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Relation between Wiener-type topological indices of benzenoid molecules

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Abstract

The distance $d(u,v|G)$ between the vertices u and v of a molecular graph G is the length of a shortest u,v-path. We consider a class of Wiener-type topological indices $W_\lambda(G)$, defined as the sum of the terms $d(u,v|G)^\lambda$ over all pairs of vertices of G. Several special cases of $W_\lambda(G)$, namely for $\lambda = +1$ (the original Wiener number) as well as for $\lambda = -2, -1$, +1/2, +2 and +3, were previously studied in the chemical literature, and found applications as molecular structure-descriptors. We establish a relation between $W_{\lambda+1}$ and W_λ, applicable for benzenoid molecules, phenylenes, chemical trees, and other types of molecular graphs.

1. Introduction

One of the oldest, best studied and most often applied molecular-graph-based structure-descriptor [1] is the Wiener topological index [2]

$$W = W(G) = \sum_{u,v} d(u,v|G). \tag{1}$$

If Eq. (1) G stands for a molecular graph, $d(u,v|G)$ is the distance (= number of edges in a shortest path) between the vertices u and v of G, and the summation embraces all pairs of vertices of G. The Wiener index was introduced in 1947. After a latent period of almost half century, within only a few years, a plethora of generalizations and extensions of the Wiener-index-concept has been put forward. Many (but not all) of these Wiener-type indices can be expressed in terms of the quantities

$$W_\lambda = W_\lambda(G) = \sum_{u,v} d(u,v|G)^\lambda, \tag{2}$$

where, clearly, W_1 coincides with the ordinary Wiener index.

First of all, the Wiener-type topological indices W_{-2}, W_{-1}, and $W_{-1/2}$ were introduced in the works [3–6], respectively. The quantity W_{-2} was named '*Harary index*' [3], but later the same name was used for W_{-1} [4]; other authors call W_{-1} the '*reciprocal Wiener index*' [5]. Klein et al. [7] demonstrated that the so-called '*hyper-Wiener index*' [8] can be expressed as $WW = (1/2)W_1 + (1/2)W_2$. In another work [9] Klein et al. established the expression $(1/6)W_3 + (1/2)W_2 + (1/3)W_1$ for a

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structure-descriptor earlier considered by Tratch et al. [10]. The quantity W_λ, as given by Eq. (2) and with λ being an unspecified continuous variable, was studied for the first time by one of the present authors [11]. In the work [12] some properties of W_λ were investigated for $-10 \leqslant \lambda \leqslant 10$.

Note that all the papers [3–12] appeared within less than 10 years.

In view of the works [3–12] on various Wiener-type topological indices, it may be of some value to search for properties of W_λ that hold for any value of λ. In this Letter we report such a relation, connecting $W_{\lambda+1}$ with W_λ, applicable to benzenoid molecules and a variety of other molecular graphs.

In order to deduce this relation we need some preparations.

2. Wiener-type indices of disconnected graphs

The definition (2) of W_λ requires that the graph G be connected. As a consequence, practically the entire research on the Wiener index and its congeners, done so far, was restricted to connected graphs. Yet, this restriction can be overcome.

Denote by $d(G,k)$ the number of pairs of vertices of the graph G that are at distance k, and note that this quantity is well defined for both connected and disconnected graphs. In particular, $d(G,0) =$ number of vertices of G, and $d(G,1) =$ number of edges of G. Then the right-hand side of Eq. (2) can be rewritten as

$$W_\lambda = W_\lambda(G) = \sum_{k \geqslant 1} d(G,k) k^\lambda. \tag{3}$$

Formula (3) may be viewed as the definition of the Wiener-type indices of disconnected graphs. Since we consider only finite (molecular) graphs, the above sum is always finite. It is easy to see that if G consists of components $G_1, G_2, \ldots, G_p$, then

$$W_\lambda(G) = W_\lambda(G_1) + W_\lambda(G_2) + \cdots + W_\lambda(G_p).$$

3. Benzenoid systems and their elementary cuts

Benzenoid systems (molecular graphs of benzenoid hydrocarbons) have been extensively studied in chemical graph theory [13]. A self-explanatory example of a benzenoid system is depicted in Fig. 1.

An *elementary cut* of a benzenoid system B is a straight line segment, passing through the middle of some edges, orthogonal to these edges, that intersects the perimeter of B exactly two times. Elementary cuts of benzenoid systems have been much studied (see, for instance, [14–19]). Illustrative examples thereof are found in Fig. 1.

Every edge of a benzenoid system is intersected by exactly one elementary cut. A benzenoid system with h hexagons and n_i internal vertices has $\gamma = 2h + 1 - n_i$ distinct elementary cuts [18].

Elementary cuts are, in fact, just a diagrammatic presentation of the Djoković–Winkler relation Θ [20,21], known in the theory of so-called '*partial cubes*', namely isometric subgraphs of hypercubes [22]. (Benzenoid systems are partial cubes [15].)

