

# *Internet* Electronic Journal of **Molecular Design**

July 2005, Volume 4, Number 7, Pages 491–500

Editor: Ovidiu Ivanciuc

Special issue dedicated to Professor Danail Bonchev on the occasion of the 65<sup>th</sup> birthday

## **On the Degeneracy of Topological Index $J$**

Damir Vukičević<sup>1</sup> and Alexandru T. Balaban<sup>2</sup>

<sup>1</sup> Department of Mathematics, University of Split, Nikole Tesle 12, HR–21000 Split, Croatia

<sup>2</sup> Texas A&M University at Galveston, Department of Marine Sciences, 5007 Avenue U,  
Galveston, TX 77551, USA

Received: May 24, 2004; Revised: January 24, 2005; Accepted: January 27, 2005; Published: July 31, 2005

### **Citation of the article:**

D. Vukičević and A. T. Balaban, On the Degeneracy of Topological Index  $J$ , *Internet Electron. J. Mol. Des.* **2005**, 4, 491–500, <http://www.biochempress.com>.

## On the Degeneracy of Topological Index $J^\#$

Damir Vukičević<sup>1,\*</sup> and Alexandru T. Balaban<sup>2,\*</sup>

<sup>1</sup> Department of Mathematics, University of Split, Nikole Tesle 12, HR–21000 Split, Croatia

<sup>2</sup> Texas A&M University at Galveston, Department of Marine Sciences, 5007 Avenue U,  
Galveston, TX 77551, USA

Received: May 24, 2004; Revised: January 24, 2005; Accepted: January 27, 2005; Published: July 31, 2005

---

*Internet Electron. J. Mol. Des.* 2005, 4 (7), 491–500

### Abstract

The topological index  $J$  is one of the widely used indices for QSAR and QSPR studies, and has the advantage of discriminating nonisomorphic graphs that represent molecules of restricted size. It is of interest to see if this property can be generalized for any connected graph. A proof is provided for the theorem stating that for almost all connected graphs  $G$  there is a nonisomorphic graph  $G'$  such that  $G$  and  $G'$  have the same topological index  $J$ . Since the index  $J$  is among the least degenerate topological indices, our results imply that *a fortiori* other topological indices are even more degenerate. Hence, none of them can be used in discrimination of general graphs.

**Keywords.** Balaban index; topological index  $J$ ; degeneracy; topological index; molecular descriptor.

---

## 1 INTRODUCTION

Among molecular descriptors, topological indices [1–9] occupy a well-established place and are frequently used for quantitative structure–activity relationship (QSAR) studies [10]. By analogy, one uses similar acronyms for physical–chemical properties (QSPR) or toxicities (QSTR).

For saturated hydrocarbons, their connected and hydrogen-depleted graph consists in vertices symbolizing carbon atoms and edges symbolizing single C–C covalent bonds. The topological index  $J$  [11–12] (average distance sum connectivity) was modeled after the Randić index  $\chi$  [13] and it was designed to be both less degenerate (by using topological distance sums instead of vertex degrees as for  $\chi$ ), and less dependent on the graph size and cyclicity (by compensating through the use of the number of edges and the cyclomatic number  $\mu$ ).

Indeed, for an infinitely long linear graph (idealized polyethylene) it was proved [14] that the value of  $J$  becomes equal to the number  $\pi$ , and for idealized infinite polymers having chains with

---

# Dedicated on the occasion of the 65<sup>th</sup> birthday to Danail Bonchev.

\* Correspondence author; E-mail: [vukicevi@pmfst](mailto:vukicevi@pmfst) and [balabana@tamug.edu](mailto:balabana@tamug.edu).

regularly placed branches such as poly(propylene) or poly(isobutene), the value of  $J$  is a rational multiple of  $\pi$  (in the two above examples  $J$  is  $3\pi/2$  and  $2\pi$ , respectively).

A computer program was published for computing index  $J$  [15]. For molecules having heteroatoms and/or multiple bonds, suitable changes were proposed [16–18]. It was found that the index  $J$  parallels in many ways the less discriminating Wiener index, e.g. in the way these indices order alkane isomers [19,20]. An application of  $J$  for polymers was described [21]. The index  $J$  has found many applications; the most interesting of these was developed by Lahana and his coworkers [22], and it involved index  $J$  along with 12 other molecular descriptors for reducing the number of possible immunosuppressive decapeptides in a virtual library of about 250,000, by a factor of 10,000, resulting in improving the activity of the lead decapeptide about 100 times. Another interesting application of  $J$  and  $\chi$  was published by Bermudez *et al.* [23], and it involved adding to these indices contributions of hydrogen bonding for computing pairwise associations between nucleotide bases in transfer RNA of *E. coli* for clustering tRNA into two groups, confirming Wong's coevolution theory of the genetic code [24]: biological evolution led to gradually increasing numbers of amino acids till they reached the present number of 20, and thus the 64 triplet codons had to be reassigned from time to time according to evolving biochemical pathways.

