MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **88** (2022) 461–470
ISSN: 0340–6253
doi: 10.46793/match.88-2.461D

Wiener Index of Families of Unicyclic Graphs Obtained From a Tree

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(Received April 1, 2022)

Abstract

The Wiener index $W(G)$ of a graph G is the sum of distances between all vertices of G. The Wiener index of a family $\mathcal{G}$ of connected graphs is defined as the sum of the Wiener indices of its members, $W(\mathcal{G}) = \sum_{G\in\mathcal{G}} W(G)$. Let U_e be a unicyclic graph obtained by replacing an edge e of a tree T with a fixed length cycle. A simple relation between Wiener indices of the family $\{U_e \,|\, e \in E(T)\}$ and a tree T is presented for certain positions of the cycle.

1 Introduction

In this article, all graphs are undirected, connected, without loops or multiple edges. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The cardinality of $V(G)$ is called the *order* of the graph G and is denoted by n_G. The *distance* $d_G(u, v)$ between vertices u and v of G is the number of edges in a shortest path connecting them. The distance of a vertex v of a graph G is the sum of distances from v to all vertices of the graph, $d_G(v) = \sum_{u\in V(G)} d_G(v, u)$. The *Wiener index* of a graph G is a distance-based topological index introduced as structural descriptor for acyclic organic molecules [20]:

$$W(G)=\sum_{u,v\in V(G)} d(u,v)=\frac{1}{2}\sum_{v\in V(G)} d_G(v).$$

It has found numerous applications in organic chemistry and related fields (see selected books [1, 14, 16, 17, 19] and reviews [2, 9, 11, 15, 18]).

In this paper, we study the Wiener index of families of graphs which may arise as the result of structural transformations of a given graph. For example, attaching a cycle to tree vertices generates a family of unicyclic graphs. The Wiener index of a family $\mathcal{G}=\{G_1,G_2,\ldots,G_r\}$ of connected graphs is defined as the sum of the Wiener indices of its members,

$$W(\mathcal{G})=W(G_1)+W(G_2)+\cdots+W(G_r).$$

In this case, values of $W(\mathcal{G})$ depend on the structures of several graphs. It is clear that if all graphs of a family $\mathcal{G}$ are isomorphic to the simple path or the complete graph of order n, then $W(\mathcal{G})$ takes extremal values among all families of cardinality r with n-vertex graphs. Properties of the Wiener index for some families of acyclic structures and benzenoid graphs were studied in [3–8, 10].

Denote by P_n and C_n the simple path and the simple cycle of order n, respectively. In is known that $W(P_n)=n(n^2-1)/6$, $d_{C_n}(v)=n^2/4$ and $W(C_n)=n^3/8$ for even n, $d_{C_n}(v)=(n^2-1)/4$ and $W(C_n)=n(n^2-1)/8$ for odd n [13]. The edge k-subdivision of an edge $e\in E(G)$ is the graph G_e constructed by replacing e with path $P_{k+2}=(v_1,v_2,\ldots,v_k)$ in a graph G. Vertices v_i, $i=1,2,\ldots k$, are called the *subdivision vertices* of e.

Let U_e be a unicyclic graph obtained by replacing edge $e=(u,v)$ of a tree T of order n with a cycle of length c and let $\mathcal{U}_c=\{U_e\,|\,e\in E(T)\}$. In general case, the calculating formula for the Wiener index $W(U_e)$ should include the distance of vertices u and v in T. It is shown that the Wiener index of the family $\mathcal{U}_c$ can be expressed in terms of $W(T)$ for certain positions of the cycle. This also allows the finding the average value of the Wiener index of graphs in $\mathcal{U}_c$.

2 Main result

Let $T_{e,k}$ and $T_{e,m}$ be trees obtained by k- and m-subdivision an edge e of a tree T, respectively. Then the process of replacing the edge e with cycle C_{k+m+2} can be represented as a join of $T_{e,k}$ and $T_{e,m}$ as shown in Fig. 1. Namely, the corresponding vertices of the trees are identified with the exception of the subdivision vertices. We calculate the Wiener index of the resulting graph U_e through distance characteristics of $T_{e,k}$ and $T_{e,m}$.

