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Topological Indices of a Kind of Altans

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ABSTRACT

Altans are a class of molecular graphs introduced recently. These graphs are attractive to many chemists and mathematicians. A topological index is a numerical invariant calculated for a description of molecular graphs. In this paper, we compute a few topological indices of Altans such as Wiener index, second Zagreb index, atom-bond connectivity (ABC) index, ABC_4 index, etc.

1. INTRODUCTION

In First-time Altans, having been obtained from benzenoids by adding a ring to all outer vertices of valence two [1], were introduced as planner systems. Later, Ivan Gutman generalized altans to arbitrary graphs [3]. In this paper, we follow Gutman's model for altans. Suppose Γ is an arbitrary connected graph of order n, S is a subset of Γ of cardinality k and $V(\Gamma) = \{0,1,\dots,n-1\}$. Consider $S_0 = \{n, n+1, \dots, n+k-1\}$ and $S_1 = \{n+k, n+k+1, \dots, n+2k-1\}$. We map the pair (Γ, S) to the pair (Γ_1, S_1) by adding the cycle C of cardinality $2k$ with operation $A(G,S)$, where C is the circle $C = \{n, n+k, n+1, n+k+1, \dots, n+k-1, n+2k-1, n\}$. Finally, we attach C to Γ by edges between S and S_0 of the form (s_i, s_{n+i}) where $0 \le i \le k$ and S_i is the i-th vertex of

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S. The vertices of degree 2 of C are the new peripheral root of the altan; suppose $A(G,S) = (\Gamma_1, S_1)$. By continue of this method, iterated altans by $A^n(G,S)$, called the n-th altan of (G,S), can be obtained. For example, by considering $\Gamma = C_6$ and $S = \{0,1,2,3,4,5\}$, the graph in Figure 1 is extended to the one depicted in Figure 2.

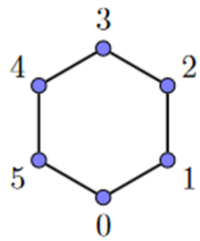

Figure 1. Benzene molecule (C_6).

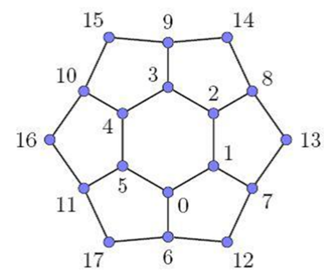

Figure 2. Altan of benzene by considering $S = \{0,1,2,3,4,5\}$.

By continuing to use this method, we can obtain the altan of Figure 3 and finally the altan with n circles.

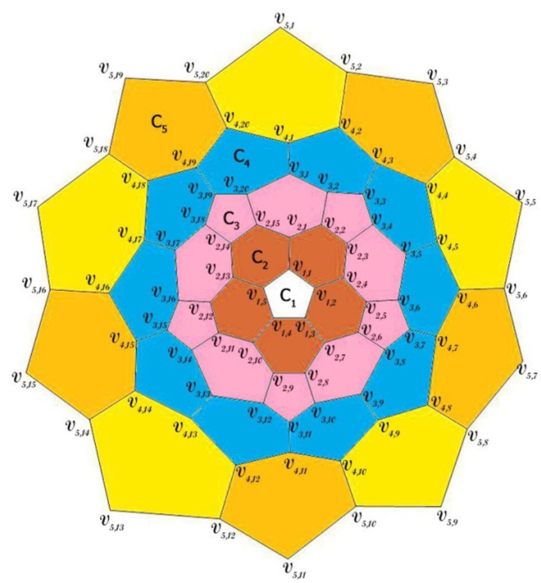

Figure 3. Altan with n circles.

First, we denote the circles of this altan by $C_i, 1 \leq i \leq n$. Also, we mark the vertices of C_1 by $v_{i,1}$, $1 \leq i \leq 5$, the vertices of C_2 by $v_{i,2}$, where $1 \leq i \leq 15$ and finally the vertices of other cycles by $v_{i,j}$, where $1 \leq i \leq 20$ and $1 \leq j \leq n$.

Up to now, many papers published about computation of some topological indices. For example see the references [6,7,8,9,10,11,12,13]. In this paper, we compute some topological indices for this kind of altans.

