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SOME TOPOLOGICAL INDICES OF AN INFINITE 1,3-ADAMANTANE ARRAY

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ABSTRACT. A topological index is a real number related to a molecular graph, which is a graph invariant. In this paper, formulas for calculating the Szeged index, Wiener index and edge Wiener index of an infinite array of 1,3-adamantane are presented.

Keywords: *Szeged index, Wiener index, edge Wiener index, 1,3-adamantane.*

1. INTRODUCTION

Let G = (V, E) be a simple molecular graph. The sets of vertices *V*(*G*) and edges *E*(*G*) of *G* represent atoms and bonds, respectively [1]. The graph *G* is said to be connected if for every vertex *x* and *y* in *V* (*G*) there exists a path connecting them. The distance *d* (*u,v*) between vertices *u* and *v* of a connected graph *G* is the number of edges in a minimum path from *u* to *v*.

A topological index is a real number related to a molecular graph, which is a graph invariant. There are several topological indices already defined. The Wiener index (*W*) is the first topological index that was introduced in 1947 by Harold Wiener [2]. It is defined as the sum of distances between all pairs of vertices in the graph. The Szeged index (Sz) is another topological index, introduced by Ivan Gutman [3]. To define the Szeged index of a graph G, we assume that *e* = *uv* is an edge connecting the vertices *u* and *v*. Suppose $n_u(e)$ is the number of vertices of *G* lying closer to *u* and $n_v(e)$ is the number of vertices of *G* lying closer to *v*, then the Szeged index of the graph *G* is defined as $Sz(G) = \sum_{e=uv\in E(G)}[n_u(e)n_v(e)]$; notice that vertices equidistant to *u* and *v* are not taken into account. For details and other related topological indices, the reader is invited to consult refs. [4-17].

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In this paper, formulas for calculating the Szeged index, Wiener index and edge Wiener index of an infinite array of 1,3-adamantane (see Figure 1) are presented.

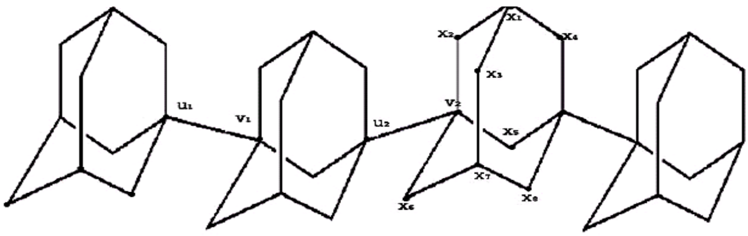

Figure 1. Tetrameric 1, 3-adamantane.

2. MAIN RESULTS

In this section, we will derive the formulas for calculating Sz index, Wiener index and edge Wiener index of an infinite array of 1,3-adamantane.

2.1. Szeged index of adamantane array A[n]

In the following we compute the index *Sz(A[n])* for an infinite array of 1, 3-adamantane.

We partition the edge set in two parts: first part is the set of edges which link all the adamantane units together, and second part is the set of edges which belong to adamantane units.

We name the edges in the first part the *linked edges* and consider $e = u_i v_i$ as a member of that part. *A[n]* has *n - 1* linked edges. Let $e = u_i v_i$ be a *linked edge* then we see that $n_{u_i}(e) = 10i$ and $n_{v_i}(e) = 10(n - i)$. Each adamantane unit has 12 edges, Figure 1. We consider the kth adamantane. For the edges $e = uv$ of that adamantane unit we have:

If $e = uv = x_1x_2, u_kx_5, x_6x_7$
then $n_u(e) = 10(n-k)+6$ and $n_v(e) = 10(k-1)+4$.

If $e = uv = x_1x_4, v_{k-1}x_5, x_7x_8$
then $n_u(e) = 10(n-k)+4$ and $n_v(e) = 10(k-1)+6$.

If $e = x_1x_3, x_2v_{k-1}, v_{k-1}x_6, x_4u_k, u_kx_8, x_3x_7$
then $n_u(e) = 10(n-1)+6$ and $n_v(e) = 4$.

Theorem 1. The Szeged index of an infinite array of 1,3-adamantane is calculated by formula:

$$Sz(A[n]) = \frac{350}{3}n^3 + 240n^2 - \frac{206}{3}n$$

Proof. $Sz(A[n]) = \sum_{e=uv}(n_u(e)n_v(e))$

$$= 100\sum_{i=1}^{n-1} i(n-i) + 3\sum_{k=1}^{n}(10(n-k)+6)(10(k-1)+4)$$

$$+ 3\sum_{k=1}^{n}(10(n-k)+4)(10(k-1)+6) + 6\sum_{k=1}^{n}4(6+10(n-1))$$

$$= \frac{50}{3}(n^3-n) + 100n^3 + 240n^2 - 52n$$

$$= \frac{350}{3}n^3 + 240n^2 - \frac{206}{3}n.$$

2.2. Wiener index of A[n]

In the following we obtain the wiener index of *A[n]*:

For this we first divide the graph to two parts: consider the first adamantane unit as part one A1, and A_{m-1} for the rest of the graph. By this way we can prove that $W(A_m) = W(A_1) + W(A_{m-1}) + d(A_1, A_{m-1})$; we have:

$$\sum_{m=2}^{n}(W(A_m) - W(A_{m-1})) = \sum_{m=2}^{n}(W(A_1) + d(A_1, A_{m-1}))W(A_n)W(A_n)$$

$$= n\,W(A_1) + \sum_{m=2}^{n} d(A_1, A_{m-1}). \qquad \text{(I)}$$

Theorem 2. $W(A_n) = 50n^3 + 80n^2 - 34n$.

