Computer Science Journal of Moldova, vol.**30**, no.3(90), 2022

Wiener Index of Some Brooms

Julian D. Allagan

Abstract

In the field of chemical graph theory, a Wiener (topological) index is a type of a molecular descriptor that is calculated based on the molecular graph of alkanes. It gives the sum of geodesic distances (or shortest paths) between all pairs of vertices of the graph. We found and prove the Wiener indices of some Brooms, which are Caterpillars, giving several unknown sequences that are now added to the collection of the largest Online Encyclopedia of Integer Sequences.

Keywords: Wiener Index, Brooms, Sequences.

1 Introduction

Suppose G is a simple graph and $v \in V(G)$. The distance between two vertices $u, v \in V(G)$, often denoted by $d_G(u, v)$, is the length (number of edges) of their shortest path in G; this is also known as a *geodesic distance*. The *eccentricity* of a vertex v, written as $\epsilon(v)$, is the maximum of the distance between v and any other vertex $u \in V$, i.e., $\epsilon(v) = \max\limits_{u \in V}\{d_G(v, u)\}$. Further, the *diameter* d of a graph is the maximum eccentricity of any vertex in the graph, i.e., $d = \max\limits_{v \in V} \epsilon(v)$. These parameters are often useful in classifying acyclic (tree-like) graphs. A topological index, a numerical value, is often used to describe chemical structures in the areas of chemical graph theory, molecular topology, and mathematical chemistry. One of the well-studied indices is the Wiener topological index (W), introduced in 1947 by Harry Wiener [12]. In graph theory, the *Wiener index* of a graph G, denoted by $W(G)$, is the sum of the distances between all unordered pairs of vertices of G. This index is used to describe and even predict

doi:10.56415/csjm.v30.20

several physical and chemical properties of molecules such as density, viscosity and velocity. Details of some of these reviews can be found in [4], [6], [8], [9], [11], for instance.

Throughout this article, we denote the n^{th} *triangular number* by $T_n = \dfrac{n(n+1)}{2} = 1+2+3+4+5+6+\ldots+n$. Moreover, we denote the k^{th} *tetrahedral number* by $T_n^k = \sum_k T_n$, the sum of the first k n^{th} triangular numbers.

Suppose $P_n := v_1 - v_2 - \ldots - v_{n-1} - v_n$, denotes a path on $n \geq 3$ vertices. By sequentially connecting k leaves to some vertex v_i, with $2 \leq i \leq n-1$, we obtain a *Caterpillar*. We denote a Caterpillar on $n+k$ vertices by P_n^k, where P_n is referred to as *stem* or *backbone*; observe that the diameter of P_n^k is the length of P_n. If every internal vertex is adjacent to at least one of the k new pendant vertices, then P_n^k is said to be *complete*. Caterpillars have been used in chemical graph theory to represent the structure of benzenoid hydrocarbon molecules, eg., [3] and [5]. Due to their importance, we present the formulae of several Wiener values for some Caterpillars. In particular, we found that the Wiener values, as sequences, of these Caterpillars which contain exactly one vertex of degree greater than 2 do not currently exist in the largest Online Encyclopedia of Integer Sequences (OEIS) [10]. We hope to submit these values and their formulae for the record.

It is easy to see that, for any complete graph K_n, $W(K_n) = \binom{n}{2}$. Further, it is well-known that the Wiener indices of a star graph S_n and a path graph P_n are $(n-1)^2$ and $\dfrac{(n-1)n(n+1)}{6}$, respectively. See [1] and [5], for instance. Further, it is shown [4] that, for any tree T on n vertices, $W(S_n) < W(T) < W(P_n)$.

As an example for finding Wiener indices, we present a proof for the Wiener index of a path, after the next proposition.

Proposition 1. $\displaystyle\sum_{j=2}^{n} \binom{j}{2} = \binom{n+1}{3}$ *holds for all* $n \geq 2$

Proof. The case when $n = 2$ is trivial. Let's assume for all $k \geq 2$,

$\sum_{j=2}^{k}\binom{j}{2}=\binom{k+1}{3}$. It follows that

$$\begin{aligned}\sum_{j=2}^{k+1}\binom{j}{2} &= \sum_{j=2}^{k}\binom{j}{2}+\binom{k+1}{2}\\ &= \binom{k+1}{3}+\binom{k+1}{2}\\ &= \binom{k+2}{3}.\end{aligned}$$

Hence the result by induction.