In a previous publication [25], it was proved that the highly discriminating index  $J$  starts to become degenerate for acyclic graphs with  $n > 11$  ( $n$  is the number of vertices), for monocyclic graphs with  $n > 7$ , and for polycyclic graphs with even smaller  $n$  values. Thus, despite the fact that  $J$  has a higher discriminating ability than most other single topological indices, it may be inferred that for almost any graph  $J$  is degenerate. A formal proof of this conjecture is the object of the present paper.

## 2 NOTATIONS

Let  $x$  be any real number. By  $\lfloor x \rfloor$  we denote the largest integer smaller than  $x$  and by  $\lceil x \rceil$  we denote the smallest integer larger than  $x$ . Let  $S$  be any finite set; by  $|S|$ , we denote its cardinality, i. e. the number of elements in  $S$ . Let  $G$  be a simple connected graph (i. e. a connected graph without loops or multiple edges). By  $V(G)$  we denote the set of vertices of  $G$ , and by  $E(G)$  the set of edges of  $G$ . Also we denote their cardinalities by  $v(G) = |V(G)|$  and  $e(G) = |E(G)|$ . Let  $x, y \in V(G)$ . By  $d_G(x)$ , we denote the degree of vertex  $x$ , and by  $d_G(x, y)$  the topological distance between vertices  $x$  and  $y$ . We also define the sum of all distances from vertex  $x$  by  $D_G(x) = \sum_{v \in V(G)} d_G(x, v)$ .

The Balaban index  $J(G)$  is defined by

$$J(G) = \frac{e(G)}{e(G) - (v(G) - 1) + 1} \cdot \sum_{uv \in E(G)} (D_G(u) D_G(v))^{-1/2} \quad (1)$$

For the sake of simplicity, we define  $E_G(uv) = (D_G(u)D_G(v))^{-1/2}$ . The last relationship can be rewritten as

$$J(G) = \frac{e(G)}{e(G) - (v(G) - 1) + 1} \cdot \sum_{e \in E(G)} E_G(e) \quad (2)$$

Let  $G_n$  be the set of all simple graphs  $G$  such that  $V(G) = SV = \{v_1, v_2, \dots, v_n\}$ , where  $n$  is an arbitrary number. Note that  $n = v(G)$  for each graph in the class  $G_n$ . Denote by:

- 1)  $C_n$  the set of all connected graphs with the set of vertices  $SV$ .
- 2)  $D_n$  the set of all graphs with the set of vertices  $SV$  such that at least two of them are not connected and have no common neighbors.
- 3)  $D'_n$  the set of all graphs with the set of vertices  $SV$  such that  $v_1$  and  $v_2$  are not connected and have no common neighbors.
- 4)  $L_n$  the set of all graphs with the set of vertices  $SV$  with maximum degree at least  $\frac{1}{2}n + n^{2/3}$ .
- 5)  $L'_n$  the set of all graphs with the set of vertices  $SV$  such that  $d_G(v_1) \geq \frac{1}{2}n + n^{2/3}$ .
- 6)  $S_n$  the set of all graphs with the set of vertices  $SV$  with minimum degree at most  $\frac{1}{2}n - n^{2/3}$ .
- 7)  $S'_n$  the set of all graphs with the set of vertices  $SV$  such that  $d_G(v_1) \leq \frac{1}{2}n - n^{2/3}$ .
- 8)  $W_n$  the set of connected graphs  $G$  with the set of vertices  $SV$  such that there is a graph  $G'$  such that  $G$  and  $G'$  are nonisomorphic and that they have the same Balaban index.