Proof. In Graph theory it has been defined that $d(G,u) = \sum_{x \in V(G)} d(u,x)$; thus

$$d(A_1, x_1) = d(A_1, x_7) = d(A_1, u) = d(A_1, v) = 18,$$

$$d(A_1, x_2) = d(A_1, x_3) = d(A_1, x_4) = d(A_1, x_5) = d(A_1, x_6) = d(A_1, x_8) = 20$$

$$\Rightarrow \; W(A_1) = \frac{1}{2}\sum_{u,v \in V(A_1)} d(u,v) = 96.$$

As in the following $d(A_1, A_{m-1})$ based on m is:

$$d(A_1, A_{m-1}) = 360(m-1) + 100(1+4+7+\cdots)$$

in which the number of sentences in the second parenthesis is m-1. Finally by constituting *W(A₁)* and $d(A_1, A_{m-1})$ in relation (I) the polynomial of $W(A_n)$ based on n will obtain:

$$W(A_n) = n\,W(A_1) + \sum_{m=2}^{n} d(A_1, A_{m-1}) = 96n + \sum_{m=2}^{n} (150m^2 + 10m - 160)$$
$$= 50n^3 + 80n^2 - 34\,n$$

2.3. Edge Wiener index of A[n]

In the following we obtain the edge Wiener index of *A[n]* , denoted by $W_e(A[n])$.

We consider the k[th] adamantane and then compute the summation of all distances of each edge, from all other edges of the graph. Then one can see that $d(G,e) = \sum_{e' \in E(G)} d(e,e')$. Then we compute the following polynomials:

$$d(G,x_1x_2) = d(G,x_6x_7) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{67}{2}\,n - 52\,k + 11,$$
$$d(G,x_1x_3) = d(G,x_3x_7) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{67}{2}\,n - 39\,k - 2,$$
$$d(G,x_1x_4) = d(G,x_7x_8) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{41}{2}\,n - 26\,k - 2,$$
$$d(G,x_4u_k) = d(G,x_8u_k) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{15}{2}\,n - 13\,k - 2,$$
$$d(G,v_{k-1}x_2) = d(G,x_6v_{k-1}) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{67}{2}\,n - 65\,k + 24,$$
$$d(G,x_5u_k) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{15}{2}\,n - 26\,k + 11,$$
$$d(G,x_5v_{k-1}) = \frac{39}{2}n^2 + 39k^2 - 39\,nk + \frac{41}{2}\,n - 52\,k + 24.$$

Now we consider the *linked edge* $u_k v_k$ and find the distance of $u_k v_k$ from all other edges of graph:

$d(G,u_kv_k) = \frac{39}{2}\,n^2 + 39\,k^2 - 39\,nk - \frac{11}{2}\,n + 2$. Thus:

Theorem 3. $W_e(A[n]) = \frac{169}{2}\,n^3 + 13\,n^2 - \frac{49}{2}\,n - 1.$

Proof 1. $W_e(G) = \frac{1}{2}\sum_{e,e' \in E(G)} d(e,e') =$

$$\frac{1}{2}\left(\sum_{k=1}^{n}(234\,n^2 + 468\,k^2 - 468\,nk + 285\,n - 468\,k + 93) + \sum_{k=1}^{n-1}\left(\frac{39}{2}\,n^2 + 39\,k^2 - 39\,nk - \frac{11}{2}\,n + 2\right)\right)$$

$$\Rightarrow \quad W_e(TA[n]) = \frac{169}{2}\,n^3 + 13\,n^2 - \frac{49}{2}\,n - 1.$$

Proof 2. Consider the first adamantane unit and edge u_1v_1 as A_1, and the other remained parts of graph A_2. Then we the edge Wiener index of A_n is as follows:

$$W_e(A_n) = n\,W_e(A_1) + \sum_{m=2}^{n} d(A_1, A_{m-1}).$$

Now we obtain $W_e(A_1)$: it can be seen that the sum of all distances between each edge of adamantane array, and all other edges of adamantane is equal to 12 and the summation of all distances between u_1v_1 and all other edges of adamantane equals 15. According to these we obtain: $W_e(A_1) = \frac{1}{2}(12)(12) + 15 = 87$. To find the formula of $W_e(A_n)$ it is enough to obtain (A_1, A_{m-1}):

$d(A_1, A_{m-1})$ = (the summation of all distances of adamantane A_1 from the adamantanes of A_{m-1})

+ (the summation of all distances of adamantane A_1 from the linked edges of A_{m-1})

+ (the distances of u_1v_1 from the adamantanes of A_{m-1})

+ (the distances of u_1v_1 from all linked edges of A_{m-1}).

Then we conclude that:

$$d(A_1, A_{m-1}) - 360(m-1) + 144\,(1+4+7+\cdots) + 15(m-2) + 12(3+6+9+\cdots) + 15(m-1) + 12(3+6+9+\cdots) + (2+5+8+\cdots).$$

In this polynomial the number of sentences in the second parenthesis is m-1 and in other sequences is m-2. Thus $d(A_1, A_{m-1}) = \frac{507}{2}m^2 - \frac{455}{2}m - 40$.

By constituting $W_e(A_1)$ and $d(A_1, A_{m-1})$ in relation I the final result would is as follows:

$$W_e(A_n) = n\,W_e(A_1) + \sum_{m=2}^{n} d(A_1, A_{m-1}) = 87\,n + \sum_{m=2}^{n}\left(\frac{507}{2}m^2 - \frac{455}{2}m - 40\right)$$

$$\Rightarrow W_e(TA[n]) = \frac{169}{2}n^3 + 13\,n^2 - \frac{49}{2}n + 14$$

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