□

Corollary 1. *The Wiener index of a path P_n is $W(P_n)=\binom{n+1}{3}$, $n \geq 2$.*

Proof. Suppose the vertices of the path are $v_1, v_2, \ldots, v_n$. We proceed to add the distances between v_i, v_j, for each $i \neq j$. As such, we compute $\sum_{j>i}^{n} d(v_i, v_j)$ which is equal to $\binom{n-i+1}{2}$, for each i, with $1 \leq i \leq n$. Now,

$$\begin{aligned}W(P_n) &= \sum_{i=1}^{n-1}\sum_{j>i}^{n} d(v_i, v_j)\\ &= \sum_{i=1}^{n-1}\binom{n-i+1}{2}\\ &= \sum_{j=2}^{n}\binom{j}{2},\end{aligned}$$

for all $n \geq 2$. The result follows from Proposition 1.

Alternatively, given the n^{th} triangular number T_n, we have

$$\begin{aligned}
W(P_n) = \sum_{j=1}^{n-1} T_j &= \sum_{j=1}^{n-1} \frac{j(j+1)}{2} \\
&= \frac{1}{2}\left(\sum_{i=1}^{n-1} j^2 + \sum_{i=1}^{n-1} j\right) \\
&= \frac{1}{2}\left(\frac{n(n-1)[2(n-1)+1]}{6} + \frac{n(n-1)}{2}\right) \\
&= \frac{(n-1)n(n+1)}{6} \\
&= \binom{n+1}{3}.
\end{aligned}$$

□

Remark 1.

Recall that, the n^{th} *rising factorial* and the n^{th} *falling factorial* denoted respectively by $x^{\overline{n}}$ and $x^{\underline{n}}$, are $x^{\overline{n}} = x(x+1)(x+2)\cdots(x+n-1) = \prod_{k=1}^{n}(x+k-1) = \prod_{k=0}^{n-1}(x+k)$ and $x^{\underline{n}} = x(x-1)(x-2)\cdots(x-n+1) = \prod_{k=1}^{n}(x-k+1) = \prod_{k=0}^{n-1}(x+k)$. Although the previous result (and upcoming ones) can be written in either format, i.e., $W(P_n) = \frac{(n-1)^{\overline{3}}}{3!} = \frac{(n+1)^{\underline{3}}}{3!}$, it is beyond the interest of this article.

2 Wiener index of Comb graphs

Suppose $P_n := v_1 - v_2 - \ldots - v_{n-1} - v_n$ denotes a path on $n \geq 3$ vertices. By sequentially connecting a single leaf to each vertex v_i, with $2 \leq i \leq n-1$, we obtain a *Complete Caterpillar* P_n^{n-2} which is commonly known as a *Comb* or a *Centipede*. Figure 2 is an example.

For the next result, we define the following: Suppose $G = (V, E)$ denotes a graph with an ordered list of vertices $(v_1, v_2, \ldots, v_n)$. We

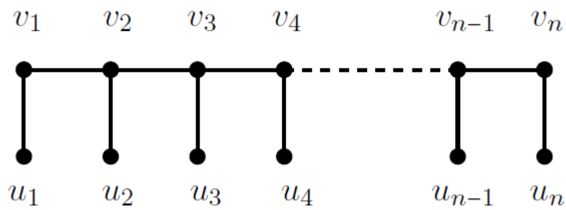

Figure 1. Comb graph on $2n$ vertices

denote and define the s^{th} *partial Wiener (index)* of G by $W^s(G)$ and $W^s(G) = \sum_{j>s} d(v_s, v_j)$, respectively. Thus, the 1^{st} *Partial Wiener (index)* of G is the sum of the distances between v_1 and any other vertex $v_j \in V$, $j > 1$. The special case when $G = K_2$, $W^1(G) = 1 = W(G)$.

Lemma 1. *Suppose G is any graph with an ordered list of vertices $(v_1, v_2, \ldots, v_n)$. It follows that* $W(G) = \sum_{k=1}^{n-1} \sum_{j>s} d(v_s, v_j)$.