More formally, we can write:

$$\begin{aligned} C_n &= \{G \in G_n : G \text{ is connected graph}\} \\ D_n &= \{G \in G_n : G \notin C_n \text{ or } \text{diam}(G) > 2\} \\ D'_n &= \{G \in G_n : \text{vertices } v_1 \text{ and } v_2 \text{ are not connected or } d_G(v_1, v_2) > 2\} \\ L_n &= \left\{G \in G_n : \text{the maximum degree of } G \text{ is at least } \frac{1}{2}n + n^{2/3}\right\} \\ L'_n &= \left\{G \in G_n : d_G(v_1) \geq \frac{1}{2}n + n^{2/3}\right\} \\ S_n &= \left\{G \in G_n : \text{the minimum degree of } G \text{ is at most } \frac{1}{2}n - n^{2/3}\right\} \\ S'_n &= \left\{G \in G_n : d_G(v_1) \leq \frac{1}{2}n - n^{2/3}\right\} \\ W_n &= \left\{G \in C_n : \text{there is a graph } G' \text{ such that } G \text{ and } G' \text{ are } \right. \\ &\quad \left. \text{nonisomorphic and } J(G) = J(G')\right\} \end{aligned} \quad (3)$$

In order to prove our main result, we shall need the Stirling formula:

$$\lim_{n \rightarrow \infty} \frac{n!}{\left(\frac{n}{e}\right)^n \sqrt{2\pi n}} = 1 \quad (4)$$

### 3 RESULTS AND DISCUSSION

Let us give an auxiliary result:

**Lemma** Let  $a$  and  $b$  be arbitrary natural numbers and let  $x_1, x_2, \dots, x_a$  be any fixed real numbers. The number of sums of  $b$  summands from  $\{x_1, \dots, x_a\}$  is at most  $\min\{a^b, (b+1)^a\}$ .

**Proof:** The number of different sums is at most the number of ordered  $b$ -tuples from the set  $\{x_1, \dots, x_a\}$ , hence it is at most  $a^b$ . Note that each sum can be rewritten in the form  $k_1 \cdot x_1 + k_2 \cdot x_2 + \dots + k_a \cdot x_a$ , where  $k_i$  is the number of occurrences of the number  $x_i$  in the observed sum, for each  $i=1, \dots, a$ . Also, note that  $0 \leq k_i \leq b$ , for each  $i=1, \dots, a$ . Hence each of the sums is uniquely determined by the  $a$ -tuple of the numbers  $(k_1, k_2, \dots, k_a)$  where  $0 \leq k_i \leq b$ , for each  $i=1, \dots, a$  and  $k_1 + \dots + k_a = b$ . The number of these  $a$ -tuples is at most  $(b+1)^a$ . This lemma is proved.

Let us prove the following theorem:

**Theorem 1.** We have  $\lim_{n \rightarrow \infty} \frac{|W_n|}{|C_n|} = 1$ .

**Proof:** The last relation is equivalent to  $\lim_{n \rightarrow \infty} \frac{|C_n \setminus W_n|}{|C_n|} = 0$ . Obviously,  $\lim_{n \rightarrow \infty} \frac{|C_n \setminus W_n|}{|C_n|} \geq 0$ . Hence it is sufficient to prove that

$$\lim_{n \rightarrow \infty} \frac{|C_n \setminus W_n|}{|C_n|} \leq 0 \quad (5)$$

Note that  $|C_n \setminus W_n| \leq |G_n \setminus W_n| \leq |D_n| + |L_n| + |S_n| + |(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)|$ , hence

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{|C_n \setminus W_n|}{|C_n|} &= \lim_{n \rightarrow \infty} \frac{|C_n \setminus W_n|}{|G_n|} \cdot \frac{|G_n|}{|C_n|} \leq \\ &\leq \lim_{n \rightarrow \infty} \frac{|D_n| + |L_n| + |S_n| + |(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)|}{|G_n|} \cdot \frac{|G_n|}{|G_n| - |G_n \setminus C_n|} \leq \\ &\leq \lim_{n \rightarrow \infty} \frac{|D_n| + |L_n| + |S_n| + |(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)|}{|G_n|} \cdot \frac{|G_n|}{|G_n| - |D_n|} \end{aligned}$$

Therefore, it is sufficient to prove that

$$\lim_{n \rightarrow \infty} \frac{|D_n|}{|G_n|} \leq 0 \quad (6)$$

$$\lim_{n \rightarrow \infty} \frac{|L_n|}{|G_n|} \leq 0 \quad (7)$$

$$\lim_{n \rightarrow \infty} \frac{|S_n|}{|G_n|} \leq 0 \quad (8)$$

$$\lim_{n \rightarrow \infty} \frac{|(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)|}{|G_n|} \leq 0 \quad (9)$$