2. SOME TOPOLOGICAL INDICES OF ALTAN

The Wiener index of a connected graph is the sum of all distances between its distinct vertices. In fact, the Wiener index of a connected graph Γ, defined in [5] as:

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

where V is the set of vertices of Γ, and $d(u,v)$ is the distance between vertices u and v.

Lemma 1. The sum of all distances between vertices of C_1 and all other vertices of the altan with n circles such that $n > 10$ is denoted by $D(C_1)$ and is equal to $D(C_1) = 100n^2 - 650n + 5545$. For $n \leq 10$, the sum of all distances between vertices of C_1 and all other vertices of the altan with n circles can be taken from the Table 1.

Table 1. The sum of all distances between vertices of C_1 and all other vertices of the altan with n circles, $n \leq 10$.

Number of Cycles	1	2	3	4	5	6	7	8	9	10
$\boldsymbol{D(C_1)}$	30	245	705	1345	2165	3165	4350	5725	7290	9045

Proof. By using simple computation, it is effortless to obtain the table above. Suppose $n > 10$. Since C_1 is a symmetric pentagon, it would suffice to compute the sum of all distances between $v_{1,1}$ and other vertices of the altan, and deduce it for other vertices of C_1. By using straightforward computation, we can infer that the sum of all distances between $v_{1,1}$ and vertices of C_1 and C_2 are 6 and 43 respectively. In Table 1, the sum of all distances between $v_{1,1}$ and vertices of C_i, $3 \leq i \leq 10$, are specified. Obviously, we can conclude that there is a regular case for distances between $v_{1,1}$ and vertices of C_i, $i \geq 11$. Therefore, distances between $v_{1,1}$ and vertices of C_{i+1} can be computed by using the distances between $v_{1,1}$ and vertices of C_i.

If i is even, then the distances between $v_{1,1}$ and vertices of $C_i, 3 \leq i \leq n$, are as follows :

$$d(v_{1,1}, v_{i,k}) = \begin{cases} d\left(v_{1,1}, v_{i,k-1}\right) + 1 & If\ \ k\ \ is\ \ odd, \\ \min\{d(v_{1,1}, v_{i,k-1}), d(v_{1,1}, v_{i,k+1})\} & If\ \ k\ \ is\ \ even. \end{cases}$$

If i is odd, then the distances between $v_{1,1}$ and vertices of $C_i, 3 \leq i \leq n$, are as follows:

$$d(v_{1,1}, v_{i,k}) = \begin{cases} \min\{d(v_{1,1}, v_{i,k-1}), d(v_{1,1}, v_{i,k+1})\} & If\ \ k\ \ is\ \ odd, \\ d\left(v_{1,1}, v_{i,k-1}\right) + 1 & If\ \ k\ \ is\ \ even. \end{cases}$$

Using by the above relations, the sum of distances between $v_{1,1}$ and other vertices of altan is computed in follow:

$$D(v_{1,1}) = 6 + 43 + 92 + \sum_{i-3}^{5} (i(4 + 2(i-3)) + 4(5 + 2(i-3)) + (6-i)(6 + 2(i-3)) + 10) + \sum_{i-4}^{6} (i(4 + 2(i-3)) + 4(5 + 2(i-3)) + (6-i)(6 + 2(i-3))) + \sum_{i-6}^{9} (i(4 + 2(i-3)) + (10-i)(5 + 2(i-3)) + 10) + \sum_{i-6}^{9} (i(4 + 2(i-3)) + (10-i)(5 + 2(i-3))) + \sum_{i-10}^{n-1} (i(4 + 2(i-3)) + 10) + \sum_{i-11}^{n} (i(4 + 2(i-3)) = 20n^2 - 130n + 1109.$$

Since C_1 is symmetric, the relations above show that the sum of distances between all vertices of C_1 and those of altan with n circles such that $n > 10$ is $D(C_1) = 5(20n^2 - 130n + 1109) = 100n^2 - 650n + 5545$. ■

Lemma 2. The sum of all distances between vertices of C_2 and all other vertices which belong to circles C_i, $i \geq 2$, of the altan with n circles such that $n > 11$ is $D(C_2) = 350n^2 - 460n - 1920$. For $n \leq 11$, the sum of all distances between vertices of C_2 and all other vertices of the altan with $n \geq 2$ circles can be derived from the Table 2.