Proof. From the definitions of s^{th} partial Wiener and the (full) Wiener index of G, it follows that $W(G) = \sum_{s=1}^{n-1} W^s(G)$, giving the result. $\square$

Theorem 2. *Suppose G^n denotes a Comb on $2n$ vertices. Then* $W(G^n) = \dfrac{n(2n^2+6n-5)}{3}$ *for all $n \geq 1$.*

Proof. Let $G^1 := u_1 - v_1$, a path on 2 vertices. We add two pendant vertices u_2, v_2, such that u_2 is adjacent to v_2 and v_2 is adjacent to v_1. The resulting graph is a Comb, denoted by G^2, which is isomorphic to P_4. Thus, $W^1(G^1) = d(u_1, v_1) = T_1$ and $W^2(G^1) = T_0$ since $W^2(G^1) = W^1(G^1 \setminus \{u_1\})$. Further, $W^1(G^2) = \sum_{w \in V(G^2)} d(u_2, w) = T_3$ and $W^2(G^2) = \sum_{w \in V(G^2)} d(u_2, w) = T_2$. So, when $G = P_4$, by definition of partial Wieners,

$$\begin{aligned} W(G) &= W^1(G^1) + W^2(G^1) + W^1(G^2) + W^2(G^2) \\ &= T_0 + T_1 + T_2 + T_3 \\ &= 10. \end{aligned}$$

Iteratively, for each $k \geq 1$, we form G^k from a previously formed Comb G^{k-1}, by adding the pair of vertices (u_k, v_k) such that u_k is adjacent to v_k and v_k is adjacent to $v_{k-1} \in V(G^{k-1})$. Thus, the vertices of G^k can be seen as the ordered list $(u_1, v_1, u_2, v_2, \ldots, u_k, v_k)$. With each such pair $(u_k, v_k) \notin V(G^{k-1})$ we compute and add the first and second partial Wieners of G^k, $k \geq 3$. So, given u_k, $W^1(G^k) = \sum_{w \in V(G^k)} d(u_k, w)$. Because $d(u_k, u_{k-1}) = T_3$ and $d(u_k, u_1) = T_{k+1}$, for all $k \geq 2$, it follows that

$$\begin{aligned} W^1(G^k) &= T_3 + \sum_{j=1}^{k-2} (T_{3+j} - T_{1+j}) \\ &= (T_{k+1} - T_{k-1}) + (T_k - T_{k-2}) + \ldots + (T_5 - T_3) + \\ &\quad +(T_4 - T_2) + T_3 \\ &= T_{k+1} + T_k - T_2, \ k \geq 3. \end{aligned}$$

Similarly, given (u_k, v_k), we compute the second partial Wieners of G^k, i.e., $W^2(G^k) = \sum_{w \in V(G^k)} d(v_k, w)$. Because $d(v_k, u_{k-1}) = T_2$ and $d(v_k, u_1) = T_k$, for all $k \geq 3$, it follows that

$$\begin{aligned} W^2(G^k) &= T_2 + \sum_{j=1}^{k-2} (T_{2+j} - T_j) \\ &= (T_k - T_{k-2}) + (T_{k-1} - T_{k-3}) + \ldots + (T_4 - T_2) + \\ &\quad +(T_3 - T_1) + T_2 \\ &= T_k + T_{k-1} - T_1, \ k \geq 3. \end{aligned}$$

Therefore, for all $n \geq 1$,

$$\begin{aligned}
W(G) &= \sum_{k=1}^{n} W^1(G^k) + \sum_{k=1}^{n} W^2(G^k) \\
&= \sum_{k=1}^{2} W^1(G^k) + \sum_{k=1}^{2} W^2(G^k) + \sum_{k=3}^{n} W^1(G^k) + \sum_{k=3}^{n} W^2(G^k) \\
&= T_1 + T_2 + T_3 + \sum_{k=3}^{n} W^1(G^k) + \sum_{k=3}^{n} W^2(G^k) \\
&= T_1 + T_2 + T_3 + \sum_{k=3}^{n} (T_{k+1} + 2T_k + T_{k-1} - T_2 - T_1) \\
&= T_1 + T_2 + T_3 + \sum_{k=3}^{n} (T_{k+1} + 2T_k + T_{k-1}) - \sum_{k=3}^{n} (T_2 + T_1)\,.
\end{aligned}$$