Let us prove relationship (6). We have

$$\lim_{n \rightarrow \infty} \frac{|D_n|}{|G_n|} \leq \lim_{n \rightarrow \infty} \frac{\binom{n}{2} \cdot |D'_n|}{|G_n|}$$

Let  $G$  be any graph in  $D'_n$ . Note that  $v_1 v_2 \notin E(G)$ . Also for each  $v_j, j = 3, \dots, n$  at least one of the edges  $v_1 v_j$  and  $v_2 v_j$  is not in  $E(G)$ . Therefore  $|D'_n| = 3^{n-2} \cdot 2^{\frac{(n-2)(n-3)}{2}}$ . It follows that

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{\binom{n}{2} \cdot |D'_n|}{|G_n|} &= \lim_{n \rightarrow \infty} \frac{\binom{n}{2} \cdot 3^{n-2} \cdot 2^{\frac{(n-2)(n-3)}{2}}}{2^{\frac{n(n-1)}{2}}} = \lim_{n \rightarrow \infty} \frac{\binom{n}{2} \cdot 3^{n-2}}{2^{2n-3}} = \\ &= \lim_{n \rightarrow \infty} \left[ \frac{\binom{n}{2} \cdot 8 \cdot \left(\frac{3}{4}\right)^n}{9} \right] = \lim_{n \rightarrow \infty} \left[ \sqrt[n]{\frac{\binom{n}{2} \cdot 8 \cdot \left(\frac{3}{4}\right)^n}{9}} \right] \end{aligned}$$

Note that  $\lim_{n \rightarrow \infty} \left[ \sqrt[n]{\frac{\binom{n}{2} \cdot 8 \cdot \left(\frac{3}{4}\right)^n}{9}} \right] = \frac{3}{4}$ . Therefore,  $\lim_{n \rightarrow \infty} \left[ \sqrt[n]{\frac{\binom{n}{2} \cdot 8 \cdot \left(\frac{3}{4}\right)^n}{9}} \right] = 0$ .

Now, let us prove relationship (7). We have

$$\lim_{n \rightarrow \infty} \frac{|L_n|}{|G_n|} \leq \lim_{n \rightarrow \infty} \frac{n \cdot |L'_n|}{|G_n|}$$

Let  $G$  be any graph in  $L'_n$ . Note that at least  $\frac{1}{2}n + n^{2/3}$  of edges in  $\{v_1 v_2, v_1 v_3, \dots, v_1 v_n\}$  are in  $E(G)$ .

Hence, we have less than  $\binom{n-1}{\lceil \frac{1}{2}n + n^{2/3} \rceil}$  choices for these edges. Therefore,

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{|L_n|}{|G_n|} &\leq \lim_{n \rightarrow \infty} \frac{n \cdot \binom{n-1}{\lceil \frac{1}{2}n + n^{2/3} \rceil} \cdot 2^{\frac{(n-1)(n-2)}{2}}}{2^{\frac{n(n-1)}{2}}} = \lim_{n \rightarrow \infty} \frac{n \cdot \binom{n-1}{\lceil \frac{1}{2}n + n^{2/3} \rceil}}{2^{n-1}} \leq \lim_{n \rightarrow \infty} \frac{n \cdot \binom{n}{\lceil \frac{1}{2}n + n^{2/3} \rceil}}{2^{n-1}} \\ &= \lim_{n \rightarrow \infty} \frac{n}{2^{n-1}} \cdot \frac{n!}{\left(\lceil \frac{1}{2}n + n^{2/3} \rceil\right)! \cdot \left(\lceil \frac{1}{2}n - n^{2/3} \rceil\right)!} \end{aligned}$$