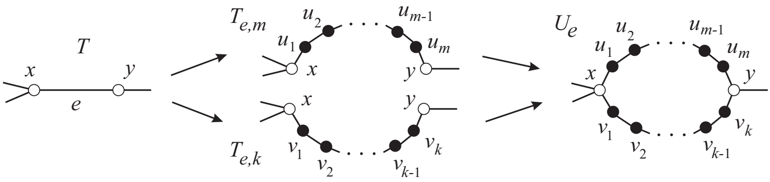

Figure 1. Replacing an edge e of a tree T with cycle C_{k+m+2}.

The following two lemmas are useful for computing the Wiener index of families of trees obtained by edge subdivisions [6].

Lemma 1. *For k-subdivisions $T_{e_1}, T_{e_2}, \ldots, T_{e_{n-1}}$ of edges $e_1, e_2, \ldots, e_{n-1}$ of a tree T of order n,*

$$\begin{aligned} & W(T_{e_1}) + W(T_{e_2}) + \cdots + W(T_{e_{n-1}}) = \\ & = \quad (3k+n-1)W(T) + (n-1)\binom{k+1}{3} + 2\binom{k}{2}\binom{n}{2}. \end{aligned}$$

The next result shows that the distances of all subdivision vertices can be expressed through the Wiener index of the initial tree.

Lemma 2. *For subdivision vertices $v_1, v_2, \ldots, v_k$ of k-subdivision of edges $e_1, e_2, \ldots, e_{n-1}$ of an n-vertex tree T,*

$$\sum_{i=1}^{n-1} \big(d_{T_{e_i}}(v_1) + \cdots + d_{T_{e_i}}(v_k) \big) = 2k\, W(T) + \frac{1}{6}\, k(k-1)(n-1)(2k+3n+2).$$

Let the family $\mathcal{U}_{k+m+2} = \{U_e \,|\, e \in E(T)\}$ be obtained from an arbitrary tree T as described above. Then there is a simple relation between quantities $W(\mathcal{U}_{k+m+2})$ and $W(T)$ for certain positions of cycle C_{k+m+2}.

Theorem 1. *For the Wiener index of the family* $\mathcal{U}_{k+m+2}$*,* $k \le m \le k+2$*,*

$$W(\mathcal{U}_{k+m+2}) = (n + 2k + 3m - 1)W(T) + \\ + \frac{1}{8}(n-1)\left[\,4n\left[\,k(k-1) + m(m-1)\,\right] + (k+m)^2(k+m+2) + \phi\,\right],$$

where $\phi = 4(k-m)$ *if* $k+m$ *is even, and* $\phi = 3k - 5m + 2$ *if* $k+m$ *is odd.*

Proof. Consider an arbitrary tree T of order n. Let U_e be a unicyclic graph obtained by replacing an edge $e = (x, y)$ of T with cycle C_{k+m+2}, where $k \ge 0$ and $m \ge k$. To apply Lemmas 1 and 2, graph U_e is constructed as follows. First, k- and m-subdivisions are applied to the edge e in two copies of the tree T. Further, the corresponding vertices of the resulting trees $T_{e,k}$ and $T_{e,m}$ are identified as depicted in Fig. 1. Since $k \le m$, it is obvious that $d_{U_e}(v) = d_{T_{e,k}}(v)$ for all $v \in V(U_e) \setminus \{u_1, u_2, \ldots, u_m\}$. Since $m \le k+2$, the length of path $(u_1, u_2, \ldots, u_m, y)$ does not exceed the length of path $(u_1, x, v_1, v_2, \ldots, v_k, y)$ and, therefore, $d_{U_e}(u_i) = d_{T_{e,m}}(u_i)$ for all $i = 1, 2, \ldots, m$. Then

$$\begin{aligned} W(U_e) &= W(T_{e,k}) + \sum_{i=1}^{m} d_{U_e}(u_i) - W(P_m) + \sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j) \\ &= W(T_{e,k}) + \sum_{i=1}^{m} d_{T_{e,m}}(u_i) - W(P_m) + \sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j). \qquad (1) \end{aligned}$$

The last term of equation (1) can be easily calculated through the Wiener index of cycle C_{k+m+2} as follows:

$$\begin{aligned} \sum_{i=1}^{m}\sum_{j=1}^{k} d_{U_e}(u_i, v_j) &= W(C_{k+m+2}) - \sum_{i<j}^{m} d_{P_m}(u_i, u_j) - \sum_{i<j}^{k} d_{P_k}(v_i, v_j) \\ &\quad - d_{C_{k+m+2}}(x) - d_{C_{k+m+2}}(y) + d_{U_e}(x, y) \\ &= W(C_{k+m+2}) - W(P_m) - W(P_k) \\ &\quad - d_{C_{k+m+2}}(x) - d_{C_{k+m+2}}(y) + (k+1). \end{aligned}$$