Thus, we have

$$\begin{aligned}
W(G) &= T_1 + T_2 + T_3 + \sum_{k=1}^{n+1} T_k + 2\sum_{k=1}^{n} T_k \\
&+ \sum_{k=1}^{n-1} T_k - \left(\sum_{k=1}^{3} T_k + 2\sum_{k=1}^{2} T_k + T_1 \right) - (n-2)(T_2 + T_1) \\
&= 3T_n + T_{n+1} + 4\sum_{k=1}^{n-1} T_k - (4n+1) \\
&= \frac{3n(n+1)}{2} + \frac{(n+1)(n+2)}{2} + 2n(n-1) - 4n - 1 \\
&= \frac{2n^3}{3} + 2n^2 - \frac{5n}{3},
\end{aligned}$$

giving the result for all $n \geq 1$. □

Here, in Table 2, we present the first ten values of the Wiener of Combs. We note that Emeric Deutsch had submitted (in 2011) this formula to OEIS as **A192023** [10] and yet, we have no record of the proof of the result.

Table 1. The first ten values of the Wiener of a Comb graph on $2n$ vertices

n	1	2	3	4	5	6	7	8
$\frac{2n^3}{3} + 2n^2 - \frac{5n}{3}$	1	10	31	68	125	206	315	456

3 Wiener Index of Brooms

A Caterpillar that is obtained by adding $k \geq 1$ pendant vertices to the first (or last) internal vertex of P_n is called a *Broom*. We denote it as B_n^k. The graphs generated in the special cases when $k = 1$ and $k = 2$ are called, respectively, *Sling* and *Tridon*. Figure 2 shows a Tridon.

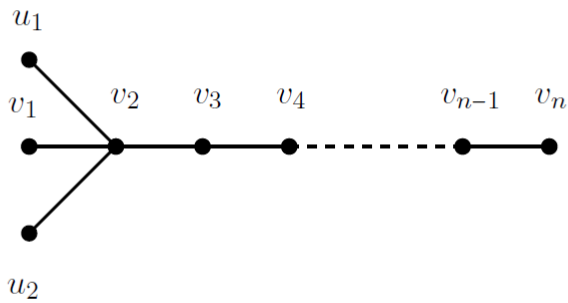

Figure 2. A Tridon B_n^2 on $n + 2$ vertices

Theorem 3. *Suppose B_n^k denotes a Broom on $n + k$ vertices. Then $W(B_n^k) = 2T_k + kT_{n-1} + W(P_n)$ for all $n \geq 3$, $k \geq 1$.*

Proof. Let T_n denote the n^{th} triangular number and u_i, $i = 1 \ldots, k$, the pendant vertices. Consider a main path P_n, for $n \geq 3$, giving $W(P_n)$. With each additional pendant vertex u_i connected to $v_2 \in P_n$, we have $d(u_i, v) = T_{n-1}$, for each $v \in P_n$ and $v \neq v_1$. This gives $\sum_{j=1}^{k} T_{n-1}$ for each u_i, $i = 1, \ldots, k$. Finally $d(u_i, v_1) = 2 = d(u_i, u_j)$ with $i \neq j$, giving $\sum_{j=1}^{k} 2j$. Together, we have

$$\begin{aligned} W(B_n^k) &= \sum_{j=1}^{k} 2j + \sum_{j=1}^{k} T_{n-1} + W(P_n) \\ &= 2\sum_{j=1}^{k} j + \sum_{j=1}^{k} T_{n-1} + W(P_n) \\ &= 2T_k + kT_{n-1} + W(P_n), \end{aligned}$$

giving the result. □

Corollary 2. *If B_n^n denotes a Broom on $2n$ vertices of which $n+2$ are pendant, then $W(B_n^n) = \frac{2n^3}{3} + \frac{n^2}{2} + \frac{5n}{6}$, for all $n \geq 3$ vertices.*

Proof. From Theorem 3 when $k = n$, there are exactly $n + 2$ pendant vertices and we have

$$\begin{aligned} W(B_n^1) &= 2T_n + nT_{n-1} + W(P_n) \\ &= n(n+1) + \frac{n^2(n-1)}{2} + \frac{(n+1)n(n-1)}{6} \\ &= \frac{2n^3}{3} + \frac{n^2}{2} + \frac{5n}{6}. \end{aligned}$$

□

This formula and several of its values are submitted and they are approved in OEIS [10] as **A349416**. In Table 3, we list the first ten values.