$$\begin{aligned}
 & n \cdot \left(\frac{n}{e}\right)^n \cdot \sqrt{2\pi n} \\
 = & \lim_{n \rightarrow \infty} \frac{n \cdot \left(\frac{n}{e}\right)^n \cdot \sqrt{2\pi n}}{2^{n-1} \cdot \left[ \left( \frac{\left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor}{e} \right)^{\left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor} \cdot \sqrt{2\pi \left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor} \cdot \left( \frac{\left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor}{e} \right)^{\left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor} \cdot \sqrt{2\pi \left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor} \right]} \\
 = & \lim_{n \rightarrow \infty} \frac{n}{2^{n-1}} \frac{\sqrt{n}}{\sqrt{\left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor} \sqrt{2\pi \left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor}} \cdot \frac{n^n}{\left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor^{\left\lfloor \frac{1}{2}n + n^{2/3} \right\rfloor} \cdot \left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor^{\left\lfloor \frac{1}{2}n - n^{2/3} \right\rfloor}} \\
 \leq & \lim_{n \rightarrow \infty} \frac{2n^{3/2}}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \cdot \frac{1}{(1 + 2n^{-1/3})^{\frac{1}{2}n + n^{2/3}} \cdot (1 - 2n^{-1/3} - n^{-1})^{\frac{1}{2}n - n^{2/3} - 1}} \\
 = & \lim_{n \rightarrow \infty} \frac{2n^{3/2} \cdot (1 - 2n^{-1/3} - n^{-1})}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \cdot \frac{1}{(1 - 4n^{-2/3} - n^{-1} - 2n^{-4/3})^{\frac{1}{2}n} \cdot \left(\frac{1 + 2n^{-1/3}}{1 - 2n^{-1/3} - n^{-1}}\right)^{n^{2/3}}} \\
 \leq & \lim_{n \rightarrow \infty} \frac{2n^{3/2}}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \cdot \frac{1}{\left[ \left(1 - \frac{1}{\frac{1}{4}n^{2/3}}\right)^{\frac{1}{4}n^{2/3}} \cdot \frac{\frac{1}{2}n}{\frac{1}{4}n^{2/3}} \cdot \left(1 + \frac{1}{\frac{1-2n^{-1/3}}{4n^{-1/3}}}\right)^{\frac{1-2n^{-1/3}}{4n^{-1/3}} \cdot \frac{n^{2/3}}{1-2n^{-1/3}}} \right]} \\
 & \cdot \frac{1}{\left(\frac{1-4n^{-2/3} - n^{-1} - 2n^{-4/3}}{1-4n^{-2/3}}\right)^{\frac{1}{2}n} \cdot \left(\frac{1-2n^{-1/3}}{1-2n^{-1/3} - n^{-1}}\right)^{n^{2/3}}} \\
 = & \lim_{n \rightarrow \infty} \frac{2n^{3/2}}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \cdot \frac{1}{e^{-2n^{1/3}} \cdot e^{\frac{4n^{1/3}}{1-2n^{-1/3}}}} \\
 & \cdot \frac{1}{\left(1 - \frac{n^{-1} + 2n^{-4/3}}{1-4n^{-2/3}}\right)^{\frac{1}{n^{-1} + 2n^{-4/3}} \cdot \frac{n^{-1} + 2n^{-4/3}}{1-4n^{-2/3}} \cdot n} \cdot \frac{1}{\left(1 - \frac{n^{-1}}{1-2n^{-1/3}}\right)^{\frac{1}{n^{-1}} \cdot \frac{n^{-1}}{1-2n^{-1/3}} \cdot n^{2/3}}} \\
 = & \lim_{n \rightarrow \infty} \frac{2n^{3/2}}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \cdot \frac{1}{e^{\frac{2n^{1/3} + 4}{1-2n^{-1/3}}} \cdot e^{-1}}
 \end{aligned}$$

$$= \lim_{n \rightarrow \infty} \left[ \left( \frac{2n^{3/2} \cdot e}{\sqrt{\left(\frac{1}{2}n + n^{2/3}\right)} \sqrt{2\pi \left(\frac{1}{2}n - n^{2/3} - 1\right)}} \right)^{\frac{1}{n^{1/3}}} \cdot \frac{1}{e^{1-2n^{-1/3}}} \right]^{n^{1/3}} = 0$$

Now, let us prove relationship (8). We have

$$\lim_{n \rightarrow \infty} \frac{|S_n|}{|G_n|} \leq \lim_{n \rightarrow \infty} \frac{n \cdot |S'_n|}{|G_n|}$$

Let  $G$  be any graph in  $S'_n$ . Note that at most  $\frac{1}{2}n - n^{2/3}$  of edges in  $\{v_1v_2, v_1v_3, \dots, v_1v_n\}$  are in  $E(G)$ .