Summing equation (1) for all edges $e \in E(T)$, we have

$$\begin{aligned} W(\mathcal{U}_{k+m+2}) &= \sum_{e\in E(T)} W(U_e) = \sum_{e\in E(T)} W(T_{e,k}) + \sum_{e\in E(T)} \sum_{i=1}^{m} d_{T_{e,m}}(u_i) \\ &- (n-1)W(P_m) + (n-1)\,[\,W(C_{k+m+2}) - W(P_m) \\ &- W(P_k) - 2d_{C_{k+m+2}}(x) + (k+1)\,]. \end{aligned}$$

Substitution expressions from Lemmas 1 and 2 into this equality completes the proof. ■

Graphs of the family $\mathcal{U}_{k+m+2}$ are relevant to chemical unicyclic structures when m and k are both small. Examples of such graphs will be considered in the subsequent sections.

Denote by $W_{\rm avr}(\mathcal{U})$ the average value of the Wiener index of unicyclic graphs in a family $\mathcal{U}$, i.e. $W_{\rm avr}(\mathcal{U}) = W(\mathcal{U})/|\,\mathcal{U}\,|$. Theorem 1 shows that $W_{\rm avr}(\mathcal{U})$ can be calculated in terms of the characteristics of the initial tree and parameters of a given cycle. In general case, quantity $W_{\rm avr}(\mathcal{U})$ may be a fractional number or the realization of integer $W_{\rm avr}(\mathcal{U})$ by graphs may not exists. Obviously, a family $\mathcal{U}$ obtained from the star contains graphs G with $W(G) = W_{\rm avr}(\mathcal{U})$.

3 Odd cycles

If edges of a tree are replaced by an odd cycle ($k+m$ is odd), then $m = k+1$, $k \geq 0$. Since $T_{e,0}$ coincides with T, triangles arise in unicyclic graphs when $k = 0$. We have only one suitable way of inserting an odd cycle.

Corollary 1. *Let a family of unicyclic graphs $\mathcal{U}_{2k+3}$ be obtained from a tree T of order n by replacing its edges with odd cycle C_{2k+3}, $k \geq 0$. Then*

$$W(\mathcal{U}_{2k+3}) = (5k+n+1)W(T) + \frac{1}{2}(n-1)k(2nk+2k^2+5k+3),$$

and the average value of the Wiener index of graphs of the family is

$$W_{\rm avr}(\mathcal{U}_{2k+3}) = \left(1 + \frac{5k+2}{n-1}\right) W(T) + \frac{1}{2}\,k(2nk+2k^2+5k+3).$$

The last equation may be useful for estimating how the Wiener index changes on average under such edge cyclization. Quantity $W_{\rm avr}(\mathcal{U}_{2k+3})$ is integer if $W(T)$ or $5k+2$ are divisible by $n-1$. For instance, $W_{\rm avr}(\mathcal{U}_{2k+3})$ is integer if a tree T has order 8 and cycles have length 5. For small cycles, expressions of Corollary 1 have a simple form.

Corollary 2. *For the families of unicyclic graphs with 3-, 5- or 7-membered cycles,*

$$\begin{aligned} W(\mathcal{U}_3) &= (n+1)W(T), \\ W(\mathcal{U}_5) &= (n+6)W(T) + (n-1)(n+5), \\ W(\mathcal{U}_7) &= (n+11)W(T) + (n-1)(4n+21), \end{aligned}$$

and the average values of the Wiener index of unicyclic graphs are

$$\begin{aligned} W_{\rm avr}(\mathcal{U}_3) &= \left(1+\frac{2}{n-1}\right)W(T), \\ W_{\rm avr}(\mathcal{U}_5) &= \left(1+\frac{7}{n-1}\right)W(T) + n + 5, \\ W_{\rm avr}(\mathcal{U}_7) &= \left(1+\frac{12}{n-1}\right)W(T) + 4n + 21. \end{aligned}$$

For unicyclic graphs with triangles, $W_{\rm avr}(\mathcal{U}_3) \to W(T)$ if $n \to \infty$. As an illustration, consider families of unicyclic graphs with cycles of length 3, 5, and 7 shown in Fig. 2. Wiener indices are indicated near graph diagrams. By Corollary 2, $W(\mathcal{U}_3) = 7 \cdot 32 = 224$, $W(\mathcal{U}_5) = 12 \cdot 32 + 55 = 439$, and $W(\mathcal{U}_7) = 17 \cdot 32 + 225 = 769$. All average values are fractional.