Corollary 3. *If B_n^1 denotes a Sling graph, then $W(B_n^1) = \frac{n^3}{6} + \frac{n^2}{2} - \frac{2n}{3} + 2$, for all $n \geq 3$ vertices.*

Table 2. The first eight values of the Wiener of a Broom graph on $2n$ vertices (of which $n+2$ are pendant)

n	3	4	5	6	7	8	9	10
$\frac{2n^3}{3}+\frac{n^2}{2}+\frac{5n}{6}$	25	54	100	167	259	380	534	725

Proof. By definition, a Sling is a Broom on $k=1$ pendant vertex. So, when $k=1$, the result in Theorem 3 becomes

$$\begin{aligned} W(B_n^1) &= 2T_1 + T_{n-1} + W(P_n) \\ &= 2 + \frac{(n-1)n}{2} + W(P_n) \\ &= 2 + \frac{n(n-1)}{2} + \frac{(n+1)n(n-1)}{6} \\ &= \frac{n^3}{6} + \frac{n^2}{2} - \frac{2n}{3} + 2. \end{aligned}$$

□

This formula is now approved in OIES as **A349417**. We found later that such values are also equivalent to the sequence **A005581**+2 which carries many combinatorics and algebraic meanings. For instance, **A005581** gives the number of inscribable triangles within a $(n+4)$-gon sharing with them its vertices but not its sides, according to Lekraj Beedassy [10].

In Table 3, we present the first ten values of the Wiener index of a Sling.

Table 3. The first eight values of the Wiener of a Sling graph on $n+1$ vertices

n	3	4	5	6	7	8	9	10
$\frac{n^3}{6}+\frac{n^2}{2}-\frac{2n}{3}+2$	9	18	32	52	79	114	158	212

Corollary 4. *If B_n^2 is a Tridon graph, then* $W(B_n^2) = \frac{n^3}{6} + n^2 - \frac{7n}{6} + 6$ *for all* $n \geq 3$.

Proof. By definition, we obtain the Wiener value of a Tridon from Theorem 3, when $k = 2$, in which we have

$$\begin{aligned} W(B_n^2) &= 2T_2 + 2T_{n-1} + W(P_n) \\ &= 6 + 2\frac{(n-1)n}{2} + W(P_n) \\ &= 6 + n(n-1) + \frac{(n+1)n(n-1)}{6} \\ &= \frac{n^3}{6} + n^2 - \frac{7n}{6} + 6 \end{aligned}$$

after an expansion. □

This formula and several of its values are submitted and they are approved in OEIS [10] as **A349418** .Table 3 shows the first ten values.

Table 4. The first eight values of the Wiener of a Tridon graph on $n+2$ vertices

n	3	4	5	6	7	8	9	10
$\frac{n^3}{6} + n^2 - \frac{7n}{6} + 6$	16	28	46	71	104	146	198	261

4 Wiener index of 2-Extended Brooms

Here, we present a generalization of Brooms, by extending the original definition from adding pendant vertices to adding paths. Suppose $P_n := v_1 - v_2 - \ldots - v_{n-1} - v_n$ denotes a path on $n \geq 3$ vertices. By sequentially adding some path graph P'_m, on $m \geq 1$ vertices to some v_i, $2 \leq i \leq n-1$, we obtain an m-Extended Broom which we denote by $B_n^k(m)$. The special case when $m = 1$ is a (regular) Broom, i.e., $B_n^k(1) = B_n^k$. Here, we present the case when $m = 2$.

For the upcoming result, for simplicity, let $G^k = B_n^k(2)$ denote a 2-Extended Broom obtained by adding $k \geq 1$ $P_k' := u_{1k} - u_{2k}$ to $v_2 \in P_n$, for $k \geq 1$. See Figure 3 for the case when $k = 2$.

