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Chemical Graphs Constructed of Composite Graphs and Their q-Wiener Index

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Abstract

The Wiener index W is the sum of distances between all pairs of vertices of a connected graph. Recently Zhang et al. [*MATCH Commun. Math. Comput. Chem.* **67** (2012) 347] considered the q-analog of W, motivated by the theory of hypergeometric series. We obtain explicit formulas for the q-Wiener index of cluster and corona of graphs, of which thorny and bridge graphs are special cases. Using these formulas, the q-Wiener indices of several classes of chemical graphs are computed.

1 Introduction

In this paper we are concerned with simple and connected graphs. Let G be such a graph. Its vertex is denoted by $V(G)$.

The distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or $d(u,v)$ for short). It is defined as the length of a shortest path connecting u and v [3].

The diameter of the graph G, denoted by d_G, is the maximum distance between two vertices of G.

Let $d(G,k)$ be the number of pairs of vertices of the graph G that are at distance k. Note that $d(G,0)$ and $d(G,1)$ are equal to the number of vertices and edges, respectively. Then the Wiener index of G is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \sum_{k\geq 1} d(G,k) \ .$$

For details of the history, mathematical theory, and chemical applications of the Wiener index see [5, 12, 21, 25].

Let q be a positive real number, $q \neq 1$. Three different variants of the q-Wiener index were considered so far [26], viz.,

$$\begin{aligned} W_1(G,q) &= \sum_{\{u,v\}\subseteq V(G)} [d(u,v)]_q \\ W_2(G,q) &= \sum_{\{u,v\}\subseteq V(G)} [d(u,v)]_q \, q^{d_G - d(u,v)} \\ W_3(G,q) &= \sum_{\{u,v\}\subseteq V(G)} [d(u,v)]_q \, q^{d(u,v)} \ . \end{aligned}$$

Where

$$[k]_q = \frac{1-q^k}{1-q} = 1 + q + q^2 + \cdots + q^{k-1} \ .$$

Obviously, $\lim_{q\to 1}[k]_q = k$, and therefore,

$$\lim_{q\to 1} W_1(G,q) = \lim_{q\to 1} W_2(G,q) = \lim_{q\to 1} W_3(G,q) = W(G) \ .$$

The possible chemical interpretation and applications of the invariants $W_i(G,q)$ are analyzed in [26]. The three q-Wiener indices are mutually related as:

$$W_2(G,q) = q^{d_G - 1} \, W_1(G, 1/q) \tag{1}$$

$$W_3(G,q) = (1+q)\, W_1(G,q^2) - W_1(G,q) \ . \tag{2}$$

In addition, we have the following relations [26]:

$$W_1(G,q) = \sum_{k\geq 1} [k]_q \, d(G,k)$$

$$W_2(G,q) = \sum_{k\geq 1}[k]_q\, q^{d_G-k}\, d(G,k)$$

$$W_3(G,q) = \sum_{k\geq 1}[k]_q\, q^{k}\, d(G,k)\ .$$

Recently [19], formulas are obtained for computing the q-Wiener indices of some compound trees.

The counting polynomial

$$H(G,\lambda) = \sum_{k=1}^{d_G} d(G,k)\,\lambda^k$$

was first put forward by Hosoya [16] (see also [13] and the references cited therein). Hosoya himself called it Wiener polynomial, but eventually the more appropriate name "Hosoya polynomial" has been accepted [4,13]. The mathematical connections between the q-Wiener indices and $H(G,q)$ are established in [26], viz.,

$$W_1(G,q) = \frac{1}{1-q}\left[\binom{n}{2} - H(G,q)\right]$$

$$W_2(G,q) = \frac{q^{d_G}}{1-q}\left[H(G,1/q) - \binom{n}{2}\right]$$

$$W_3(G,q) = \frac{1}{1-q}\left[H(G,q) - H(G,q^2)\right].$$

In view of the relations (1) and (2), in what follows we shall report only expressions for $W_1(G,q)$ The corresponding formulas for $W_2(G,q)$ and $W_3(G,q)$ could then be established by means of Eqs. (1) and (2), respectively.

Throughout this paper, C_n , P_n , K_n , and S_n denote the cycle, path, complete, and star graphs on n vertices. Our other notations are standard and taken mainly from [14].

