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REMARKS ON THE BALABAN INDEX

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Abstract. The Balaban index was defined by A. T. Balaban in 1982 as $J = J(G) = \mu(G) \sum_{uv \in E(G)} (D_u D_v)^{-1/2}$, where $\mu(G) = m/(m-n+2)$ and $D_u = \sum_{x \in V(G)} d(u,x)$. In this paper we compute some bounds of the Balaban index and then by means of group action we compute the Balaban index of vertex transitive graphs.

1. Introduction. In theoretical chemistry molecular structure descriptors are used to compute properties of chemical compounds. Throughout this paper, 'graph' means a simple connected graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. If $x, y \in V(G)$ then the distance $d(x,y)$ between x and y is defined as the length of a minimum path connecting x and y. Then the eccentricity of vertex u is defined as $\varepsilon(u) = \max\{d(x,u) \mid x \in V(G)\}$. The radius $r(G)$ and diameter $d(G)$ of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. The Wiener number or Wiener index is the first topological index based

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on the distance between any pair of vertices. By using this number, Wiener computed the boiling point of paraffin. See [1] for more details about the Wiener index.

Nowadays many topological indices have been defined for QSAR and QSPR studies and one of them is the Balaban index. The Balaban index was defined about 30 years ago by A. T. Balaban as follows [2]:

$$J = J(G) = \mu(G) \sum_{uv \in E(G)} (D_u D_v)^{-1/2},$$

Where $\mu(G) = m/(m - n + 2)$ and $D_u = \sum_{x \in V(G)} d(u, x)$. This topological index appears to be a very useful molecular descriptor with attractive properties. The goal of this paper is computing some bounds of the Balaban index. We obtain a general formula for the Balaban index of vertex transitive graphs. We apply our formula to two vertex transitive fullerene graphs, namely C_{20} and C_{60}. Here our notations are standard and mainly taken from the standard book of graph theory such as [3]. We encourage readers to refer to [4–8] to study some properties of Balaban index.

2. Results and Discussion.

2. Results and Discussion. In this section we first obtain some new bounds of the Balaban index and then by means of a vertex transitive graph we obtain some new equalities for this topological index.

2.1. Bounds of the Balaban Index. Before calculating some bounds of the Balaban index we compute this topological index for some well-known graphs:

Example 1. Let S_n be a star graph on $n + 1$ vertices. It is easy to see that for the central vertex denoted by u, $D_u = \underbrace{1 + 1 + 1 + \cdots + 1}_{n} = n$. For other vertices such as v, $D_v = \underbrace{2 + 2 + \cdots + 2}_{n-1} = 2n - 2$. This implies for every edge $e = uv$, $D_u D_v = n(2n - 2)$ and so,

$$J(S_n) = \frac{n^2}{\sqrt{2n(n-1)}}.$$

Example 2. Suppose K_n denotes a complete graph on n vertices. For every vertex u, $D_u = n-1$. Hence

$$J(K_n) = \frac{n^2(n-1)^2}{4(n-1)} = \frac{n^2(n-1)}{4}.$$

Recall that in 1975, the Randić index [9] of G was introduced by the chemist Milan Randić as:

$$R\left(G\right) = \frac{1}{\sqrt{d_u d_v}},$$

Where the degree of vertex u is denoted by d_u. In the following Theorem we obtain a relationship between the Randic index and the Balaban index:

Theorem 3.

$$J\left(G\right) \leq \frac{m}{m-n+2} R\left(G\right).$$

Proof. By using definition we have $D_u = 1n_1 + 2n_2 + \cdots + \varepsilon_u n_{\varepsilon_u} \geq d_u$. Thus for every edge $e = uv$, $D_u D_v \geq d_u d_v$ and this completes the proof. □

Here we define the modified Randic index by replacing the degree of vertex with its eccentricity. On the other hand, the modified Randic index is as follows:

$$R\left(G\right) = \frac{1}{\sqrt{\varepsilon_u \varepsilon_v}},$$

where the eccentricity of vertex u is denoted by ε_u. In the following Theorem we compare the Balaban index with the modified Randic index:

Theorem 4.

$$J\left(G\right) \leq \frac{m}{m-n+2} MR\left(G\right).$$

Proof. According to proof of Theorem 3, $D_u \geq \varepsilon_u$, for any vertex u in $V(G)$. By using definition of the Balaban index the proof is straightforward. □

Theorem 5. *Let $D(G)$ denotes the diameter of graph G, then*

$$\frac{m}{(m-n+2)D(G)} \leq J\left(G\right) \leq \frac{m^2}{m-n+2}.$$

P r o o f. Since $D_u \geq 1$, so $J\left(G\right) \leq \dfrac{m}{m-n+2}\sum\limits_{uv\in E(G)} 1 = \dfrac{m^2}{m-n+2}$. On the other hand, $D_u \leq D(G)(n-1)$ and $m \geq n-1$. Hence,

$$J\left(G\right) \geq \frac{m}{m-n+2}\sum_{uv\in E(G)}\frac{1}{D(G)(n-1)} \geq \frac{m^2}{(m-n+2)(n-1)D(G)}. \qquad \square$$