Table 2. The sum of all distances between vertices of C_2 and all other vertices of the altan with $2 \leq n \leq 11$ circles.

Number of Cycles	2	3	4	5	6	7	8	9	10	11
$\boldsymbol{D(C_2)}$	770	2200	3980	6290	9050	12285	16020	20275	25070	30430

Proof. We divide the vertices of C_2 in two parts:

The vertices located on interface of hexagons, and those not located on interface of hexagons. Thus, we consider the vertices $v_{2,1}$ and $v_{2,2}$. The sum of all distances between $v_{2,1}$ and vertices of C_2 is equal to 48. By using a method similar to Lemma 1, we can show that the sum of all distances between $v_{2,1}$ and vertices of C_i, $3 \leq i \leq 14$, is as follows:

$$D(v_{2,1}) = 48 + 94 + \sum_{i=4}^{6} (16i - 6) + \sum_{i=3}^{5} (16i + 4) + \sum_{i=4}^{6} (17i - 12) + \sum_{i=6}^{7} (17i - 2) + \sum_{i=8}^{9} (19i - 20) + \sum_{i=7}^{8} (17i + 6) + \sum_{i=10}^{n} (20i + 24) + \sum_{i=10}^{n-1} (20i + 34) + 350 = 30n^2 + 48n - 440.$$

The sum of all distances between $v_{2,2}$ and vertices of C_2 is equal to 53. Similarly, the sum of all distances between $v_{2,2}$ and vertices of C_i, $3 \leq i \leq 14$, is as follows:

$$D(v_{2,2}) = 2008 + \sum_{i=12}^{n} 10(2 + 2(i-3)) + \sum_{i=11}^{n-1} (10(2 + 2(i-3)) + 10) = 2008 + \sum_{i=12}^{n} (20i - 40) + \sum_{i=11}^{n-1} (20i - 30) = 20n^2 - 70n + 28.$$

Therefore, the sum of all distances between vertices of C_2 and all other vertices of the altan with n circles is $D(C_2) = 5(30n^2 + 48n - 440) + 10(20n^2 - 70n + 28) = 350n^2 - 460n - 1920$. ■

Lemma 3. The sum of all distances between vertices of C_3 and all other vertices of C_i, $3 \leq i \leq n$, such that $n > 12$ is $D(C_3) = 400n^2 - 200n + 10080$. For $n \leq 12$, the sum of all distances between vertices of C_3 and all other vertices of the altan with $n \geq 3$ circles can be extracted from Table 3.

Table 3. The sum of all distances between vertices of C_3 and all other vertices of the altan with $3 \leq n \leq 12$ circles.

Number of Cycles	3	4	5	6	7	8	9	10	11	12
$\boldsymbol{D(C_3)}$	1980	4400	7280	10660	14580	19080	24200	29980	36460	43680

Proof. We divide the vertices of C_3 of the form $v_{3,i}$ into two parts where i is either odd or even. Thus, we consider two vertices $v_{3,1}$ and $v_{3,2}$. By employing a method remarkably similar to Lemma 1 and preparing a table such as Table 1, the following results can be achieved:

$$D(v_{31}) = 2140 + \sum_{i=13}^{n} 10(2(i-3)) + \sum_{i=12}^{n-1} (10(2(i-3)) + 10)$$
$$= 2140 + \sum_{i=13}^{n} (20i - 60) + \sum_{i=12}^{n-1} (20i - 50)$$
$$= 20n^2 - 110n + 580.$$

$$D(v_{32}) = 1858 + \sum_{i=12}^{n} 10(1 + 2(i-3)) + \sum_{i=12}^{n-1} (10(1 + 2(i-3)) + 10)$$
$$= 1858 + \sum_{i=12}^{n} (20i - 50) + \sum_{i=11}^{n-1} (20i - 40)$$
$$= 20n^2 - 90n + 428.$$

Thus the sum of all distances between vertices of C_3 and all other vertices of $C_i, 3 \leq i \leq n$, is $D(C_3) = 10(20n^2 - 110n + 580) + 10(20n^2 - 90n + 428) = 400n^2 - 2000n + 10080$. ■

Lemma 4. The sum of all distances between vertices of C_4 and all other vertices of $C_i, 4 \leq i \leq n$, such that $n > 13$ is $D(C_4) = 400n^2 - 2800n + 12480$. For $n \leq 13$, the sum of all distances between vertices of C_4 and all other vertices of the altan with $n \geq 4$ circles can be drawn out from Ttable 4.