2 Main results

A rooted graph is a graph in which one vertex is labeled in a special way so as to be distinguished from the other vertices. This special vertex is called the root of the graph. Let G be a labeled graph on n vertices. Let $\mathbf{H}$ be a sequence of n rooted graphs $H_1, H_2, \ldots, H_n$. The rooted product $G(\mathbf{H})$ is the graph obtained by identifying the root of H_i with the i-th vertex of G, for $i = 1, 2, \ldots, n$ [7].

The cluster $G_1\{G_2\}$ of a graph G_1 and a rooted graph G_2 is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of G_2, and by identifying the root vertex of the i-th copy of G_2 with the i-th vertex of G_1, for $i = 1, 2, \ldots, |V(G_1)|$, see Fig. 1. The cluster is a special case of rooted product. In what follows, we denote the root vertex of G_2 by w, and the copy of G_2 whose root is identified with the vertex $u \in V(G_1)$ by G_2^u.

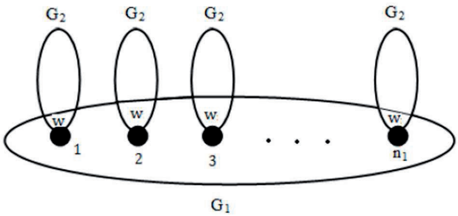

Fig. 1. The cluster $G_1\{G_2\}$.

For given graphs G_1 and G_2, their corona product, $G_1 \circ G_2$, is obtained by taking $|V(G_1)|$ copies of G_2 and joining each vertex of the i-th copy of G_2 with the i-th vertex of G_1.

2.1 q-Wiener index of the cluster of graphs

In this section we determine the q-Wiener index of the cluster $G_1\{G_2\}$. First we define for vertex $x \in V(G)$,

$$D_G(x,q) = \sum_{x \neq u \in V(G)} [d(u,x)]_q \qquad \text{and} \qquad Q_G(x) = \sum_{x \neq u \in V(G)} q^{d(u,x)} \,.$$

Theorem 2.1. Let G_1 be a graph of order n_1, and let G_2 be a graph of order n_2, rooted at the vertex w. Then

$$\begin{aligned} & W_1(G_1\{G_2\},q) = n_1\, W_1(G_2,q) \\ + \; & W_1(G_1,q)\left[Q_{G_2}(w) + \frac{1}{3}\,Q_{G_2}(w)(n_2-1) + \frac{1}{3}\,Q^2_{G_2}(w) + \frac{1}{3}\,(n_2-1)^2 + n_2\right] \\ + \; & H(G_1,q)\left[D_{G_2}(w,q) + \frac{2}{3}\,Q_{G_2}(w)D_{G_2}(w,q) + \frac{1}{3}\,(n_2-1)D_{G_2}(w,q)\right] \end{aligned}$$

$$+ \quad D_{G_2}(w,q)\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}\,Q_{G_2}(w)+1+\frac{2}{3}\,(n_2-1)\right].$$

Proof. From the definition of the cluster $G_1\{G_2\}$, the distance between the vertices of $u, v \in V(G_1\{G_2\})$ can be easily obtained bearing in mind that of $d_{G_1\{G_2\}}(u,v) = d_{G_2}(u,v)$ if $u, v \in V(G_2^x)$, and $d_{G_1\{G_2\}}(u,v) = d_{G_2}(u,w) + d_{G_1}(x,y) + d_{G_2}(v,w)$ if $u \in V(G_2^x)$, $v \in V(G_2^y)$ and $x \neq y$. These relations imply

$$W_1(G_1\{G_2\},q) = \sum_{\{u,v\}\subseteq V(G_1\{G_2\})} [d_{G_1\{G_2\}}(u,v)]_q$$

$$= \quad n_1 \sum_{\{u,v\}\subseteq V(G_2)} [d_{G_2}(u,v)]_q + \sum_{\{u,v\}\subseteq V(G_1)} [d_{G_1}(u,v)]_q$$

$$+ \quad \sum_{\{u,v\}\subseteq V(G_1)} \ \sum_{x\in V(G_2^u)-\{w\}} \ \sum_{y\in V(G_2^v)-\{w\}} [d_{G_2}(x,w)+d_{G_1}(u,v)+d_{G_2}(y,w)]_q$$

$$+ \quad \sum_{u\in V(G_1)} \ \sum_{v\in V(G_1)-\{u\}} \ \sum_{x\in V(G_2^v)-\{w\}} [d_{G_1}(u,v)+d_{G_2}(x,w)]_q$$

