CROATICA CHEMICA ACTA CCACAA **75** (2) 613–620 (2002)

ISSN-0011-1643
CCA-2820

Original Scientific Paper

On the Wiener Number of Thorn Trees, Stars, Rings, and Rods[✦,#]

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Received June 5, 2001; revised February 21, 2002; accepted February 22, 2002

The concept of thorn graphs proposed recently by Gutman is extended to the broader concept of generalized thorny graphs. The latter preserve unchanged certain parts of the parent graph while applying the procedure of thorn graph generation to the rest of the graph. Thorn stars and rods are typical examples of such generalized thorn graphs, owing to the unchanged star center, and the other-than-terminal rod vertices. Formulae are presented for the Wiener number of these and other classes of (generalized) thorn graphs.

Key words: (generalized) thorn graphs, Wiener number, thorn rings, thorn stars, thorn rods.

INTRODUCTION

The Wiener number[1] is one of the most common topological descriptors of molecular structure, an area of theoretical chemistry to which Milan Randić made significant contributions.[2,3]

Recently, Gutman[4,5] introduced the concept of »thorn graph« for any graph G* that can be obtained from a parent connected graph G by attaching $p_i \geq 0$ new vertices of degree one to each vertex i. Theorems have been derived for a special case of thorn graphs for which $p_i = a_{\max} - a_i$, where $a_{\max}$ is a constant, and a_i is the degree of the i-th vertex in G, G being a tree. For

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✦ Dedicated to Professor Milan Randić on the occasion of his 70th birthday.

Reported in part on the Second Indo-American Workshop on Mathematical Chemistry, May 30 – June 3, 2000, University of Minnesota, Duluth, Minnesota, USA.

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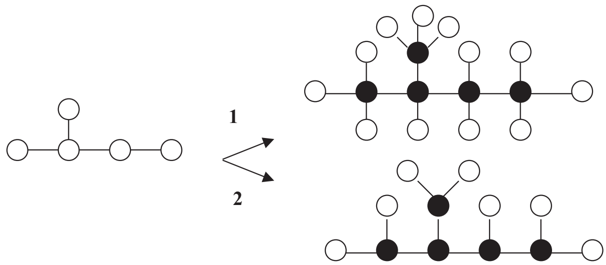
organic acyclic molecules, a_{max} = 4 or 3 for the respective classes of alkanes (as in the transformation of **1**) or polyenoids (as in **2**).



These classes of compounds have only non-terminal vertices of degree $t = a_{max}$ and terminal vertices of degree 1. Such graphs are sometimes called proper graphs.[6] One might thus regard proper graphs as a special case of thorny graphs with a uniform vertex degree t of all non-terminal vertices. We will call such graphs t-thorn graphs. The t-thorn graphs are of importance for polymer theory, especially for dendrimers.[7] The Wiener number of polymer graphs could be of use in the quantitative characterization of polymer topology,[8,9] as well as for specific structure-property relationships. Formulae for the Wiener number of dendrimer species have been reported by Gutman[10] and Diudea.[11] Recently, Dobrynin, Entringer, and Gutman[12] reviewed the studies on the Wiener index of trees.

Gutman[4] derived a formula that relates the Wiener number W of such thorn trees T* with the Wiener number of the parent graph T having n vertices:

$$W(\mathrm{T}^*) = (t-1)^2 W(\mathrm{T}) + [(t-1)n+1]^2 \ . \tag{1}$$

Bytautas, Bonchev, and Klein[13] calculated the average Wiener number for the (structural) isomer classes of alkanes and polyenoids having up to 100 carbon atoms, making use of formula (1) and a generation-series-based methodology for calculating average properties of isomer series.[14–15] In this paper we present closed-form formulae for calculating the Wiener number of several classes of thorn graphs, such as caterpillars having a chain as a parent graph, and thorn rings whose parent graph is a monocycle. We also apply the notion of generalized thorn graphs, to consider stars and rods. Such graphs preserve the vertex degrees in some essential structural fragments of the parent graph such as the central vertex of a star or the internal part of a chain, whereas the procedure of the thorn graph formation is applied to the rest of the graph vertices. The Wiener number formulae for these two classes of general graphs are also presented. The formulae are given in a form containing essential structural information; besides the number of thorns these are the rod length and the number of star arms.

THE WIENER NUMBER FORMULAE FOR THORN TREES

Caterpillars

$a = 3, b = 6$ $a = 4, b = 7$

Definition: A caterpillar is a thorn tree T*(a,b) whose nonterminal vertices $b \geq 1$ are of the same degree $a > 2$, and whose parent graph is the b-site chain graph, P_b.