Therefore, we have less than  $\binom{n-1}{\frac{1}{2}n - n^{2/3}}$  choices for these edges. Therefore,

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{|L_n|}{|G_n|} &\leq \lim_{n \rightarrow \infty} \frac{n \cdot \binom{n-1}{\left[\frac{1}{2}n - n^{2/3}\right]} \cdot 2^{\frac{(n-1)(n-2)}{2}}}{2^{\frac{n(n-1)}{2}}} \leq \lim_{n \rightarrow \infty} \frac{n \cdot \binom{n}{\left[\frac{1}{2}n - n^{2/3}\right]}}{2^{n-1}} = \\ &\lim_{n \rightarrow \infty} \frac{n \cdot \binom{n}{\left[\frac{1}{2}n + n^{2/3}\right]}}{2^{n-1}} = \{\text{as it is earlier proved}\} = 0. \end{aligned}$$

It remains to prove relationship (9). Let us bound from above  $|(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)|$ . Denote  $A_n = \{J(G) : G \in (G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)\}$ . Note that for each graph  $G \in G_n$  there are at most  $n!$  graphs  $G'$  such that  $G$  and  $G'$  are isomorphic. Therefore,

$$|(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)| \leq n! |A_n|$$

Let  $G$  be an arbitrary graph from the set  $(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)$ . Note that each vertex  $v \in V(G)$  has more than  $\frac{1}{2}n - n^{2/3}$  and less than  $\frac{1}{2}n + n^{2/3}$  neighbors and all other vertices from  $V(G) \setminus \{v\}$  are on distance 2. Therefore,

$$\begin{aligned} \frac{1}{2}n + n^{2/3} + 2 \left( n - 1 - \left( \frac{1}{2}n + n^{2/3} \right) \right) &< D_G(v) < \frac{1}{2}n - n^{2/3} + 2 \left( n - 1 - \left( \frac{1}{2}n - n^{2/3} \right) \right) \\ \frac{3}{2}n - 2 - n^{2/3} &< D_G(v) < \frac{3}{2}n - 2 + n^{2/3} \end{aligned}$$

Hence there are less than  $\lfloor 2n^{2/3} \rfloor$  possible values of  $D_G(v)$ . Therefore for each  $e \in E(G)$ , there are less than  $\lfloor 4n^{4/3} \rfloor$  possible values of  $E_G(e)$ .

Let us observe the formula  $J(G) = \frac{e(G)}{e(G) - (v(G) - 1) + 1} \cdot \sum_{e \in E(G)} E_G(e)$ . The value of the first factor



$\frac{e(G)}{e(G)-(v(G)-1)+1}$  can be chosen in  $\frac{n(n-1)}{2}+1$  ways ( $v(G)$  is prescribed and  $0 \leq e(G) \leq \frac{n(n-1)}{2}$ ). The value of the second factor  $\sum_{e \in E(G)} E_G(e)$  can be chosen in at most  $\left(\frac{n(n-1)}{2}+1\right)^{\lfloor 4n^{4/3} \rfloor} \leq \left(\frac{n(n-1)}{2}+1\right)^{4n^{4/3}}$  ways. (Note that there are at most  $\frac{n(n-1)}{2}$  summands and each of them can take one of  $\lfloor 4n^{4/3} \rfloor$  values and use Lemma 1). Therefore,  $|A_n| \leq \left(\frac{n \cdot (n-1)}{2}\right) \left(\frac{n \cdot (n-1)}{2}+1\right)^{4n^{4/3}} \leq n^2 \cdot n^{8n^{4/3}} \leq n^{10n^{4/3}}$ .

Hence,

$$|(G_n \setminus W_n) \setminus (D_n \cup L_n \cup S_n)| \leq n! \cdot n^{10n^{4/3}}$$

It is sufficient to prove that

$$\lim_{n \rightarrow \infty} \frac{n! \cdot n^{10n^{2/3}}}{2^{\frac{n(n-1)}{2}}} \leq 0$$

Let us prove this

$$\lim_{n \rightarrow \infty} \frac{n! \cdot n^{10n^{4/3}}}{2^{\frac{n(n-1)}{2}}} \leq \lim_{n \rightarrow \infty} \frac{n^n \cdot n^{10n^{4/3}}}{2^{\frac{n(n-1)}{2}}} \leq \lim_{n \rightarrow \infty} \frac{n^{11n^{4/3}}}{2^{\frac{n(n-1)}{2}}} = \lim_{n \rightarrow \infty} \left( \frac{n^{11}}{2^{\frac{n(n-1)}{4/3}}} \right)^{n^{4/3}}$$

Note that  $\lim_{n \rightarrow \infty} \left( \frac{n^{11}}{2^{\frac{n(n-1)}{4/3}}} \right) = 0$ , hence indeed  $\lim_{n \rightarrow \infty} \left( \frac{n^{11}}{2^{\frac{n(n-1)}{4/3}}} \right)^{n^{4/3}} = 0$ . This proves our theorem.