$$= \quad n_1\, W_1(G_2,q) + W_1(G_1,q) + \frac{1}{3}\,(n_2-1)^2\, W_1(G_1,q)$$

$$+ \quad \frac{1}{3}\,n_1\,(n_1-1) D_{G_2}(w,q)(n_2-1) + \frac{1}{3}\,H(G_1,q)\,D_{G_2}(w,q)(n_2-1)$$

$$+ \quad \frac{1}{3}\,H(G_1,q)\,D_{G_2}(w,q)\,Q_{G_2}(w) + \frac{1}{3}\,Q_{G_2}(w)\,W_1(G_1,q)(n_2-1)$$

$$+ \quad \frac{1}{3}\,H(G_1,q)\,D_{G_2}(w,q)\,Q_{G_2}(w) + \frac{1}{6}\,n_1\,(n_1-1) D_{G_2}(w,q)\,Q_{G_2}(w)$$

$$+ \quad \frac{1}{3}\,Q^2_{G_2}(w)\,W_1(G_1,q) + W_1(G_1,q)(n_2-1) + \frac{1}{2}\,n_1\,(n_1-1) D_{G_2}(w,q)$$

$$+ \quad H(G_1,q)\,D_{G_2}(w,q) + W_1(G_1,q)\,Q_{G_2}(w) = n_1\, W_1(G_2,q)$$

$$+ \quad W_1(G_1,q)\left[Q_{G_2}(w) + \frac{1}{3}\,Q_{G_2}(w)(n_2-1) + \frac{1}{3}\,Q^2_{G_2}(w) + \frac{1}{3}\,(n_2-1)^2 + n_2\right]$$

$$+ \quad H(G_1,q)\left[D_{G_2}(w,q) + \frac{2}{3}\,Q_{G_2}(w)\,D_{G_2}(w,q) + \frac{1}{3}\,(n_2-1) D_{G_2}(w,q)\right]$$

$$+ \quad D_{G_2}(w,q)\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}\,Q_{G_2}(w)+1+\frac{2}{3}\,(n_2-1)\right]$$

which completes the proof. ∎

Note that for given graphs G and H, the graph $G \circ H$ can be considered as the cluster of G and of $K_1 + H$, where the root of $K_1 + H$ is at the single vertex of K_1. So the formula of q-Wiener index of $G \circ H$ can be obtained by setting $G_1 \cong G$ and $G_2 \cong K_1 + H$ in Theorem 2.1.

Corollary 2.2. Let G and H be two graphs with n_1 and n_2 vertices and m_1 and m_2 edges respectively, then

$$\begin{aligned} W_1(G \circ H, q) &= n_1 \left[m_2 + n_2 + (1+q)\overline{m_2} \right] \\ &+ W_1(G_1, q) \left[1 + n_2(1+q) + \frac{1}{3} n_2^2 (q^2 + q + 1) \right] \\ &+ H(G_1, q) \left[n_2 + \frac{1}{3} n_2^2 (2q+1) \right] \\ &+ n_2 \left[\frac{1}{6} n_1 (n_1 - 1) n_2 (q+2) + \frac{n_1(n_1-1)}{2} \right] \end{aligned}$$

where $\overline{m_2}$ is the number of edges of the complement of $K_1 + H$.

Let G be a labeled graph on n vertices and let $p_1, p_2, \ldots, p_n$ be non-negative integers. The thorny graph $G^*(p_1, p_2, \ldots, p_n)$ of the graph G is obtained from G by attaching p_i pendent vertices to the i-th vertex of G, $i = 1, 2, \ldots, n$. The concept of thorny graphs was introduced in [9] and eventually found a variety of chemical applications [2, 15, 22–24], mainly related with Wiener–type indices.

The thorny graph $G^*(p_1, p_2, \ldots, p_n)$ can be viewed as the rooted product of G by the sequence of star graphs $\{S_{p_1+1}, S_{p_2+1}, \ldots, S_{p_n+1}\}$, where the root vertex of S_{p_i+1} is the vertex of degree p_i , $i = 1, \ldots, n$.