In the proof of Theorem 3, we saw $D_u = 1n_1 + 2n_2 + \cdots + \varepsilon_u n_{\varepsilon_u}$. Here, we can obtain a lower bound for the Balaban index. In other words,

$$D_u = 1n_1 + 2n_2 + \cdots + \varepsilon_u n_{\varepsilon_u} \leq (n_1 + n_2 + \cdots n_{\varepsilon_u})\varepsilon_u = n\varepsilon_u.$$

This implies $D_uD_v \leq n^2\varepsilon_u\varepsilon_v$ and we have proved the following Theorem:

Theorem 6.

$$J\left(G\right) \geq \frac{m}{n(m-n+2)}MR\left(G\right).$$

2.1. Vertex-Transitive Graphs. Groups are often used to describe symmetries of objects. This is formalized by the notion of a group action. Let G be a group and X a nonempty set. An action of G on X is denoted by GX and X is called a G-set. It induces a group homomorphism ϕ from G into the symmetric group S_X on X, where $\phi(g)x = gx$ for all $x \in X$. The orbit of x will be denoted as x^G and defined as the set of all $\phi(g)x$, $g \in G$.

A bijection σ on the vertex set of graph G is named an automorphism of the graph if it preserves the edge set. In other words, σ is an automorphism if $e = uv$ is an edge, then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Let $\mathrm{Aut}(G) = \{\alpha : V \to V, \alpha \text{ is bijection}\}$, then $\mathrm{Aut}(G)$ under the composition of mappings forms a group. We say $\mathrm{Aut}(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(u) = v$. The edge transitive graph can be defined similarly.

Lemma 7. *Suppose G is a graph, A_1, A_2, ..., A_t are the orbits of* $\mathrm{Aut}(G)$ *under its natural action on $V(G)$ and $x, y \in A_i$, $1 \le i \le t$. Then $D_x = D_y$. In particular, if G is vertex transitive then for every pair (u, v) of vertices $D_u = D_v$.*

Proof. It is easy to see that if vertices u and v are in the same orbit, then there is an automorphism ϕ such that $\phi(u) = v$. Thus

$$D_v = \sum_{y \in V(G)} d(v, y) = d(\phi(u), \phi(w)) = d(u, w) = D_u.$$

If G be a vertex transitive graph then $D_u = D_v$, $u, v \in V(G)$. This completes our proof. □

Theorem 8. *Suppose G is a vertex transitive (n, m) graph and $u \in V(G)$. Then for some integers k,*

$$J(G) = \frac{mn^2k}{2(m-n+2)W(G)}.$$

Proof. It is easy to see that every vertex transitive graph is k-regular for some k?s. Let $u \in V(G)$, by Lemma 7, we have:

$$J(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{D_u D_v}} = \frac{m}{m-n+2} \sum_{u \in V(G)} \frac{d_u}{D_u} = \frac{mnk}{(m-n+2)D_u}.$$

On the other hand, $W(G) = \frac{1}{2}\sum_{u \in V(G)} D_u = \frac{n}{2} D_u$. This implies $D_u = \frac{2}{n} W(G)$ and the proof is completed. □

As a result of the last Theorem we compute the Balaban index of some well-known vertex transitive graphs. At first, consider a polyhex nanotorus ($T[p, q]$) depicted in Fig. 1. Ashrafi et al. in [10] proved that this graph is vertex transitive. So, by Theorem 8 we can easily compute the Wiener index of a polyhex nanotorus. On the other hand this graph is 3-regular, $|V(T[p, q])| = pq$ and $|E(T[p, q])| = 6pq$. This implies:

$$J(T[p,q]) = \frac{6pq(pq)^2 \times 3}{2(6pq - pq + 2)W(T[p,q])} = \frac{9p^3q^3}{(5pq+2)W(T[p,q])}.$$

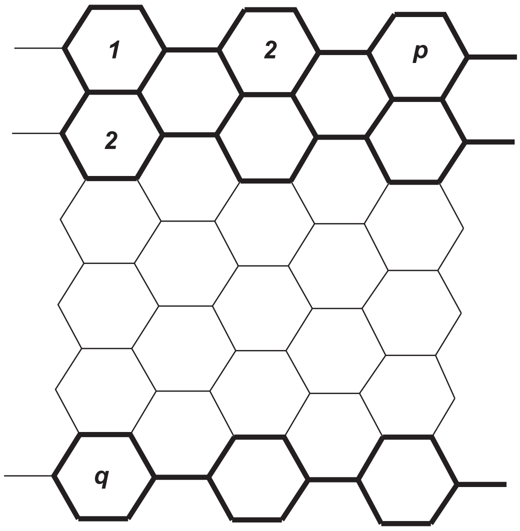

Fig. 1. A 2-dimensional lattice for $T[p, q]$

Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985 [11]. Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. They have n carbon atoms, $3n/2$ bonds, 12 pentagonal and $n/2 - 10$ hexagonal faces. The most important member of the family of fullerenes is C_{60} [12]. Some properties of fullerene graphs are studied in [13–19]. The smallest fullerene is C_{20}. It is a well-known fact that among all fullerene graphs only C_{20} and C_{60} (see Figs 2, 3) are vertex transitive. Since for every vertex of C_{20} such as u, $D_u = 50$ and for $u \in V(C_{60})$, $D_u = 278$, then