Table 4. The sum of all distances between vertices of C_4 and all other vertices of the altan with $4 \leq n \leq 12$ circles.

Number of Cycles	4	5	6	7	8	9	10	11	12	13
$\boldsymbol{D(C_4)}$	2000	4420	7300	10680	14600	19100	24220	30000	36480	43770

Proof. Similar to Lemma 3, we divide the vertices of C_4 of the form $v_{4,i}$ into two parts where i is either odd or even. Therefore, we consider two vertices $v_{4,1}$ and $v_{4,2}$. Similar to the previous lemma, the following results can be shown:

$$D(v_{4,1}) = 1858 + \sum_{i=13}^{n} 10(1 + 2(i-4)) + \sum_{i=12}^{n-1} (10(1 + 2(i-4)) + 10)$$
$$= 1858 + \sum_{i=12}^{n} (20i - 70) + \sum_{i=11}^{n-1} (20i - 60) = 20n^2 - 130n + 538.$$

$$D(v_{4,2}) = 2140 + \sum_{i=14}^{n} 10(2(i-4)) + \sum_{i=13}^{n-1} (10(2(i-4)) + 10)$$
$$= 2140 + \sum_{i=14}^{n} (20i - 80) + \sum_{i=12}^{n-1} (20i - 70)$$
$$= 20n^2 - 150n + 710.$$

Thus the sum of all distances between vertices of C_4 and all other vertices of $C_i, 4 \leq i \leq n,$ is $D(C_4) = 10(20n^2 - 130n + 538) + 10(20n^2 - 150n + 710) = 400n^2 - 2800n + 12480$. ■

Lemma 5. The sum of all distances between vertices of $C_k, k \geq 5$, and all other vertices of $C_i, 5 \leq i \leq n$, such that $n > k + 9$ is $D(C_i) = 400n^2 - 2800n + 12480$. For $n \leq k + 9$, the sum of all distances between vertices of C_k and all other vertices of the altan with $n \geq k$ circles can be obtained from Table 5.

Table 5. The sum of all distances between vertices of C_k and all other vertices of the altan with $k \leq n \leq k + 9$ circles and $k \geq 5$.

Number of Cycle	k	$k+1$	$k+2$	$k+3$	$k+4$	$k+5$	$k+6$	$k+7$	$k+8$	$k+9$
$D(C_k)$	2000	4420	7300	10680	14600	19100	24220	30000	36480	43770

Proof. By having considered the figure of the altan and computed all distances between vertices of $C_k, k \geq 5$, and all other vertices of C_i, $5 \leq i \leq n$, the following results are yielded:

If k is odd, then we have $D(v_{k,i}) = D(v_{4,i+1})$ and if k is even, then $D(v_{k,i}) = D(v_{4,i})$. Since the number of vertices v_{ki} where i is even is equal to vertices v_{ki} where $i$is odd, the result is confirmed. ■

By using the above lemmas for each case, we can compute the Wiener index. The second Zagreb index of Γ is defined as $M_2(\Gamma) = \sum_{uv \in E(\Gamma)} d(u)d(v)$, where $d(u)$ is the degree of vertex u.

Proposition 6. Let Γ be the altan in Figure 3. The second Zagreb index of Γ is $M_2(\Gamma) = 270n - 375$.

