Vertex-weightings for distance moments and thorny graphs

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Received 5 February 2004; received in revised form 18 December 2006; accepted 14 May 2007
Available online 13 June 2007

Abstract

Valence-weightings are considered for shortest-path distance moments, as well as related weightings for the so-called “Wiener” polynomial. In the case of trees the valence-weighted quantities are found to be expressible as a combination of unweighted quantities. Further the weighted quantities for a so-called “thorny” graph are considered and shown to be related to the weighted and unweighted quantities for the underlying parent graph.

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MSC: primary 05C12; 05C05; secondary 05C90

Keywords: Wiener index; Wiener polynomial; Wiener number; Distance moments; Thorny graph; Resistance distance

1. Introduction

The sum over all shortest-path distances of a (molecular) graph was introduced by Wiener \cite{29,30} as a “topological index”, i.e., a graphic invariant for use in structure–property correlations. It has been termed the “Wiener number” and much studied, as indicated in several surveys \cite{4,12,20,21,24}. Moreover a fair number of modifications or extensions of the Wiener number of a (molecular) graph have been considered. The Wiener number evidently may be viewed \cite{14} as the unnormalized first moment of the set of intersite shortest-path distances of such a graph, and the (square-root of the) second moment is involved in an index considered by Balaban \cite{1}. Further higher (unnormalized) moments \cite{17,23} of these distances have also become of interest as a novel set of graph invariants. The so-called “hyper-Wiener” index \cite{22} of Randić first defined for trees turns out to be related \cite{17} to the first two moments, so that a natural extension to cycle-containing graphs is indicated. The index of Tratch and Zefirov \cite{28} turns out to be similarly related \cite{16} to the first three moments, again thereby facilitating an extension to cycle-containing graphs. A sort of valence-weighted Wiener index arises \cite{18} in Schultz’s \cite{27} so-called “molecular topological” index, which for trees turns \cite{16} out to have a relation to unweighted moments. Estrada \cite{5,6} has proposed (and utilized) a similar vertex-weighting for higher moments. Also Gutman \cite{9} has shown how for trees a sort of double vertex-weighted Wiener index can be related to unweighted moments. Further Estrada \cite{5,7} has proposed such double vertex-weightings for higher moments. Yet a further extension of the Wiener number in terms of the so-called Wiener polynomial has been made \cite{13,26,10} with...
the realization that suitable derivatives evaluated at \( x = 1 \) yield the moments. Many of these different extensions and their applications are discussed in the book [25].

Here the various mentioned results are inter-related and unified in an extended mathematical framework. In Section 2 single and double vertex-weighted Wiener polynomials are introduced, and for the case of trees these new polynomials are proved to be related to the ordinary Wiener polynomial. In Section 3 these results for trees are then noted to lead to relations between corresponding vertex-weighted moments and unweighted moments.

Section 4 goes on to consider so-called “thorny-graphs”, which in chemistry may be viewed as the hydrogen-completed graphs of parent H-deleted graphs. These have recently been studied [11,26], and Gutman [8,11] has established a relation between the Wiener index for a thorny graph and its parent. Here weighted moments and weighted Wiener polynomials are considered for a thorny graph and are shown to be related to correspondent weighted quantities for the underlying parent graph.

In Section 5 a few additional results are noted, first concerning a relation for weighted quantities of a thorny tree to unweighted quantities of the parent tree. And second a further analog is developed for the polynomials and moments of Sections 2 and 3, now defined in terms of the so-called “resistance distance”.

Thence a range of new results are found, to unify and extend the previous work.

2. Vertex-weighted Wiener polynomials

Standard notation for a (molecular) graph \( G \) is used, and throughout the present paper \( G \) is assumed to be connected. The vertex (or site) set is \( V \), with cardinality \( N \), and the edge (or bond) set is \( E \). A connected acyclic graph is termed a tree. The shortest-path distance between vertices \( i \) and \( j \) is denoted \( D(i, j) \), the degree (or valence) of vertex \( i \) is denoted \( v_i \), and the number of length-2 paths in \( G \) is denoted \( p_2(G) \). The Wiener polynomial of \( G \) is defined as

\[
P_o(G; x) = \sum_{i<j} x^{D(i,j)}
\]

with \( x \) a dummy variable. This coincides with the definition of Hosoya [13], and Sagan et al. [26]. A corresponding (singly) vertex-weighted Wiener polynomial is defined as

\[
P_v(G; x) = \frac{1}{2} \sum_{i<j} (v_i + v_j) x^{D(i,j)+1},
\]

and a doubly vertex-weighted Wiener polynomial is

\[
P_vv(G; x) = \sum_{i<j} v_i v_j x^{D(i,j)+2},
\]

where \( v_i \) is the degree of vertex \( i \). For the case of trees (i.e., acyclic connected graphs) special results apply:

**Theorem A.** For a tree \( T \),

\[
P_v(T; x) = (x + 1) P_o(T; x) - (N - 1)x.
\]

**Proof.** First, we rewrite

\[
P_v(T; x) = x P_o(T; x) + \frac{1}{2} \sum_k \sum_{j \neq k} (v_j - 1) x^{D(j,k)+1}.
\]

Now let \( n(j) \) be the set of vertices adjacent to \( j \), whence in this last sum over vertices \( j \) the factor \( v_j - 1 \) may be replaced by a sum over the vertices \( i \in n(j) \) such that \( i \) is farther away from \( k \) than is \( j \). Evidently for a tree there are \( v_j - 1 \) such vertices \( i \) with the remaining vertex adjacent to \( j \) lying closer to \( k \) (along the path between \( j \) and \( k \)). Then for these \( v_j - 1 \) vertices \( i \) one has \( D(i, k) = D(j, k) + 1 \), and

\[
\sum_{j \neq k} (v_j - i) x^{D(j,k)+1} = \sum_{j \neq k} \sum_{D(i,k) > D(j,k)} x^{D(i,k)}.
\]
But as \( j \) ranges, the vertices \( i \) which arise are all those other than \( k \) or the neighbors of \( k \), and each such \( k \) occurs but once in a tree, so that

\[
P_v(T; x) = x P_o(T; x) + \frac{1}{2} \sum_{k \in V} \left[ \sum_{i \neq k} x^{D(i, k)} - \sum_{i \in n(k)} x \right] = (x + 1) P_o(T; x) - \frac{1}{2} \sum_{k \in V} x v_k.
\]

With the recognition that \( \sum_k v_k \) is twice the number \( e \) of edges, and that for a tree \( e = N - 1 \), one then immediately completes proof of the theorem.  

**Theorem B.** For a tree \( T \),

\[
P_vv(T; x) = (1 - x^2) P_o(T; x) + 2x P_v(T; x) - (N - 1) x - p_2(T) x^2.
\]

**Proof.** We rewrite

\[
P_vv(T; x) = x^2 P_o(T; x) + \sum_{j < k} [(v_j - 1 + v_k - 1) + (v_j - 1)(v_k - 1)] x^{D(j, k) + 2}
\]

\[
= -x^2 P_o(T; x) + 2x P_v(T; x) + \sum_{j < k} (v_j - 1)(v_k - 1) x^{D(j, k) + 2},
\]

much as in the proof of theorem A. Now the last \( j < k \) sum is to be replaced by an \( i < m \) sum first with \( i \in n(j) \) such that \( i \) is farther away from \( k \) than is \( j \) and second with \( m \in n(k) \) such that \( m \) is farther away from \( j \) than is \( k \). Evidently for a tree, there are \( v_j - 1 \) such vertices \( i \) and \( v_k - 1 \) such vertices \( m \), while \( D(i, k) = D(j, k) + 1 \), \( D(j, m) = D(j, k) + 1 \), and \( D(i, m) = D(j, k) + 2 \). Then

\[
P_vv(T; x) = -x^2 P_o(T; x) + 2x P_v(T; x) + \frac{1}{2} \sum_{i \in V} \left[ \left( \sum_{m \neq i} x^{D(i, m)} \right) - C_i \right],
\]

where \( C_i \) is a correction due to the pairs of the sites \( i, m \) with \( D(i, m) = 1 \) or 2. This correction evidently takes the form

\[
C_i = \sum_{m \in n(i)} x^1 + \sum_{m \in n(n(i))} x^2 = v_i x + p_2(T, i) x^2,
\]

where \( p_2(T, i) \) denotes the number of length-2 paths with one end at vertex \( i \). Then

\[
P_vv(T; x) = -x^2 P_o(T; x) + 2x P_v(T; x) + P_o(T_x) - \frac{1}{2} \sum_i v_i x - \frac{1}{2} \sum_i p_2(T, i) x^2.
\]

Here \( \frac{1}{2} \sum_i v_i \) gives \( N - 1 \) and \( \frac{1}{2} \sum_i p_2(T, i) \) gives \( p_2(T) \), whence the proof of the theorem is readily completed.  