We would like to establish what portion of connected graphs are graphs that have nonisomorphic graphs with the same Balaban index, more formally, we would like to calculate  $\left| \bigcup_{n \in N} W_n \right| / \left| \bigcup_{n \in N} C_n \right|$ . Unfortunately, this is impossible, because both nominator and denominator of the last ratio are infinitesimal. The best that we can do is to calculate

$$\lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right|$$

It is obvious that  $\lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right| \leq 1$ . In order to prove that  $\lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right| = 1$ , it is sufficient to prove that for each  $\varepsilon > 0$ , we have  $\lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right| > 1 - \varepsilon$ . Denote by  $n_0 = n_0(\varepsilon)$  the smallest natural number such that we have  $\frac{|W_n|}{|C_n|} > 1 - \frac{\varepsilon}{2}$  for each  $n > n_0$ . It follows that:

$$\begin{aligned} \lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right| &= \lim_{x \rightarrow \infty} \frac{\sum_{n=1}^x |W_n|}{\sum_{n=1}^x |C_n|} > \lim_{x \rightarrow \infty} \frac{\sum_{n=n_0+1}^x |C_n| \cdot \left(1 - \frac{\varepsilon}{2}\right)}{\sum_{n=1}^{n_0} |C_n| + \sum_{n=n_0+1}^x |C_n|} = \\ &= \lim_{x \rightarrow \infty} \frac{\frac{\varepsilon}{2} \cdot \sum_{n=n_0+1}^x |C_n| + \sum_{n=n_0+1}^x |C_n| \cdot (1 - \varepsilon)}{\sum_{n=1}^{n_0} |C_n| + \sum_{n=n_0+1}^x |C_n|} \end{aligned}$$

Note that  $\sum_{n=1}^{n_0} |C_n|$  is a finite number and that  $\lim_{x \rightarrow \infty} \sum_{n=n_0+1}^x |C_n|$  is an infinite number. Therefore, we can

conclude that  $\lim_{x \rightarrow \infty} \sum_{n=n_0+1}^x |C_n| \cdot \frac{\varepsilon}{2} > (1 - \varepsilon) \sum_{n=1}^{n_0} |C_n|$ . It follows that

$$\lim_{x \rightarrow \infty} \frac{\frac{\varepsilon}{2} \cdot \sum_{n=n_0+1}^x |C_n| + \sum_{n=n_0+1}^x |C_n| \cdot (1 - \varepsilon)}{\sum_{n=1}^{n_0} |C_n| + \sum_{n=n_0+1}^x |C_n|} > \lim_{x \rightarrow \infty} \frac{(1 - \varepsilon) \sum_{n=1}^{n_0} |C_n| + \sum_{n=n_0+1}^x |C_n| \cdot (1 - \varepsilon)}{\sum_{n=1}^{n_0} |C_n| + \sum_{n=n_0+1}^x |C_n|} = 1 - \varepsilon$$

Hence, indeed  $\lim_{x \rightarrow \infty} \left| \bigcup_{n=1}^x W_n \right| / \left| \bigcup_{n=1}^x C_n \right| = 1$ .

## 4 CONCLUSIONS

From the discussion above, the following conclusion follows: *For almost all connected graphs G there is a nonisomorphic graph G' such that J(G) = J(G')*. Since index J is among the least degenerate topological indices, our results imply that *a fortiori* other topological indices are even more degenerate for general graphs. It remains to be seen whether indices with even lower degeneracy than J, such as BCUT [26–28], obey the theorem proved here.

## Acknowledgment

One of the authors (D.V.), acknowledges a support from the Ministry of Science, Education and Sports of Republic of Croatia (Grant No. 0037117).

## 5 REFERENCES

- [1] J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*. Gordon & Breach, Amsterdam, 1999.
- [2] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.
- [3] L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure–Activity Analysis*, Research Studies Press, Letchworth, 1986.
- [4] L. B. Kier and L. H. Hall, *Molecular Structure Description: The Electrotological State*; Academic Press, San Diego, 1999.
- [5] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley – VCH, New York, 2000.
- [6] M. Randić, In *Encyclopedia of Computational Chemistry* (P. v. R. Schleyer et al. Eds.), Wiley, Chichester, 1998,

pp. 3018–3032.