4 Even cycles

If edges of a tree are replaced by an even cycle ($k+m$ is even), then k and m are both even or odd, $k \geq 0$. Therefore, even cycles can be suitably inserted when $m \in \{k, k+2\}$.

Corollary 3. *Let a family of unicyclic graphs $\mathcal{U}_{k+m+2}$ be obtained from a tree T of order n by replacing its edges with even cycle C_{m+k+2}.*

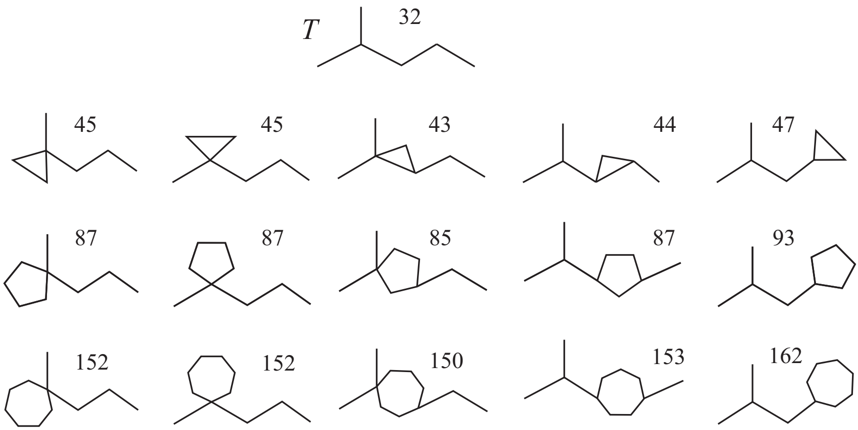

Figure 2. Families of graphs with 3-, 5- and 7-membered cycles.

Then for $m = k \geq 1$,

$$W(\mathcal{U}_{2k+2}) = (n + 5k - 1)W(T) + (n - 1)k\,[\,n(k - 1) + k(k + 1)\,],$$

and for $m = k + 2 \geq 0$,

$$W(\mathcal{U}_{2k+4}) = (n + 5k + 5)W(T) + \\ + (n - 1)[\,n(k^2 + k + 1) + (k + 1)^2(k + 2) - 1\,],$$

and the average values of the Wiener index of unicyclic graphs are

$$W_{\mathrm{avr}}(\mathcal{U}_{2k+2}) = \left(1 + \frac{5k}{n-1}\right) W(T) + k\,[\,n(k - 1) + k(k + 1)\,],$$

$$W_{\mathrm{avr}}(\mathcal{U}_{2k+4}) = \left(1 + \frac{5k+6}{n-1}\right) W(T) + n(k^2 + k + 1) + (k + 1)^2(k + 2) - 1.$$

If $m = k$, then cycles have length 4, 6, 8, etc. If $m = k + 2$, then odd k gives cycles of length 6, 10, 14, etc., while even k gives cycles of length 4, 8, 12, etc.

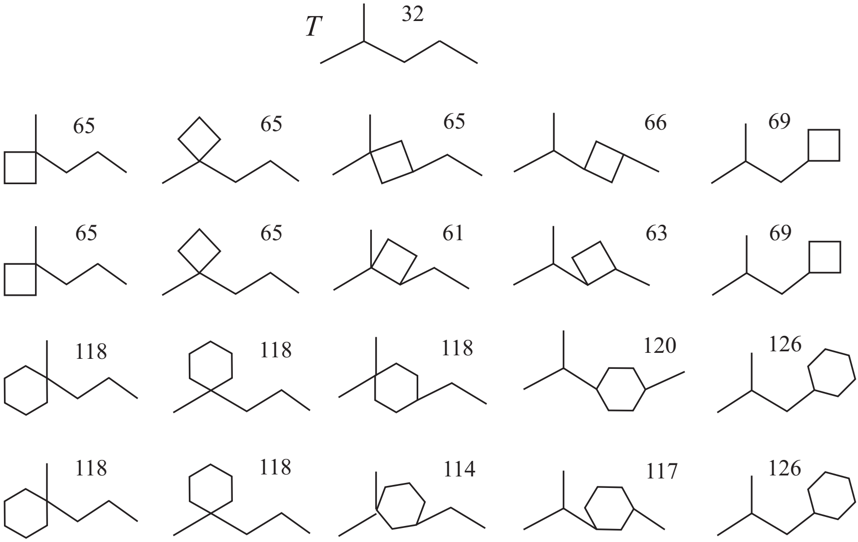

Figure 3. Families of unicyclic graphs with 4- and 6-membered cycles.