### 3. Wiener-related scalar invariants

The (unweighted) *unnormalized* \( n \)th moment for shortest-path distances is defined as

\[
W_o(G; n) = \sum_{i < j} D(i, j)^n.
\]

Here Wiener’s [29] index occurs for the case of \( n = 1 \), and various higher moments arise in several other works, as mentioned in the introduction. Corresponding unnormalized (singly) vertex-weighted \( n \)th moments are defined as

\[
W_v(G; n) = \frac{1}{2} \sum_{i < j} (v_i + v_j) D(i, j)^n.
\]
The $n = 1$ case occurs in Schultz’s [27] “molecular topological index”, and higher such moments have been considered by Estrada [7]. Unnormalized doubly vertex-weighted $n$th moments are defined as

$$W_{vv}(G; n) = \sum_{i < j} v_i v_j D(i, j)^n$$

and have been proposed by Estrada [5]. A convenient notation takes $\ast$ to denote a generic label $o$, $v$ or $vv$, so that $W_{\ast}(G; n)$ is correspondingly $W_o(G; n)$, $W_v(G; n)$, or $W_{vv}(G; n)$ — and similarly for $P_{\ast}(G; x)$, while we also define $p(\ast) = 0, 1, or 2$, for these three respective circumstances. Now:

**Proposition C.** For a connected graph $G$,

$$W_{\ast}(G; n) = \left[ \left( \frac{d}{dx} \right)^n \left[ x^{-p(\ast)} P_{\ast}(G; x) \right] \right]_{x=1}$$

and

$$P_{\ast}(G; x) = \sum_{n>0} W_{\ast}(G; n)(n!)^{-1} x^{p(\ast)} \ln(x)^n.$$

The proof of the first relation is quite immediate from the definitions of the $P_{\ast}(G; x)$ and the $W_{\ast}(G; n)$, with the result for $\ast = o$ already noted [13,26]. The second relation is developed on identifying $x = e^\zeta$ and viewing $W_{\ast}(G; n)$ as given in the first relation as

$$W_{\ast}(G; n) = \left[ \left( \frac{d}{d\zeta} \right)^n \sum_{i < j} e^{\zeta D(i, j)} \right]_{\zeta=0}.$$

Then the second relation of the proposition is obtained by making a Taylor series expansion about $\zeta = 0$ (where $\ln x$ in turn may be expanded in powers of $x - 1$).

In conjunction with Theorems A and B this proposition quite straight-forwardly leads to:

**Corollary D.** For a tree $T$,

$$W_v(T; n) = W_o(T; n) + \sum_{k=0}^n (-1)^{n-k} \binom{n}{k} W_o(T, k);$$

$$W_{vv}(T; n) = 2W_v(T; n) - W_o(T; n) + \sum_{k=0}^n \binom{n}{k} W_o(T; k)(-2)^{n-k} - (-1)^n (N - 1).$$

The results of this corollary for $W_v(T; 1)$ and $W_{vv}(T; 1)$ are established in [9].

4. Thorny graphs and Wiener-type polynomials

Granted a graph $G$ with all vertices of degree at most $t$ there is a corresponding $t$-thorny graph $G^*$ which is defined with vertex and edge sets $V^*$ and $E^*$ so as to include the correspondent sets $V$ and $E$ of $G$ along with sufficient additional degree-1 vertices and incident edges to bring the degree of each site $i \in V \subseteq V^*$ up to a degree $t$. An example of a graph $G$ and its corresponding 3-thorny graph $G^*$ is shown in Fig. 1.