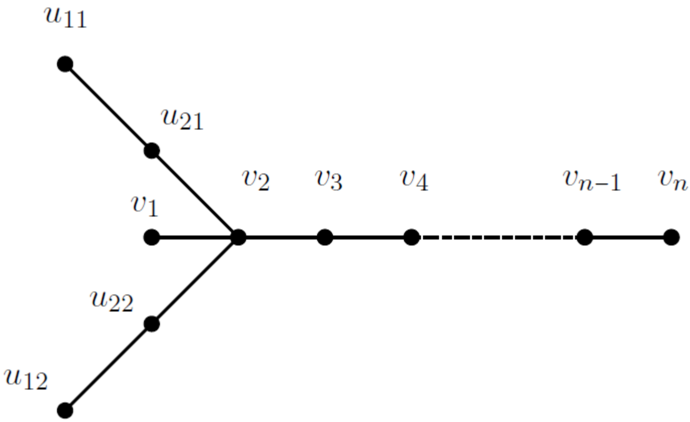

Figure 3. A 2-Extended Broom

Theorem 4. *The Wiener index of a 2-Extended Broom G^k is given by $W(G^k) = \frac{1}{6}n^3 - \frac{1}{6}n + n^2k + 6k^2 - k$ with $n \geq 3$ and $k \geq 1$.*

Proof. Consider the main path, P_n. Now, we sequentially add $P_k' := u_{1k} - u_{2k}$ to $v_2 \in P_n$, for $k \geq 1$. Knowing $W(P_n)$, we proceed to add the values of $d(u_{1k}, v)$ and $d(u_{2k}, v)$, for each $v \in P_n$ and $k \geq 1$.

Observe that $\sum_{x_k} d(u_{1k}, x_k) = T_n$ and $\sum_{y} d(u_{2k}, y) = T_{n-1}$ for every $x_k \in \{u_{2k}, v_2, v_3, \ldots, v_n\}$ and $y \in \{v_2, v_3, \ldots, v_n\}$. Further, $d(u_{1k}, v_1) = 3$ and $d(u_{2k}, v_1) = 2$.

Thus, when $k = 1$, we have

$$\begin{aligned} W(G^1) &= W(P_n) + \\ &\quad + \sum_{x_1} d(u_{11}, x_1) + \sum_{y} d(u_{21}, y) + d(u_{11}, v_1) + d(u_{21}, v_1) \\ &= W(P_n) + T_n + T_{n-1} + 2(1) + 3(1). \end{aligned}$$

When $k = 2$. We have $d(u_{12}, v_1) = 3 = d(u_{12}, u_{21})$, $d(u_{22}, v_1) = 2 = d(u_{22}, u_{21})$, and $d(u_{12}, u_{11}) = 4$, $d(u_{22}, u_{11}) = 3$. Together, with $\sum_{x_2} d(u_{12}, x_2) + \sum_{y} d(u_{22}, y)$ for every $x_2 \in \{u_{22}, v_2, v_3, \ldots, v_n\}$ and $y \in \{v_2, v_3, \ldots, v_n\}$, we have

$$W(G^2) = W(G^1)+ \\ + \sum_{x_2} d(u_{12}, x_2) + \sum_{y} d(u_{22}, y) + 2(2) + 3(2) + (3 + 4).$$

Similarly, when $k = 3$, we obtain

$$W(G^3) = W(G^1) + W(G^2) + \sum_{x_3} d(u_{13}, x_3) + \sum_{y} d(u_{23}, y) + 2(3)+ \\ + 3(3) + 7(2).$$

Thus, for all $k \geq 1$, we obtain recursively that,

$$\begin{aligned} W(G^k) = &\sum_{i=1}^{k-1} W(G^i) + \sum_{x_k} d(u_{1k}, x_k) + \sum_{y} d(u_{2k}, y) + 2\left(\sum_{i=1}^{k} i\right) \\ &+ 3\left(\sum_{i=1}^{k} i\right) + 7\left(\sum_{i=1}^{k-1} i\right) \\ &= W(P_n) + kT_n + kT_{n-1} + 2T_k + 3T_k + 7T_{k-1} \\ &= W(P_n) + k(T_n + T_{n-1}) + 5T_k + 7T_{k-1}. \end{aligned}$$

Since $W(P_n) = \dfrac{(n+1)n(n-1)}{6}$ and $T_j = \dfrac{j(j+1)}{2}$, the result follows after expansion. □

In the next two corollaries, we present two extremal cases; when $k = n$ and when $k = 1$. Both cases follow directly from the previous theorem. We present the first ten values for each case and we point out that neither sequence currently exists in OEIS [10].