Theorem 2.3. The q-Wiener index of the thorny graph $G^*(p_1, p_2, \ldots, p_n)$ is given by:

$$W_1(G^*(p_1, p_2, \ldots, p_n), q) = \sum_{i=1}^{n} W_1(S_{p_i+1}, q) + W_1(G, q)$$
$$+ \sum_{\substack{i,j=1 \\ i<j}}^{n} p_i \, p_j \left[d_G(w_i, w_j) + 2 \right]_q + \sum_{i=1}^{n} p_i \left[D_G(w_i, q) + Q_G(w_i) \right] .$$

Proof. By the definition of the thorny graph $G^*(p_1, p_2, \ldots, p_n)$, we have:

$$W_1(G^*(p_1, p_2, \ldots, p_n), q) = \sum_{\{u,v\} \subseteq V(G^*(p_1, p_2, \ldots, p_n))} \left[d_{G^*(p_1, p_2, \ldots, p_n)}(u, v) \right]_q$$

$$= \sum_{i=1}^{n} \sum_{\{u,v\}\subseteq V(S_{p_i+1})} [d_{S_{p_i+1}}(u,v)]_q + \sum_{\{u,v\}\subseteq V(G)} [d_G(u,v)]_q$$

$$+ \sum_{\substack{i,j=1\\ i<j}}^{n} \sum_{\{u,v\}\subseteq V(G)} \sum_{x\in V(S^u_{p_i+1})-\{w_i\}} \sum_{y\in V(S^v_{p_i+1})-\{w_j\}} [d_G(u,v)+2]_q$$

$$+ \sum_{i=1}^{n} \sum_{u\in V(G)} \sum_{v\in V(G)-\{u\}} \sum_{x\in V(S^v_{p_i+1})-\{w_i\}} [d_G(u,v)+1]_q$$

$$= \sum_{i=1}^{n} W_1(S_{p_i+1},q) + W_1(G,q) + \sum_{\substack{i,j=1\\ i<j}}^{n} p_i\, p_j\, [d_G(w_i,w_j)+2]_q$$

$$+ \sum_{i=1}^{n} p_i\, [D_G(w_i,q) + Q_G(w_i)]$$

which completes the proof. ■

3 Examples and corollaries

In this section we apply Theorem 2.1, Corollary 2.2, and Theorem 2.3 to the q-Wiener index of some interesting classes of graphs.

For a given graph G, its t-thorny graph $\Theta_t(G)$ is obtained by attaching t pendent vertices to each vertex of G. This graph can be represented as the cluster of G and the star graph on $t+1$ vertices S_{t+1}, where the root of S_{t+1} is on its vertex of degree t.

Corollary 2.4. By Theorem 2.1 and Proposition 2. in [26], the q-Wiener index t-thorny graph of a given graph G with n vertices is computed as:

$$\begin{aligned} W_1(\Theta_t(G),q) &= \frac{nt}{2}\,[t(1+q)+(1-q)] + W_1(G,q)\left[1+t(1+q)+\frac{t^2}{3}\,(q^2+q+1)\right] \\ &+ H(G,q)\left[t+\frac{t^2}{3}\,(2q+1)\right] + t\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}\,t\,(q+2)+1\right]. \end{aligned}$$

From the above formula and Proposition 2 in [26], the q-Wiener index of the t-thorny graph of P_n and C_n can easily be computed.

Example 2.5.

$$\begin{aligned}
W_1(\Theta_t(P_n),q) &= \frac{nt}{2}\left[t(1+q)+(1-q)\right] \\
&+ \frac{1}{2}\sum_{k=1}^{n-1}\left(k(k+1)q^{n-k-1}\right)\left[1+t(1+q)+\frac{t^2}{3}\left(q^2+q+1\right)\right] \\
&+ \sum_{i=1}^{n-1}\left(i\,q^{n-i}\right)\left[t+\frac{t^2}{3}\left(2q+1\right)\right]+t\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}t(q+2)+1\right].
\end{aligned}$$

If n is an even number, then

$$\begin{aligned}
&W_1(\Theta_t(C_n),q) = \frac{nt}{2}\left[t(1+q)+(1-q)\right] \\
+ &\left(n\sum_{k=1}^{\frac{n}{2}-1}[k]_q+\frac{n}{2}(1+q+\cdots+q^{\frac{n}{2}-1})\right)\left[1+t(1+q)+\frac{t^2}{3}(q^2+q+1)\right] \\
+ &\left(n\sum_{k=1}^{\frac{n}{2}-1}q^k+\frac{n}{2}q^{\frac{n}{2}}\right)\left[t+\frac{t^2}{3}\left(2q+1\right)\right]+t\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}t(q+2)+1\right].
\end{aligned}$$