Let $e_1 = (u_1, v_1)$ and $e_2 = (u_2, v_2)$ be two edges of a graph G. One says [19,20] that e_1 and e_2 are in relation Θ, $e_1 \Theta e_2$, if $d(u_1, u_2|G) + d(v_1, v_2|G) \neq d(u_1, v_2|G) + d(v_1, u_2|G)$.

In the case of partial cubes the relation Θ is transitive, i.e., if $e_1 \Theta e_2$ and $e_2 \Theta e_3$, then $e_1 \Theta e_3$.

If e_1 and e_2 are edges of a hexagon (or, more generally, of an even-membered cycle), then $e_1 \Theta e_2$ if and only if these edges lie opposite to each other. Then, because of the transitivity of Θ, all edges of a benzenoid system lying on an elementary cut

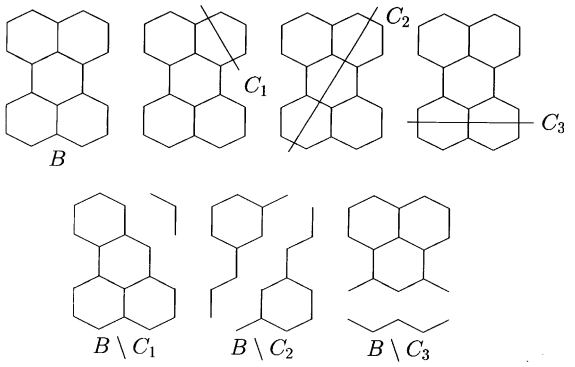

Fig. 1. A benzenoid system B (perylene), three of its elementary cuts (C_1, C_2, C_3), and the subgraphs obtained by dissecting B along C_1, C_2, and C_3. The perylene graph has a total of nine elementary cuts.

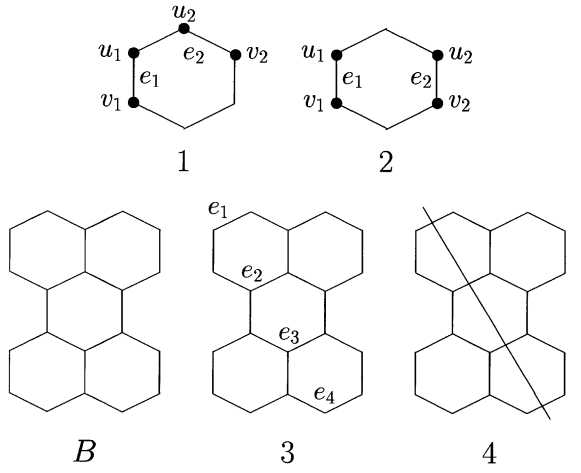

Fig. 2. Diagram 1: $d(u_1,u_2)=1,\ d(v_1,v_2)=3,\ d(u_1,v_2)=2,\ d(v_1,u_2)=2$; therefore $d(u_1,u_2)+d(v_1,v_2)=d(u_1,v_2)+d(v_1,u_2)$ implying that the edges e_1 and e_2 are not in relation Θ. Diagram 2: $d(u_1,u_2)=2,\ d(v_1,v_2)=2,\ d(u_1,v_2)=3,\ d(v_1,u_2)=3$; therefore $d(u_1,u_2)+d(v_1,v_2)\neq d(u_1,v_2)+d(v_1,u_2)$ implying that the edges e_1 and e_2 are in relation Θ. Diagram 3: The edges e_1 and e_2 lie on opposite sides of the hexagon a of the benzenoid system B; therefore $e_1\Theta e_2$. The edges e_2 and e_3 lie on opposite sides of the hexagon b, whereas e_3 and e_4 lie on opposite sides of the hexagon c; therefore $e_2\Theta e_3$ and $e_3\Theta e_4$. Then, by transitivity, $e_1\Theta e_3$, $e_1\Theta e_4$, and $e_2\Theta e_4$. The edges e_1,e_2,e_3,e_4 form a Θ-class, which is just another way of presentation of the elementary cut depicted in Diagram 4.

(and only these edges) are mutually Θ-related. One says that they form a Θ-class; an example is shown in Fig. 2.

Using the technique of Θ-relations it is possible to deduce certain results for W_λ of benzenoid systems (or, more generally, of partial cubes). This is outlined in the subsequent section.

4. The main result

If B is a benzenoid system, then for any real (or complex) value of the parameter λ,

$$W_{\lambda+1}(B)=\gamma W_\lambda(B)-\sum_C W_\lambda(B\setminus C). \tag{4}$$

In Eq. (4) C stands for an elementary cut, and the summation goes over all elementary cuts of B; the total number of elementary cuts of B is denoted by γ. As already mentioned, $\gamma=2h+1-n_i$. Recall also that $W_\lambda(B\setminus C)$ is computed using formula (3) that is applicable to disconnected graphs.

