2006) 39–54.

[19] I. Gutman, S. Klavžar and B. Mohar (eds.), Fifty Years of the Wiener Index, MATCH Commun. Math. Comput. Chem. 35 (1997) 1–259.

[20] I. Gutman, S. Klavžar and B. Mohar (eds.), Fiftieth Anniversary of the Wiener Index, Discrete Appl. Math. 80(1) (1997) 1–113.

[21] I. Gutman, L. Popović, and L. Pavlović, Elementary edge-cuts in the theory of benzenoid hydrocarbons—an application, MATCH Commun. Math. Comput. Chem. 36 (1997) 217–229.

[22] W. Imrich and S. Klavžar, *Product Graphs: Structure and Recognition*, John Wiley & Sons, New York, 2000.

[23] S. Karmarkar, S. Karmarkar, S. Joshi, A. Das and P. V. Khadikar, Novel application of Wiener vis-à-vis Szeged indices in predicting polychlorinated biphenyls in the environment, J. Serb. Chem. Soc. 62 (1997) 227–234.

[24] P. V. Khadikar, On a novel structural descriptor PI, Nat. Acad. Sci. Lett. 23 (2000) 113–118.

[25] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. Dobrynin and I. Gutman, The Szeged index and an analogy with the Wiener index, J. Chem. Inf. Comput. Sci. 35 (1995) 547–550.

[26] P. V. Khadikar, S. Karmarkar and V. K. Agrawal, Relationships and relative correlation potential of the Wiener, Szeged and PI indices, Nat. Acad. Sci. Lett. 23 (2000) 165–170.

[27] P. V. Khadikar, S. Karmarkar and V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, J. Chem. Inf. Comput. Sci. 41 (2001) 934–949.

[28] P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmarkar and V. K. Agrawal, Novel PI indices of hexagonal chains, J. Math. Chem. 29 (2001) 143–150.

[29] P.V. Khadikar, S. Karmarkar, V.K. Agrawal, J. Singh, A. Shrivastava, I. Lukovits and M.V. Diudea, Szeged index - Applications for drug modeling, Lett. Drug. Design & Disc. 2(8) (2005) 606–624.

[30] P. V. Khadikar, S. Karmarkar and R. G. Varma, The estimation of PI index of polyacenes, Acta Chim. Slov. 49 (2002) 755–771.

[31] I. Gutman and S. Klavžar, Chemical graph theory of fibonacenes, MATCH Commun. Math. Comput. Chem. 55 (2006) 39–54.

[32] S. Klavžar, I. Gutman, B. Mohar, Labeling of benzenoid systems which reflects the vertex–distance relations, J. Chem. Inf. Comput. Sci. 35 (1995) 590–593.

[33] S. Klavžar, I. Gutman and A. Rajapakse, Wiener numbers of pericondensed benzenoid hydrocarbons, Croat. Chem. Acta 70 (1997) 979–999.

[34] S. Klavžar, P. Žigert and I. Gutman, An algorithm for the calculation of the hyper-Wiener index of benzenoid hydrocarbons, Comput. Chem. 24 (2000) 229–233.

[35] K. C. Mathur, S. Singh, S. Mathur and P. V. Khadikar, Modeling polychlorinated biphenyls (PBCs)in environment, Poll. Res. 18 (1999) 405–409.

[36] S. Simić, I. Gutman and V. Baltić, Some graphs with extremal Szeged index, Math. Slovaca 50 (2000) 1–15.

[37] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.

[38] E. Wilkeit, Isometric embeddings in Hamming graphs, J. Combin. Theory Ser. B 50 (1990) 179–197.

[39] J. Žerovnik, Szeged index of symmetric graphs, J. Chem. Inf. Comp. Sci. 39 (1999) 77–80.