If n is an odd number, then

$$\begin{aligned}
&W_1(\Theta_t(C_n),q) = \frac{nt}{2}\left[t(1+q)+(1-q)\right] \\
+ &\left(n\sum_{k=1}^{\frac{n-1}{2}}[k]_q\right)\left[1+t(1+q)+\frac{t^2}{3}\left(q^2+q+1\right)\right] \\
+ &\left(n\sum_{k=1}^{\frac{n-1}{2}}q^k\right)\left[t+\frac{t^2}{3}\left(2q+1\right)\right]+t\,\frac{n_1(n_1-1)}{2}\left[\frac{1}{3}t(q+2)+1\right].
\end{aligned}$$

Our next example is about the bridge graph constructed on a given graph G. Let G be a graph rooted at vertex w and let n be a positive integer. The bridge graph $B_d(G,w)$ is the graph obtained by taking d copies of G and by connecting the vertex w of the i-th copy of G to the vertex w of the $i+1$-th copy of G by an edge for $i=1,2,\ldots,d-1$, as shown in Fig. 2. The bridge graph $B_d(G,w)$ can be represented as the cluster of d vertex path P_d and the graph G.

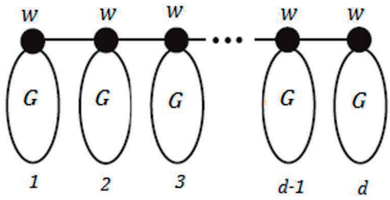

Fig. 2. The bridge graph $B_d(G,w)$

Corollary 2.6. Let G be a graph rooted at vertex w, then

$$\begin{aligned}
&W_1(B_d(G,w),q) = d\,W_1(G,q)\\
+\ &\frac{1}{2}\sum_{k=1}^{d-1}\left(k(k+1)q^{d-k-1}\right)\left[Q_G(w)+\frac{1}{3}\,Q_G(w)(|V(G)|-1)\right]\\
+\ &\frac{1}{2}\sum_{k=1}^{d-1}\left(k(k+1)q^{d-k-1}\right)\left[\frac{1}{3}\,Q_G^2(w)+\frac{1}{3}\,(|V(G)|-1)^2+|V(G)|\right]\\
+\ &\sum_{k=1}^{d-1}(k\,q^{d-k})\left[D_G(w,q)+\frac{2}{3}\,Q_G(w)\,D_G(w,q)+\frac{1}{3}\,(|V(G)|-1)D_G(w,q)\right]\\
+\ &D_G(w,q)\,\frac{d(d-1)}{2}\left[\frac{1}{3}\,Q_G(w)+1+\frac{2}{3}\,(|V(G)|-1)\right].
\end{aligned}$$

Consider now the square comb lattice $Cq(N)$ with open ends, possessing $N=n^2$ vertices (see Fig. 3). This graph can be represented as the cluster $P_n\{P_n\}$, where the root of P_n is on its pendent vertex.

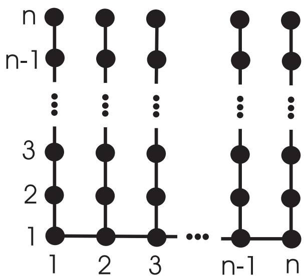

Fig. 3. The the square comb lattice $Cq(N)$.

Example 2.7. Using Corollary 2.6 and Proposition 2. in [26], the q-Wiener index of the square comb lattice $Cq(N)$ with $N = n^2$ vertices is given by:

$$\begin{aligned} W_1(Cq(N), q) &= \frac{1}{6}\sum_{k=1}^{n-1} k(k+1)q^{n-k-1}\left[n^2+4n+1+\left(\sum_{k=1}^{n-1} q^k\right)^2 + (n+2)\sum_{k=1}^{n-1} q^k\right] \\ &+ \frac{1}{3}\sum_{k=1}^{n-1} k\, q^{n-k} \sum_{k=1}^{n-1}[k]_q \left[2\sum_{k=1}^{n-1} q^k + n + 2\right] \\ &+ \frac{n(n-1)}{6}\sum_{k=1}^{n-1}[k]_q \left[2n+1+\sum_{k=1}^{n-1} q^k\right]. \end{aligned}$$

Using Corollary 2.6, we can get the following results for the bridge graph constructed on the cycle C_m, see Fig. 4 for the case $m = 6$. Note that because of the symmetry of the graph C_m, any vertex of this graph can be assumed as its root vertex.