If $G$ is imagined to be the H-deleted graph of an alkane, then the 4-thorny graph $G^*$ is the H-included graph. In addition to the studies [25,2], thorny graphs were defined by Cayley [3]. The cyclomatic number of $G$ is $\mu(G) = e(G) - N + k(G)$ where $e = e(G)$ is the number of edges of $G$ and $k(G)$ is the number of components. It now follows that:

**Proposition E.** Let $G$ be an $N$-vertex graph with every vertex of degree at most $t$, and let the cyclomatic number of $G$ be $\mu(G)$. Then the $t$-thorny graph $G^*$ contains $N$ vertices of degree $t$ and $(t - 2)N + 2 - 2\mu(G)$ vertices of degree 1.
The proof is fairly straightforward, and the result is in essence long-recognized in chemistry, in that for an \( N \)-carbon hydrocarbon without multiple bonds there are \( 2N + 2 - 2\mu(G) \) H-atoms, which is the result for a connected graph and \( t = 4 \). For the \( t \)-thorny case each vertex of \( G \) when forming \( G^* \) may be viewed to contribute \( t \) half-bonds of which \( e = \mu(G) + N - k(G) \) pairs contribute to whole bonds in both \( G \) and \( G^* \), thence leaving \( Nt - 2e \) half-bonds to be connected to additional degree-1 sites in \( G^* \). This \( t \)-thorny result for the connected case was also noted in [30].

**Theorem F.** Let \( G \) be an \( N \)-vertex connected graph with every vertex of degree at most \( t \), and let \( G^* \) be the corresponding \( t \)-thorny graph.

\[
P_o(G^*; x) = (1 + tx)^2 P_o(G; x) - 2(1 + tx)P_v(G; x) + P_vv(G; x) + \left[ Nt - 2e \right] x + \left[ p_2(G) + 2e(1 - t) + N \right] x^2.
\]

**Proof.** Let \( D \) and \( D^* \) be the respective shortest-path distance functions for \( G \) and \( G^* \), and for \( i' \in V \) let the set of adjacent degree-1 vertices in \( G^* \) be denoted \( n^*(i') \). That is, though \( i' \) is a vertex of \( G \), the vertices of \( n^*(i') \) are not in \( G \) but rather only in \( G^* \). Then

\[
D^*(i, j) = \begin{cases} 
D(i, j), & i, j \in V, \\
D(i, j) + 1, & i \in n^*(i'), j \in V, \\
D(j', j''), & i \in n^*(i'), j \in V, \ j \in n^*(j'), j' \in V,
\end{cases}
\]

so that the sum over vertices in the definition of \( P(G^*; x) \) may be partitioned amongst those vertices in \( V \) and the different \( n^*(i') \), with \( i' \in V \). The part of this summation where both indices \( i \) and \( j \) belong to \( G \) is just

\[
\sum_{i<j} x^{D(i,j)} = P_o(G; x).
\]

The part of the summation where \( i \in V \) and \( j \in n^*(i) \) is

\[
\sum_{i \in V} \sum_{j \in n^*(i)} x^{D(i,j)+1} = \sum_{i \in V} (t - v_i) x = [Nt - 2e] x,
\]

where we recognize that \( \sum_i v_i = 2e \). The remaining part of the summation where one index is in \( V \) and the other is not may be written as

\[
\sum_{i' < j} x^{D(i',j)+1} + \sum_{i' < j'} x^{D(i,j') + 1} = \sum_{i < j} (t - v_i + t - v_j) x^{D(i,j)+1} = 2tx P_o(G; x) - 2P_v(G; x).
\]
Next we consider the part of the summation where neither index \((i, j)\) is in \(V\), but both are attached to the same vertex of \(V\),
\[
\sum_{i' \in V} \sum_{i < j} x^2 = x^2 \sum_{i \in V} \left( t - v_i \right),
\]
since there are \(\left( \frac{t - v_i}{2} \right)\) pairs of distinct vertices in \(n^*(i)\). This sum can be expressed as
\[
\frac{1}{2} \sum_{i \in V} [t^2 - t - 2tv_i + v_i^2 + v_j]x^2,
\]
yielding
\[
\left[ N \left( \frac{t}{2} \right) - 2et + 2e + \sum_{i \in V} \left( \frac{v_i}{2} \right) \right] x^2.
\]
The last sum in the square brackets is equal to the number of all paths of length 2 in \(G\), \(p_2(G)\), so that this total contribution becomes
\[
\left[ p_2(G) + 2e(1 - t) + N \left( \frac{t}{2} \right) \right] x^2.
\] (4.4)

And next the remaining part of the summation where neither index \(i\) or \(j\) is in \(V\) is
\[
\sum_{i' \in V} \sum_{i \notin V} \sum_{j \notin V} x^{D(i', j')+2} = \sum_{i < j} (t - v_i)(t - v_j)x^{D(i, j)+2}
\]
\[
= t^2 x^2 P_o(G; x) - 2tx P_v(G; x) + P_{vv}(G; x).
\] (4.5)

Finally, addition of these five formulae (4.1)–(4.5) together leads to the expression of the theorem for \(P_o(G; n)\).