Corollary 4. *For the families of unicyclic graphs with cycles of length 4 and 6, we have*

$$W(\mathcal{U}_4) = \begin{cases} (n+4)W(T) + 2(n-1), & \textit{if } m = k = 1, \\ (n+5)W(T) + (n-1)(n+1), & \textit{if } m = 2, k = 0, \end{cases}$$

$$W(\mathcal{U}_6) = \begin{cases} (n+9)W(T) + 2(n-1)(n+6), & \textit{if } m = k = 2, \\ (n+10)W(T) + (n-1)(3n+11), & \textit{if } m = 3, k = 1, \end{cases}$$

and the average values of the Wiener index of unicyclic graphs are

$$W_{\text{avr}}(\mathcal{U}_4) = \begin{cases} \left(1 + \frac{5}{n-1}\right) W(T) + 2, & \textit{if } m = k = 1, \\ \left(1 + \frac{6}{n-1}\right) W(T) + n + 1, & \textit{if } m = 2, k = 0, \end{cases}$$

$$W_{\text{avr}}(\mathcal{U}_6) = \begin{cases} \left(1 + \frac{10}{n-1}\right) W(T) + 2(n+6), & \textit{if } m = k = 2, \\ \left(1 + \frac{11}{n-1}\right) W(T) + 3n + 11 & \textit{if } m = 3, k = 1. \end{cases}$$

As an example, consider families of unicyclic graphs with cycles of length 4 and 6 shown in Fig. 3. By Corollary 4, $W(\mathcal{U}_4) = 10 \cdot 32 + 10 = 330$ (the first row, $m = k = 1$), $W(\mathcal{U}_4) = 9 \cdot 32 + 35 = 323$ (the second row, $m = 2, k = 0$), $W(\mathcal{U}_6) = 15 \cdot 32 + 120 = 600$ (the third row, $m = k = 2$), and $W(\mathcal{U}_6) = 14 \cdot 32 + 145 = 593$ (the last row, $m = 3, k = 1$). Graphs of the families in the first and the third rows contain unicyclic graphs U with "average" structure. Namely, $W(U) = W_{\mathrm{avr}}(\mathcal{U}_4) = 66$ and $W(U) = W_{\mathrm{avr}}(\mathcal{U}_6) = 120$.

***Acknowledgment*:** The study was carried out within the framework of the state contract of the Sobolev Institute of Mathematics (project number FWNF-2022-0017).

References

[1] D. Bonchev, D. H. Rouvray (Eds.), *Chemical Graph Theory — Introduction and Fundamentals*, Gordon & Breach, New York, 1991.

[2] D. Bonchev, The Wiener number — some applications and new developments, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry. Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 58–88.

[3] A. A. Dobrynin, On the Wiener index of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 707–726.

[4] A. A. Dobrynin, On the Wiener index of certain families of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 565–574.

[5] A. A. Dobrynin, Wiener index of hexagonal chains with segments of equal length, in: M. Dehmer, F. Emmert-Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications*, Chapman and Hall/CRC, New York, 2014, pp. 81–109.

[6] A. A. Dobrynin, Wiener index of subdivisions of a tree, *Siberian El. Math. Rep.* **16** (2019) 1581–1586.

[7] A. A. Dobrynin, On the Wiener index of the forest induced by contraction of edges in a tree, *MATCH Commun. Math. Comput. Chem.* **86** (2020) 321–326.

[8] A. A. Dobrynin, On the Wiener index of two families generated by joining a graph to a tree, *Discr. Math. Lett.* **9** (2022) 44–48.

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

[10] A. A. Dobrynin, E. Estaji, Wiener index of certain families of hexagonal chains, *J. Appl. Math. Comput.* **59** (2019) 245–256.

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

[12] R. C. Entringer, Distance in graphs: trees, *J. Comb. Math. Comb. Comput.* **24** (1976) 65–84.

[13] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czech. Math. J.* **26** (1976) 283–296.

[14] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[15] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.

[16] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[17] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1982.

[18] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: developments and applications, *Croat. Chem. Acta* **68** (1995) 105–129.

[19] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, Chapman& Hall/CRC, Boca Raton, 2018.

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