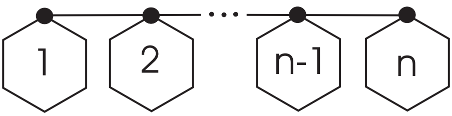

Fig. 4. The bridge graph constructed on the cycle C_6 .

Example 2.8. Let n and m be positive integers, $m \geq 3$

$$A = 2\sum_{k=1}^{\frac{m}{2}-1} q^k + q^{\frac{m}{2}} \qquad , \qquad B = 2\sum_{k=1}^{\frac{m}{2}-1}[k]_q + [\frac{m}{2}]_q$$

$$A' = 2\sum_{k=1}^{\frac{m-1}{2}} q^k \qquad , \qquad B' = 2\sum_{k=1}^{\frac{m-1}{2}}[k]_q$$

If m is even, then

$$\begin{aligned} & W_1(P_n\{C_m\}, q) \\ = & \frac{1}{2}\sum_{k=1}^{n-1} k(k+1)q^{n-k-1}\left[A + \frac{1}{3}A(m-1) + \frac{1}{3}A^2 + \frac{1}{3}(m-1)^2 + m\right] \end{aligned}$$

$$+ \sum_{k=1}^{n-1} k\, q^{n-k} \left[B + \frac{2}{3}\, AB + \frac{1}{3}\,(m-1)B\right]$$

$$+ \frac{n(n-1)}{2}\, B\left[\frac{1}{3}\, A + \frac{2}{3}\, m + \frac{1}{3}\right] + nm \sum_{k=1}^{\frac{m}{2}-1} [k]_q + \frac{mn}{2}\,(1 + \cdots + q^{\frac{m}{2}-1})\ .$$

If m is odd, then

$$\begin{aligned} & W_1(P_n\{C_m\}, q) \\ = \ & \frac{1}{2}\sum_{k=1}^{n-1} k(k+1)q^{n-k-1}\left[A' + \frac{1}{3}\,A'(m-1) + \frac{1}{3}\,A'^2 + \frac{1}{3}\,(m-1)^2 + m\right] \\ + \ & \sum_{k=1}^{n-1} k\, q^{n-k}\left[B' + \frac{2}{3}\,A'B' + \frac{1}{3}\,(m-1)B'\right] + \frac{n(n-1)}{2}\,B'\left[\frac{1}{3}\,A' + \frac{2}{3}\,m + \frac{1}{3}\right] \\ + \ & nm \sum_{k=1}^{\frac{m-1}{2}} [k]_q\ . \end{aligned}$$

For a given graph G, the graph $K_2 \circ G$ is called the bottleneck graph of G. By Corollary 2.2, we have:

Example 2.9. Let G be a graph with n vertices and m edges, then

$$W_1(K_2 \circ G, q) = n(3+q) + n^2\,(2 + 2q + q^2) - 2qm + 1\ .$$

In particular, the q-Wiener index of the bottleneck graph of P_n is equal to

$$W_1(K_2 \circ P_n, q) = n^2\,(2 + 2q + q^2) + n(3-q) + 2q + 1\ .$$

A caterpillar or caterpillar tree is a tree in which all the vertices are within distance 1 of a central path. If we delete all pendent vertices of a caterpillar tree, then we obtain a path. Thus, caterpillars are thorny graphs whose parent graph is a path, see Fig. 5.

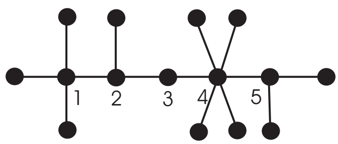

Fig. 5. A caterpillar tree obtained by attaching pendent vertices to P_5.

Example 2.10. Using Theorem 2.3, the q-Wiener index of caterpillar tree $P_n^*(p_1,\ldots,p_n)$ is given by:

$$W_1(P_n^*(p_1,p_2,\ldots,p_n),q)=\sum_{i=1}^{n}\left[\binom{p_i+1}{2}+\binom{p_i}{2}q\right]+W_1(P_n,q)$$

$$+\sum_{\substack{i,j=1\\ i<j}}^{n}p_i\,p_j\,[d_{P_n}(w_i,w_j)+2]_q+\sum_{i=1}^{n}p_i\,[D_{P_n}(w_i,q)+Q_{P_n}(w_i)]\ .$$

Caterpillar trees are used in chemical graph theory to represent the structure of benzenoid hydrocarbon molecules [6, 8, 17, 18]. In addition, the caterpillar tree $P_n^*(3,2,2,\ldots,2,3)$ is the plerogram–type [10,11] molecular graph of the normal alkane with n carbon atoms.