Now also:

**Theorem G.** Let \(G\) and \(G^*\) be as in Theorem F. Then
\[
P_v(G^*; x) = tx[x^2 + (t + 1)x + 1]P_o(G; x) - x(2tx + t + 1)P_v(G; x) + xP_{vv}(G; x)
\]
\[
+ \left[ p_2(G) + 2e(1 - t) + N \left( \frac{t}{2} \right) \right] x^3 + \left[ N \left( \frac{t + 1}{2} \right) - e(t + 1) \right] x^2.
\]

**Proof.** The result is proved in much the same fashion as Theorem F. The \(i, j\)-summation over vertices of \(V^*\) as appears in the definition of \(P_v(G^*; x)\) is similarly partitioned into different contributions. The part where both \(i\) and \(j\) belong to \(V\) is
\[
\frac{1}{2} \sum_{i < j} (t + t)x^{D(i, j)+1} = tx P_o(G; x),
\] (4.6)

where it has been recognized that the degrees of two such vertices are both \(t\) when considered as members of \(G^*\). The part of the summation where \(i \in V\) and \(j \in n^*(i)\) is
\[
\sum_{i \in V} \sum_{j \in n^*(i)} \frac{t + 1}{2} x^{D(i, j)+1} = \frac{t + 1}{2} \sum_{i \in V} x^2(t - v_i) = \frac{t + 1}{2} [Nt - 2e] x^2,
\] (4.7)

where this time it is recognized that the degrees of the two vertices as they occur in \(G^*\) are \(t\) and 1 (thereby giving rise to the \((t + 1)/2\) factor). The remaining part of the summation where one index is in \(v\) and the other is not is
\[
\frac{1}{2} \sum_{i' < j} \sum_{i \in n^*(i')} (t + 1)x^{D(i', j)+2} + \frac{1}{2} \sum_{i < j'} \sum_{j \in n^*(j')} (t + 1)x^{D(i, j')+2} = \frac{1}{2} (t + 1) \sum_{i < j} (t - v_i + t - v_j)x^{D(i, j)+2},
\]
thus yielding
\[(t + 1)[tx^2P_o(G; x) - xP_v(G; x)]. \tag{4.8}\]

Next the part of the summation where neither index \(i\) or \(j\) is in \(V\), but both are attached to the same site of \(V\), is
\[
\sum_{i' \in V} \sum_{i < j} \frac{1 + 1}{2} xD(i', j')^3 + 3 = \sum_{i \in V} \left(t - v_i \right)^2,
\]
thus yielding
\[
\left[p_2(G) + 2e(1 - t) + N \left(\frac{t}{2}\right)\right]x^3. \tag{4.9}\]

And next the remaining part of the summation where neither index \(i\) or \(j\) is in \(V\) is
\[
\sum_{i' < j_1 \in e^*(i')} \sum_{j_1 \in e^*(j')} \frac{1 + 1}{2} xD(i', j')^3 + 3 = \sum_{i < j} (t - v_i)(t - v_j)xD(i, j)^3
\]
\[
= t^2x^3P_o(G; x) - 2tx^2P_v(G; x) + xP_{vv}(G; x). \tag{4.10}\]

Addition of (4.6)–(4.10) together leads to the expression of the theorem for \(P_v(G^*; x)\).

Yet further we have:

**Theorem H.** Let \(G\) and \(G^*\) be as in Theorem F. Then
\[
P_{vv}(G^*; x) = t^2x^2(1 + x)^2P_o(G; x) - 2tx^2(1 + x)P_v(G; x) + x^2P_{vv}(G; x)
\]
\[
+ t[2Nt - 2e]x^3 + \left[p_2(G) + 2e(1 - t) + N \left(\frac{t}{2}\right)\right]x^4.
\]

The proof although somewhat detailed is of the same form as the two previous ones, and is not gone through here.