Corollary 5. *The Wiener index of a 2-Extended Broom G^n on $3n$ vertices is given by* $W(G^n) = \dfrac{7}{6}n^3 + 6n^2 - \dfrac{7n}{6}$ *with* $n \geq 3$.

Table 5. The first eight values of a 2-Extended Broom G^n on $3n$ vertices

n	3	4	5	6	7	8	9	10
$\frac{7}{6}n^3 + 6n^2 - \frac{7n}{6}$	82	166	290	461	686	972	1326	1755

Table 5 shows some of the values of $W(G^n)$.

Corollary 6. *The Wiener index of a 2-Extended Broom G^1 on $n+2$ vertices is given by* $W(G^1) = \frac{1}{6}n^3 + n^2 - \frac{1}{6}n + 5$ *with* $n \geq 3$.

Table 6 shows some of the values of $W(G^1)$.

Table 6. The first eight values of a 2-Extended Broom G^1 on $n+2$ vertices

n	3	4	5	6	7	8	9	10
$\frac{1}{6}n^3 + n^2 - \frac{1}{6}n + 5$	18	31	50	76	110	153	206	270

References

[1] D. Bonchev and N. Trinajstić, "Information theory, distance matrix, and molecular branching," *Journal of Chemical Physics*, vol. 67, no. 10, pp. 4517-–4533, 1977.

[2] E. R. Canfield, R. W.Robinson, and D. H. Rouvray, "Determination of the Wiener molecular branching index for the general tree," *J. Comput. Chem.*, vol. 6, pp. 598–609, 1985.

[3] A. Coja-Oghlan, S.O. Krumke, and T. Nierhoff, "Scheduling a server on a caterpillar network—a probabilistic analysis," in *6^th Workshop on Models and Algorithms for Planning and Scheduling Problems*, (France), pp. 48–50, 2003.

[4] A.A. Dobrynin, R. Entringer, and I. Gutman, "Wiener Index for trees: Theory and Applications," *Acta Appl. Math.*, vol. 66, pp. 211–249, 2001. DOI: https://doi.org/10.1023/A:1010767517079.

[5] S. El-Basil, "Caterpillar (Gutman) trees in chemical graph theory," *Topics in Current Chemistry*, vol. 153, pp. 273–289, 1990.

[6] D. Papazova, M. Dimov, and D. Bonchev, "Calculation of gas chromatographic retention indices of isoalkanes based on a topological approach," *Journal of Chromatography*, vol. 188, no. 2, pp. 297–303, 1980.

[7] D. H. Rouvray and R. B. King, *Topology in Chemistry: Discrete Mathematics of Molecules*, Horwood Publishing Ltd., Chichester, 2002, pp. 89–112.

[8] D. H. Rouvray and B. C. Crafford, "The dependence of physicochemical properties on topological factors," *South African Journal of Science*, vol. 72, pp. 47–51, 1976.

[9] D. H. Rouvray and W. Tatong, "Novel applications of topological indices," *Zeitschriftf ür Naturforschung*, vol. 41, pp. 1238–1244, 1986.

[10] N. J. A. Sloane et al., *The On-Line Encyclopedia of Integer Sequences*, [Online]. Available: `https://oeis.org`, Accessed on: November 2021.

[11] L. I. Stiel and G. Odos, "The normal boiling points and critical constants of saturated aliphatic hydrocarbons," *American Institute of Chemical Engineers*, vol. 8, no. 4, Article ID 5276529, 1962.

[12] H. Wiener, "Structural determination of paraffin boiling points," *J. Amer. Chem. Soc.*, vol. 69, pp. 17–20, 1947.

Julian D. Allagan

Received May 30, 2022
Accepted June 02, 2022

Julian Allagan
Elizabeth City State University
Elizabeth City, North Carolina, U.S.A
E–mail: `adallagan@ecsu.edu`