Example 2.11. Using Example 2.10, the q-Wiener index of the caterpillar tree $P_n^*(p,2,2,\ldots,2,p)$ is given by:

$$\begin{aligned}W_1(P_n^*(p,2,2,\ldots,2,p),q) &= 2\left[\binom{p+1}{2}+\binom{p}{2}q\right]+(3+q)(n-2)\\ &+ \frac{1}{2}\sum_{k=1}^{n-1}k(k+1)q^{n-k-1}+\sum_{\substack{i,j=1\\ i<j}}^{n}p_i\,p_j\,[d_{P_n}(w_i,w_j)+2]_q\\ &+ \sum_{i=1}^{n}p_i\,[D_{P_n}(w_i,q)+Q_{P_n}(w_i)]\ .\end{aligned}$$

In particular, for $p=3$, we arrive at:

Example 2.12. The q-Wiener indices of the plerograms of ethane, propane, and butane are

$$\begin{aligned}W_1(P_2^*(3,3),q) &= 9q^2+21q+28\\ W_1(P_3^*(3,2,3),q) &= 9q^3+27q^2+45q+55\\ W_1(P_4^*(3,2,2,3),q) &= 9q^4+21q^3+44q^2+64q+91\ .\end{aligned}$$

Let $T_1,\ldots,T_m$, $m\geq 2$, be trees with disjoint vertex sets of orders $n_1,\ldots,n_m$, respectively. Let $w_i\in V(T_i)$, $i=1,2,\ldots,m$. Any tree T on more than two vertices can be viewed as being obtained by joining a new vertex u to each of the vertices

$w_1, w_2, \ldots, w_m$. In following, we state a theorem from [19], that makes it possible to recursively calculate the q-Wiener index of any tree.

Lemma 2.13. Let T be a tree on $n \geq 3$ vertices, whose structure is specified above, then

$$\begin{aligned} W_1(T,q) &= \sum_{i=1}^{m} W_1(T_i,q) + q\sum_{i=1}^{m} d_{T_i}(w_i,1) + q^2 \sum_{i=1}^{m}(n-1-n_i)\, d_{T_i}(w_i,1) \\ &+ (n-1) - (1-q)q^2 \sum_{1\leq i<j\leq m} d_{T_i}(w_i,1)d_{T_j}(w_j,1) \\ &+ \frac{1+q}{2}\left[(n-1)^2 - \sum_{i=1}^{m} n_i^2\right] \end{aligned}$$

where $d_{T_i}(w_i,1) = \sum\limits_{u\in V(T_i)} [d(u,w_i)]_q$.

The ordinary Bethe tree $B_{d,k}$ is a rooted tree of k levels whose root vertex has degree d, the vertices from levels 2 to $k-1$ have degree $d+1$, and the vertices at level k have degree 1, see Fig. 6. Using Lemma 2.13, we get the following relation for the q-Wiener index of $B_{d,k}$.

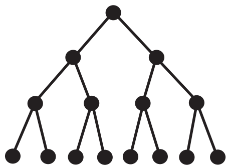

Fig. 6. The ordinary Bethe tree $B_{2,4}$.

Corollary 2.14. The q-Wiener index of the ordinary Bethe tree $B_{d,k}$ is given by

$$\begin{aligned} W_1(B_{d,j},q) &= d\,W_1(B_{d,j-1},q) + qd\left[\sum_{m=0}^{j-3}\left(\sum_{i=m+1}^{j-2} q^m\, d^i\right)\right] \\ &+ q^2\,(d^j-d)\left[\sum_{m=0}^{j-3}\left(\sum_{i=m+1}^{j-2} q^m\, d^i\right)\right] + \sum_{i=1}^{j-1} d^i \\ &- (1-q)q^2\binom{d}{2}\left[\sum_{m=0}^{j-3}\left(\sum_{i=m+1}^{j-2} q^m\, d^i\right)\right]^2 \end{aligned}$$

$$+ \quad \frac{1+q}{2}\left[\left(\sum_{i=1}^{j-1} d^i\right)^2 - d\left(\sum_{m=0}^{j-2} d^m\right)^2\right]$$

where $3 \le j \le k$ and

$$W_1(B_{d,3},q) = \frac{d^4}{2}\left(q^3+q^2+q+1\right) + d^3\left(1+q+\frac{(1-q)q^2}{2}\right) + d^2\left(1-q^2\right) + \frac{d}{2}(1-q)\ .$$