$$J(C_{20}) = \frac{150}{50} = 3, \quad J(C_{60}) = \frac{2025}{4 \times 278} = 1.821.$$

Lemma 9. *Suppose G is a graph, A_1, A_2, ..., A_t are the orbits of* $\mathrm{Aut}(G)$ *under its natural action on $E(G)$ and $x, y \in A_i$, $1 \leq i \leq t$. Then*

$$J(G) = \frac{m}{(m-n+2)} \sum_{i=1}^{t} \sum \_xy \in E(A_i) \frac{1}{\sqrt{D_x D_y}}.$$

In particular, if G is an edge transitive (n, m) graph and $e = uv \in E(G)$

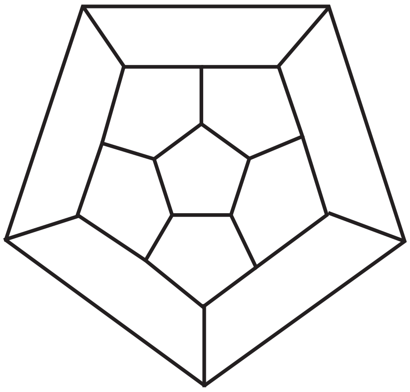

Fig. 2. 2-dimensional graph of fullerene C_{20}

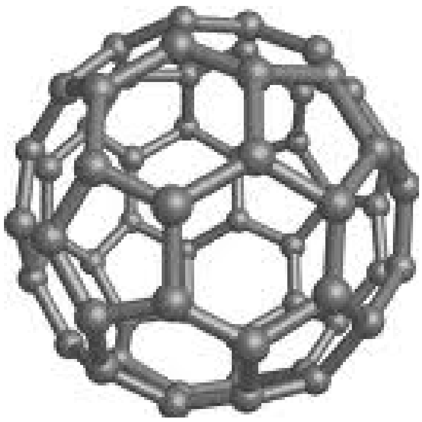

Fig. 3. 3D graph of fullerene C_{60}

is an arbitrary edge, then

$$J(G) = \frac{m^2}{(m-n+2)\sqrt{D_u D_v}}.$$

P r o o f. The proof is similar to the proof of Lemma 7. □

A hypercube (Fig. 4)is defined as follows:

The vertex set of the hypercube $H_n$consists of all n-tuples $b_1 b_2 \ldots b_n$ with $b_i \in \{0,1\}$. Two vertices are adjacent if the corresponding tuples differ in precisely one place. Darafsheh [20] proved H_n is vertex and edge transitive. So we have:

Theorem 10.

$$J\left(H_n\right) = \frac{n2^{n-1}}{2^{n-1}(n-2)+2}.$$

P r o o f. Since H_n is edge transitive by Lemma 9,

$$J\left(G\right) = \frac{m^2}{(m-n+2)\sqrt{D_u D_v}}.$$

Because it is vertex transitive according to Lemma 7, $J\left(G\right) = \dfrac{m^2}{(m-n+2)D_u}$. But H_n has exactly 2^n vertices, $n2^{n-1}$ edges and for every vertex u, $D(u) = n.2^{n-1}$. $\square$

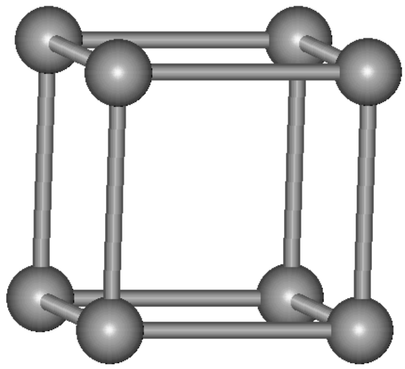

Fig. 4. Hyper cube H_3

3. Conclusion.

Topological descriptors are very important tools in chemical graph theory. Among them topological indices role a fundamental map in predicting chemical phenomena. In other words, topological indices are numerical parameters which are graph invariant and they are used in development of quantitative structure-activity relationships (QSARs). One of the most important topological indices is Balaban index defined by A. T. Balaban. In this paper some new bounds of this topological index were computed. We also studied the properties of the Balaban index for vertex-transitive graphs.

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