In order to verify Eq. (4) we need the following facts about the relation Θ in the case when the graph G is a partial cube, cf. [22,23]:

(i) G is a connected graph.
(ii) A path P in G is a geodesic if and only if no two different edges of P are in relation Θ.
(iii) Let $F_1,F_2,\ldots,F_\gamma$ be the Θ-classes of G. Then for $i=1,2,\ldots,\gamma$, the subgraph $G\setminus F_i$ consists of two connected components.

Proof of Eq. (4).

Consider a partial cube G and let $F_1,F_2,\ldots,F_\gamma$ be its Θ-classes. Define an auxiliary quantity X as

$$X=\sum_{i=1}^{\gamma} W_\lambda(G\setminus F_i).$$

Let u and v be arbitrary vertices of G. By property (i) their distance is well-defined, $d(u,v|G)=k\geqslant 1$. Let P be a u,v-geodesic. By property (ii), the edges of P belong to different Θ-classes, say to $F_1,F_2,\ldots,F_k$. By property (iii), u and v belong to different components of $G\setminus F_i$ for $i=1,\ldots,k$, but are in the same component for $i=k+1,\ldots,\gamma$.

Therefore, $d(u,v|G\setminus F_i)=k$ for $i=k+1,\ldots,\gamma$, and the pair u,v contributes $(\gamma-k)$-times to X. Summing these contributions over all pairs of vertices of B we arrive at:

$$\begin{aligned}X&=\sum_{k\geqslant 1}(\gamma-k)d(G,k)k^\lambda\\&=\gamma\sum_{k\geqslant 1}d(G,k)k^\lambda-\sum_{k\geqslant 1}d(G,k)k^{\lambda+1}\\&=\gamma W_\lambda(G)-W_{\lambda+1}(G),\end{aligned}$$

resulting in the identity

$$\gamma W_\lambda(G)-W_{\lambda+1}(G)=\sum_{i=1}^{\gamma}W_\lambda(G\setminus F_i). \tag{5}$$

In the case of benzenoid systems, the Θ-classes in (5) may be replaced by elementary cuts, and Eq. (4) follows.

5. Discussion and concluding remarks

In the special cases $\lambda=0$ and $\lambda=1$ formula (4) can be significantly simplified.

For a connected n-vertex graph G, $W_0(G) = \binom{n}{2}$. If, in turn, G possesses two components, with n_1 and n_2 vertices, then $W_0(G) = \binom{n_1}{2} + \binom{n_2}{2}$. Bearing these relations in mind, we get from (4):

$$W(B) = \gamma\binom{n}{2} - \sum_C \left[\binom{n_1(C)}{2} + \binom{n_2(C)}{2}\right],$$

where $n_1(C)$ and $n_2(C)$ count the vertices of the two components of $B\backslash C$. Taking into account that for all elementary cuts, $n_1(C) + n_2(C) = n$, and that there are γ distinct elementary cuts, we arrive at a remarkably simple, previously reported [17], expression for the Wiener index:

$$W(B) = \sum_C n_1(C)n_2(C).$$

Setting $\lambda = 1$ we obtain from (4)

$$W_2(B) = \gamma W(B) - \sum_C W(B\backslash C),$$

from which follows a new connection between the Wiener and hyper-Wiener indices of benzenoid systems:

$$WW(B) = \frac{\gamma+1}{2} W(B) - \frac{1}{2}\sum_C W(B\backslash C). \qquad (6)$$

Identity (5) holds for all partial cubes. There are molecular graphs, other than benzenoid systems, that are partial cubes. Of them, phenylenes and (chemical) trees deserve particular attention.

In the case of phenylenes formula (4) is applicable without any modification. For a phenylene with h hexagons, $\gamma = 3h$.

In the case of (chemical) trees, each edge belongs to a different Θ-class. Then Eq. (4) reduces to [24]:

$$W_{\lambda+1}(T) = (n-1)W_\lambda(T) - \sum_e W_\lambda(T-e). \qquad (7)$$

where T stands for an n-vertex tree, and the summation goes over all edges e of T.

From identity (7) we straightforwardly arrive at the following special case of Eq. (6):

$$WW(T) = \frac{n}{2} W(T) - \frac{1}{2}\sum_e W(T-e), \qquad (8)$$

that was earlier communicated in [25]. In reality, after the discovery of relation (8) [25], efforts have been made to understand its origin and extend the range of its validity. This resulted first in formula (7) [24] and eventually in (4) and (5).

Thus, by applying certain advanced proof techniques of graph theory [22], we could shed some light on the perplexed and hitherto concealed relations between various Wiener-type topological indices. These results enable a better insight into the structure-dependency of these structure-descriptors and also make easier their calculation.

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