Denote by $C(d,k,n)$ the unicyclic graph obtained by attaching the root vertex of $B_{d,k}$ to the vertices of the n-vertex cycle C_n, see Fig. 7. For more information about this graph, see [1]. It is easy to see that $C(d,k,n)$ is the cluster of C_n and $B_{d,k}$. So by Theorem 2.1 and Corollary 2.14, we get the q-Wiener index of $C(d,k,n)$.

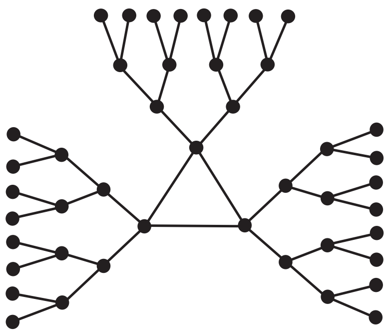

Fig. 7. The unicyclic graph $C(2,4,3)$.

Example 2.15. Let

$$A = \sum_{m=1}^{k-2} (dq)^m \quad , \quad B = \sum_{m=0}^{k-2}\left(\sum_{i=m+1}^{k-1} q^m\, d^i\right) \quad , \quad C = \sum_{m=1}^{k-1} d^m\ .$$

Then the q-Wiener index of the unicyclic graph $C(d,k,n)$ is given by

$$W_1(C(d,k,n),q) = n\, W_1(B_{d,k},q)$$

$$+ \quad \left(n\sum_{m=1}^{\frac{n}{2}-1}[m]_q + \frac{n}{2}\left(1+q+\cdots+q^{\frac{n}{2}-1}\right)\right)\left[A + \frac{1}{3}AC + \frac{1}{3}A^2 + \frac{1}{3}C^2 + C + 1\right]$$

$$+ \left(n \sum_{m=1}^{\frac{n}{2}-1} q^m + \frac{n}{2} q^{\frac{n}{2}} \right) \left[B + \frac{2}{3} AB + \frac{1}{3} CB \right] + B \, \frac{n(n-1)}{2} \left[\frac{1}{3} A + 1 + \frac{2}{3} C \right].$$

Denote by $P(d,k,n)$ the tree obtained by attaching the root vertex of $B_{d,k}$ to the vertices of P_n, see Fig. 8. For more information about this classes of trees, see [20]. It is easy to see that $P(d,k,n)$ can be considered as the bridge graph $B(B_{d,k}, B_{d,k}, \ldots, B_{d,k}; w, w, \ldots, w)$, where w denotes the root vertex of $B_{d,k}$. So by Corollaries 2.6 and 2.14, we get the q-Wiener index of $P(d,k,n)$.

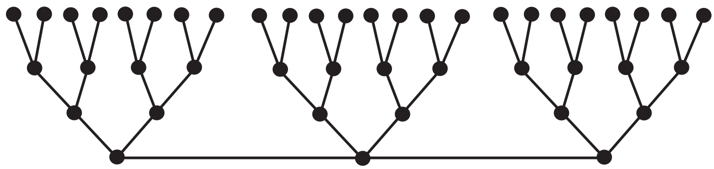

Fig. 8. The tree $P(2,4,3)$.

Example 2.16. The q-Wiener index of the tree $P(d,k,n)$ is given by:

$$W_1(P(d,k,n),q) = n\, W_1(B_{d,k},q) + \frac{1}{2} \left(\sum_{m=1}^{n-1} m(m+1)\, q^{n-m-1} \right) \left[A + \frac{1}{3} AC \right]$$

$$+ \frac{1}{2} \left(\sum_{m=1}^{n-1} m(m+1)\, q^{n-m-1} \right) \left[\frac{1}{3} A^2 + \frac{1}{3} C^2 + C + 1 \right]$$

$$+ \left(\sum_{m=1}^{n-1} m\, q^{n-m} \right) \left[B + \frac{2}{3} AB + \frac{1}{3} CB \right] + B \, \frac{n(n-1)}{2} \left[\frac{1}{3} A + 1 + \frac{2}{3} C \right].$$

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