5. Further results and resistance distance

There are a few further items to note. First the use of Proposition C and Corollary D, Theorems F, G, and H lead quite readily to:

**Corollary I.** For an \(N\)-vertex tree \(T\) with every vertex of degree at most \(t\), let \(T^*\) be the corresponding \(t\)-thorny tree. Then
\[
W_o(T^*; n) = (t - 1)^2 \sum_{k=0}^{n} \binom{n}{k} W_o(T; k)2^{n-k} + N \left(\frac{t}{2}\right)2^n + N(t - 1) + 1;
\]
\[
W_v(T^*; n) = W_o(T^*; n) + (t - 1)^2 \sum_{k=0}^{n} \binom{n}{k} W_o(T; k) + N \left(\frac{t}{2}\right);
\]
\[
W_{vv}(T^*; n) = 2W_v(T^*; n) - W_o(T^*; n) + (t - 1)^2W_o(T; n).
\]

The result here for \(W_o(T^*; 1)\) is established by Gutman [8].

But also some of the definitions and results can be neatly extended in yet another direction, involving the so-called “resistance distance”. One imagines unit resistors on each edge of a graph \(G\) and lets \(\Omega(i, j)\) denote the effective resistance between \(i\) and \(j\) when the poles of a battery are connected to the vertices \(i\) and \(j\). It turns out that \(\Omega(i, j)\) is [19] a distance function on \(G\); it also has much more purely mathematical methods of definition [15], and is termed
the resistance distance on $G$. Thence the polynomials and moments of Sections 2 and 3 might also be extended with definitions where $\Omega$ replaces the shortest-path distance $D$, thusly

$$P'_o(G; x) = \sum_{i < j} x^{\Omega(i,j)};$$

$$P'_v(G; x) = \frac{1}{2} \sum_{i < j} (v_i + v_j)x^{\Omega(i,j)+1};$$

$$P'_{vv}(G; x) = \sum_{i < j} v_i v_j x^{\Omega(i,j)+2}.$$

And similarly for the $W'_\star(G; n), \star = o, v, vv$. Then one has:

**Proposition J.** For a connected graph $G$ the result of Proposition C holds with $P_\star(G; x)$ and $W_\star(G; n)$, respectively, replaced by $P'_\star(G; x)$ and $W'_\star(G; n)$, for $\star = o, v, vv$.

Next the resistance distance $\Omega$ is generally different from $D$, but it is the same for trees. Indeed whenever there is but one path between two vertices $i$ and $j$, $\Omega(i, j) = D(i, j)$, all as is quite reasonable from an intuitive physical point of view. Further whenever all the paths between $i$ and $j$ pass through a vertex $k$, then

$$D(i, j) = D(i, k) + D(k, j) \quad \text{and} \quad \Omega(i, j) = \Omega(i, k) + \Omega(k, j),$$

again as intuitively physically reasonable. Now the first of these relations is the essential property of $D$ used in developing Theorems F, G, and H; in particular, this is what is used in developing the relation between $D^* \text{ and } D$. But the relation above for $\Omega$ allows one to write a similar relation between the resistance distance $\Omega^*$ for a (connected) thorny graph and $\Omega$ for the underlying parent. Thus:

**Proposition K.** Let $G$ be an $N$-vertex connected graph with every vertex of degree at most $t$, and let $G^*$ be the corresponding $t$-thorny graph. Then Theorems F, G, and H hold with $P_\star(G; x)$ replaced by $P'_\star(G; x)$ for $\star = o, v, vv$.

### 6. Overview and conclusion

As already indicated in the Introduction the present results relate to a body of previous work. In the present work substantial extension and unification is evidently attained. Many of our results have been realized only for special cases (of our general results of C, D, and I), while a number of results seem to be entirely new (as A, B, F, G, H, J, and K). The new quantities defined here are the polynomials $P'_o(G; x)$ and $P'_{vv}(G; x)$ (as well as their resistance-distance analogues), but they are seen (in Propositions C and J) to be just “transforms” of the already studied quantities $W'_o(G; n)$ and $W'_{vv}(G; n)$, and their use facilitates the result of Corollaries D and I in a neat fashion. Further it is surmised that they will be of chemical interest as molecular descriptors, paralleling the use of $P_o(G; x)$ and $W_o(G; n)$.

**Acknowledgment**

D.J.K. and T.D. acknowledge the support of the Welch Foundation of Houston, Texas, via Grant No. BD-0894.

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