Theorem: The Wiener number of a caterpillar having b branched vertices of degree a is:

$$W(T^*(a,b)) = \frac{1}{6} b(a-1)[(a-1)(b-1)(b+7) + 6(a+1)] + 1 . \quad (2)$$

Proof: We apply the formula originally used by Wiener:

$$W = \frac{1}{2} \sum_{\text{all edges}} N_i N_j \quad (3)$$

where N_i and N_j are the numbers of vertices in the left and right components to which the graph is decomposed after cutting a graph edge $\{i,j\}$, and the sum of Eq. (3) is over all edges in the graph. The total number of vertices in T*(a,b) is

$$n = (a-1)b + 2 . \quad (4)$$

Applying the Wiener constructive procedure one obtains

$$W = 1 \times (n-1) \times [(a-2)b+2] + a \times (n-a) + (2a-1) \times [n-(2a-1)] +$$

$$(3a-2) \times [n-(3a-2)] + \ldots + [(b-1)a - (b-2)] \times [n - (b-1)a + (b-2)] =$$

$$[(a-1)b+1][(a-2)b+2] + \sum_{i=1}^{b-1} [i(a-1) + 1][(a-1)(b-i) + 1]$$

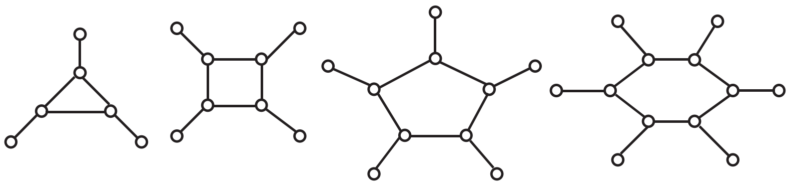
wherefrom one arrives after some elementary transformations at formula (2). For the chemically relevant cases of $a = 3$ and $a = 4$ one obtains the Wiener number as a polynomials of degree three in the number of branched vertices:

$$W(b,a = 3) = \frac{1}{3}(2b^3 + 12b^2 + 10b + 3) \tag{2a}$$

$$W(b,a = 4) = \frac{1}{2}(3b^3 + 18b^2 + 9b + 2)\ . \tag{2b}$$

It can be shown that our formula (2) along with the formula for $W(P_b)$ is a consequence of Gutman's formula (1).

Thorny Rings



$n = 3, t = 3$ $n = 4, t = 3$ $n = 5, t = 3$ $n = 6, t = 3$

Definition: A t-thorny ring has a simple cycle as the parent, and t-2 thorns at each cycle vertex.

Theorem: The Wiener number of a t-thorny ring having n ring-vertices is

$$W = \frac{1}{8}n(t-1)^2\ (n^2-a) + n(t-2)(nt-n-1) \tag{5}$$

with $a = 0$ for n – even, and $a = 1$ for n – odd.

Proof: Due to symmetry of the t-thorn ring, the Wiener number may be expressed by the sum d_1 of the distances to a ring vertex 1 and that d_2 to a terminal vertex 2:

$$W(C_n,t) = \frac{1}{2}n[d_1 + (t-2)d_2]\ . \tag{6}$$

By induction, one has

$$d_2 = d_1 + (t-1)n-2 \tag{7}$$

$$d_1(n\text{–even}) = \frac{1}{4}\,[(t-1)n^2 + 4(t-2)n];$$

$$d_1(n\text{–odd}) = \frac{1}{4}\,[(t-1)n^2 + 4(t-2)n - t + 1]\ . \tag{8}$$

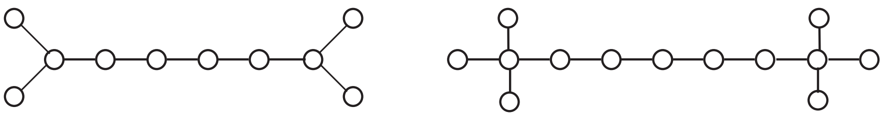
Substituting (7) and (8) into (6) one obtains Eq. (5).

Substituting in (5) $n^3/8 = C_{n\text{-even}}$ and $(n^3-n)/8 = C_{n\text{-odd}}$, one can express the Wiener number of a t-thorn ring, $W(C_{n,t})$, by the Wiener number of the parent cyclic graph, $W(C_n)$:

$$W(C_n,t) = (t-1)^2\ W(C_n) + n(t-2)\ (nt - n - 1)\ . \tag{9}$$

Eq. (9) for the thorn rings coincides with the equation given as Corollary 1.1 by Gutman[4] for the general case of thorn graphs G* obtained from a parent graph G by attaching the same number of vertices t at each of the vertices of G.

Thorn Rods



$p = 6,\ t = 3$ $\qquad$ $p = 7,\ t = 4$

Definition: A thorn rod is a graph, $P_{p,t}$, which includes a linear chain (termed »rod«) of p vertices and degree-t terminal vertices at each of the two rod ends.