- [7] M. Karelson, *Molecular Descriptors in QSAR/QSPR*, Wiley – Interscience, New York, 2000.
- [8] D. Bonchev, *Information Theoretic Indices for Characterization of Chemical Structure*, Research Studies Press – Wiley, Chichester, 1983.
- [9] N. Trinajstić, *Chemical Graph Theory*, 2<sup>nd</sup> ed. CRC Press, Boca Raton, 1992.
- [10] A. T. Balaban, In *Encyclopedia of Analytical Chemistry* (R. A. Meyers, Ed.), Wiley, Chichester, 2000, vol. 8, pp. 7288–7311.
- [11] A. T. Balaban, *Chem. Phys. Lett.* **1982**, *80*, 399–404.
- [12] A. T. Balaban, *Pure Appl. Chem.* **1983**, *55*, 199–206.
- [13] M. Randić, *J. Am. Chem. Soc.* **1975**, *97*, 6609–6615.
- [14] A. T. Balaban, N. Ionescu–Pallas and T. S. Balaban, *MATCH Commun. Math. Comput. Chem.* **1985**, *17*, 121–146.
- [15] A. T. Balaban and P. Filip, *MATCH Commun. Math. Comput. Chem.* **1984**, *16*, 163–190.
- [16] A. T. Balaban, *MATCH Commun. Math. Comput. Chem.* **1986**, *21*, 115–122.
- [17] O. Ivanciuc, T. Ivanciuc and A. T. Balaban, *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 395–401.
- [18] M. Barysz, G. Jashri, R. S. Lall, V. K. Srivastava, and N. Trinajstić, In *Chemical Applications of Topology and Graph Theory* (R. B. King, Ed.), Elsevier, Amsterdam, 1983, pp. 222–227.
- [19] A. T. Balaban, In *Topology in Chemistry: Discrete Mathematics of Molecules* (Eds. D. H. Rouvray and R. B. King), Horwood, Chichester, 2002, pp. 89–112.
- [20] A. T. Balaban, D. Mills, and S. C. Basak, *MATCH Commun. Math. Comput. Chem.* **2002**, *45*, 5–26.
- [21] T. S. Balaban, A. T. Balaban, and D. Bonchev, *J. Mol. Struct. (Theochem)* **2001**, *535*, 81–92.
- [22] G. Grassy, B. Calas, A. Yasri, R. Lahana, J. Woo, S. Iyer, M. Kaczorek, R. Floc'h, and R. Buelow, *Nature Biotechnol.* **1998**, *16*, 748–752.
- [23] C. I. Bermudez, E. E. Daza, and E. J. Andrade, *Theor. Biol.* **1999**, *197*, 193–205.
- [24] J. T. Wong, *Proc. Natl. Acad. Sci. USA*, **1975**, *72*, 1909–1912.
- [25] A. T. Balaban and L. V. Quintas, *MATCH Commun. Math. Comput. Chem* **1983**, *14*, 213–233.
- [26] R. S. Pearlman and K. M. Smith, *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 28–35.
- [27] D. T. Stanton, *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 11–20.
- [28] F. R. Burden, *J. Chem. Inf. Comput. Sci.* **1989**, *28*, 225–227.

## Biographies

**Damir Vukičević** is assistant professor of mathematics at University of Split, Croatia. He was born in 1975, and obtained degrees BSc in 1998, MA in 2000 and PhD in 2003. His research interests include discrete mathematics (especially graph theory), mathematical chemistry, algorithms and their optimization, applications of computer science (especially in chemistry). So far he co-worked with four members of Academies of Science and Arts (from Croatia, Romania, Serbia and Monte Negro) and several other distinguished scientists.

**Alexandru T. Balaban** is professor of organic and general chemistry at the Texas A&M University in Galveston. Between 1956 and 1999 he has taught organic chemistry at the Bucharest Polytechnic University, Romania. His research fields include: new syntheses of aromatic heterocycles, stable nitrogen free radicals, catalytic automerization of phenanthrene, chemical applications of graph theory (reaction graphs, enumeration of valence isomers of annulenes and their derivatives, topological indices including the “Balaban index”  $J$  used in drug design, QSAR and QSPR studies, and theoretical invariants for fullerenes). Purely graph-theoretical results derived from reaction graphs are the unique trivalent cage with girth 11, and the first of the three possible trivalent cages with girth 10. He has authored or edited 17 books, over 60 chapters in books edited by other authors, and over 650 papers published in peer-reviewed journals. He is a member of the Romanian Academy, of the American–Romanian Academy, and an Honorary Member of the Hungarian Academy of Sciences. Among his awards is the 1994 Skolnik Award of the Division of Chemical Information of the American Chemical Society.