Proof. The number of vertices of Γ is $|V| = 5 + 15 + \sum_{i=3}^{n} 20 = 20n - 20$. The sum of all degrees of vertices of Γ where n > 1 is $\sum_{v \in V(\Gamma)} d(v) = 5 \times 3 + 15 \times 3 +$

$\sum_{i=3}^{n-1}(20 \times 3) + 10 \times 3 + 10 \times 2 = 60n - 70$. Thus, the cardinality of edges of Γ is $|E| = \frac{1}{2}\sum_{v\in V(\Gamma)} d(v) = 30n - 35$. Therefore, the second Zagreb index of Γ is $M_2(\Gamma) = 9(30n - 55) + 20 \times 6 = 270n - 375$. ■

The first and the second product Zagreb index of Γ is denoted by $PM_1(\Gamma)$ and $PM_2(\Gamma)$ respectively and defined as $PM_1(\Gamma) = \prod_{uv\in E(\Gamma)}\big(d(u) + d(v)\big)$ and $PM_2(\Gamma) = \prod_{uv\in E(\Gamma)} d(u)d(v)$ [2,4].

Proposition 7. The first and the second product Zagreb index of Γ are

$$PM_1(\Gamma) = 6^{(30n-55)} \times 5^{20},\ PM_2(\Gamma) = 3^{(90n-145)} \times 2^{20}.$$

Proof. Γ has $30n - 55$ edges with vertices of degree 3 and 20 edges in circle C_n such that one edge is of degree 2 and the other one is of degree 3. So we have $PM_1(\Gamma) = (3 + 3)^{(30n-55)} \times (2 + 3)^{20} = 6^{(30n-55)} \times 5^{20}$ and $PM_2(\Gamma) = (3 \times 3)^{(3n-55)} \times (2 \times 3)^{20} = 3^{(90n-145)} \times 2^{20}$. ■

Set $M_{r,s}(\Gamma) = \sum_{u,v\in V}(d(u)^r d(v)^s + d(v)^r d(u)^s)$.

Proposition 8. $M_{r,s}(\Gamma) = 60 \times 3^r3^s n - 1103^r3^s + 20(3^r2^s + 2^r3^s)$.

Proof. Since Γ has $30n - 55$ edges with vertices of degree 3 and 20 edges in circle C_n such that one edge is of degree 2 and the other edge is of degree 3, the $M_{r,s}(\Gamma)$ index of Γ is $M_{r,s}(\Gamma) = 2 \times 3^r3^s(30n - 55) + 20(3^r2^s + 2^r3^s) = (60 \times 3^r3^s n - 1103^r3^s + 20(3^r2^s + 2^r3^s)$. ■

The atom-bond connectivity (ABC) index [8] is defined as

$$ABC(\Gamma) = \sum_{uv\in E(\Gamma)}\sqrt{\left(\frac{d(u)+d(v)-2}{d(u)d(v)}\right)}.$$

Proposition 9. The ABC index of Γ is $ABC(\Gamma) = 20n - \frac{110}{3} + 10\sqrt{2}$.

Proof. By argument similar to the above mentioned theorem, we have $ABC(\Gamma) = (30n - 55)\sqrt{\frac{3+3-2}{3\times3}} + 20\sqrt{\frac{3+2-2}{3\times2}} = 20n - \frac{110}{3} + 10\sqrt{2}$. ■

The $ABC_4(\Gamma)$ index is defined as

$$ABC_4(\Gamma) = \sum_{uv\in E(\Gamma)}\sqrt{\left(\frac{s(u)+s(v)-2}{s(u)s(v)}\right)},$$

where $s(u)$ and $s(v)$ are the sum of all vertices which adjacent to u and v respectively.

Proposition 10. The ABC_4 index of Γ is $ABC_4(\Gamma) = \frac{40}{3}n - \frac{260}{9} + 10\sqrt{\frac{14}{63}} + 20\sqrt{\frac{11}{42}}$.

Proof. By argument similar to Theorem 8, we can show that $ABC_4(\Gamma) = (30n - 65) \times \sqrt{\frac{9+9-2}{9\times 9}} + 10\sqrt{\frac{9+7-2}{9\times 7}} + 20\sqrt{\frac{6+7-2}{6\times 7}} = \frac{40}{3}n - \frac{260}{9} + 10\sqrt{\frac{14}{63}} + 20\sqrt{\frac{11}{42}}$. ■

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