Theorem: The Wiener number of a thorn rod $P_{p,t}$ is

$$W(P_{p,t}) = \frac{1}{6}\,(p^3-p) + (t-1)^2\ (p+3) + (t-1)(p^2+p-2)\ . \tag{10}$$

Proof: We proceed from the Doyle-Graver formula[16]

$$W = \binom{n+1}{3} - \sum\nolimits_u \sum_{i<j<k} n_i n_j n_k\ . \tag{11}$$

Here, n is the total number of vertices in the graph, and n_i, n_j, and n_k are the numbers of vertices in the branches i, j, and k emanating from vertex u, and the first summation is over all branched vertices. The thorn rod has only two branched vertices each one having t–1 branches of a single vertex and a large branch with $p + t - 2$ vertices. Then, from (11) one gets

$$W(\mathrm{P}_{p,t}) = \binom{n+1}{3} - 2\binom{t-1}{3} - 2\binom{t-1}{2}(p + t - 2)\ . \tag{12}$$

After substituting $n = p + 2t - 2$ and simplifying Eq. (12) one arrives at Eq. (10). The specific case with $p = 2$, corresponds to the »pom-pom« model, widely used in polymer theory:

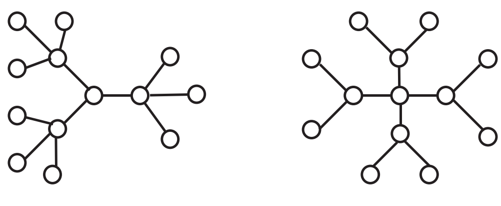
$$W(\mathrm{P}_{2,t}) = 5(t-1)^2 + 4(t-1) + 1\ . \tag{16a}$$

Corollary: The Wiener number of the t-thorn rod can be obtained from the Wiener number of the parent path graph, $W(\mathrm{P}_p)$, by the formula:

$$W(\mathrm{P}_{p,t}) = W(\mathrm{P}_p) + (t-1)^2(p+3) + (t-1)(p^2+p-2)]\ . \tag{17}$$

The proof follows directly from Eq. (16) the first term in which is exactly the Wiener number of the parent path graph.

Thorn Stars



$k = 3,\ t = 4$ $k = 4,\ t = 3$

Definition: Thorn stars are graphs obtained from a k-arm star by attaching t-1 terminal vertices to each of the star arms.

Theorem: The Wiener number of a thorn star $\mathrm{S}_{k,t}$ is

$$W(\mathrm{S}_{k,t}) = kt(2kt-k-t+1) \tag{18}$$

Proof: We proceed again from the Doyle-Graver formula (11) for the Wiener number of a branched tree. There are k+1 branched vertices in $\mathrm{S}_{k,t}$, k of which are equivalent and have t–1 branches of one vertex and one branch of

n-t vertices. The central vertex has k equivalent branches, each one with t vertices. Therefore, (11) transforms into

$$W = \binom{n+1}{3} - k\left[\binom{t-1}{3} + (n-t)\binom{t-1}{2}\right] - \binom{k}{3}t^3 \ . \tag{19}$$

Expressing the total number of vertices in $S_{k,t}$ as

$$n = kt + 1 \tag{20}$$

and substituting them in (19), one proves the theorem.

Eq. (20) shows that for a given star, the Wiener number is a quadratic function of the number of thorns t. For the chemically relevant cases of 3-arm star and 4-arm star one obtains

$$W(S_{3,t}) = 15(t–1)^2 + 24(t–1) + 9 \tag{18a}$$

$$W(S_{4,t}) = 28(t–1)^2 + 44(t–1) + 16 \tag{18b}$$

Corollary: The Wiener number of the t-thorn star, $W(S_{k,t})$, is related to the Wiener number of the parent star, $W(S_k)$, by the equation

$$W(S_{k,t}) = W(S_k) + k(t–1)[2k(t–1) + 3k–t] \tag{21}$$

The proof follows directly from comparing Eq. (18) to the equation[17]

$$W(S_k) = k^2 \ . \tag{22}$$

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SAŽETAK

O Wienerovu broju trnovitih stabala, zvijezda, prstenova i prutova

Danail Bonchev i Douglas J. Klein

Graf-teorijska koncepcija o trnovitim stablima poopćena je u koncepciju o trnovitim grafovima. Ona dopušta da izvjesni dijelovi izvornoga grafa ostanu nepromijenjeni prilikom primjene postupka generiranja trnovitih grafova na ostatak izvornoga grafa. Trnovite zvijezde i prutovi tipični su primjeri poopćenih trnovitih grafova s nepromijenjenim središtem zvijezde i nedirnutim unutarnjim čvorovima pruta. Dane su formule za izračunavanje Wienerova broja tih i drugih klasa (poopćenih) trnovitih grafova.