Bounds for the Sum-Balaban index and (revised) Szeged index of regular graphs

Hui Lei and Hua Yang*

Center for Combinatorics and LPMC-TJKLC
Nankai University, Tianjin 300071, China
E-mail: leihui0711@163.com; yanghuasunny1991@163.com

Abstract

Mathematical properties of many topological indices are investigated. Knor et al. gave an upper bound for the Balaban index of r-regular graphs on n vertices and a better upper bound for fullerene graphs. They also suggested exploring similar bounds for other topological indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index, and give upper and lower bounds for these three indices of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively.

Keywords: Sum-Balaban index; the (revised) Szeged index; regular graph; fullerene graph

1. Introduction

Thousands of topological indices are introduced to characterize the physical-chemical properties of molecules [57]. We can divide these topological indices into three types according the definitions: degree-based indices, distance-based indices and spectrum-based indices. Degree-based indices contain (general) Randić index [47], (general) zeroth order Randić index [47, 34, 35, 55], Zagreb index [29, 26, 3, 5, 20, 58], connective eccentricity index [62, 63] and so on. Distance-based indices [61, 15] include Balaban index [7, 8, 4], Wiener index [51, 50, 41, 22, 25, 33], Wiener polarity index [19, 52], Szeged index [2], Kirchhoff index [23, 24], the ABC index [32, 54], and the Harary index [1, 6], and so on. Eigenvalues of graphs [64], various of graph energies [10, 11, 36, 37, 43, 48, 38, 49,

*The corresponding author.

27, 13, 15, 30, 53], the Estrada index [39], and HOMO-LUMO index [46] belong to spectrum-based indices. Actually, there are also some topological indices defined based on both degrees and distances [60], such as degree distance [21]. From mathematical aspect, one direction to studying properties of each index is to determine the extremal values of the index among a given classes of graphs. In this paper, we focus on the bound for the Sum-Balaban index and the (revised) Szeged index.

Let $G = (V,E)$ be a simple graph. The distance between vertices u and v is denoted by $d_G(u,v)$. Let $w(u) = \sum_{a\in V} d_G(u,a)$. The *Balaban index* of G is defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv\in E} \frac{1}{\sqrt{w(u)\cdot w(v)}},$$

which was proposed by Balaban [7, 8] in 1982. It is also called the *average distance-sum connectivity index* or *Balaban J index*. Furthermore, Balaban et al. [9] proposed the concept of the *Sum-Balaban index* for a connected graph G, namely,

$$SJ(G) = \frac{m}{m-n+2} \sum_{e=uv\in E} \frac{1}{\sqrt{w(u)+w(v)}}.$$

We emphasize that many mathematical properties and results on the Balaban index and the Sum-Balaban index have been achieved, see [12, 16, 17, 45, 59, 65].

As a topological index, the Sum-Balaban index was widely used in QSAR/QSPR modeling. And several approaches have been presented for the calculation of Sum-Balaban index by taking into account the chemical nature of elements. However, many mathematical properties of Sum-Balaban index are still not studied extensively. For example, we have known that the complete graph K_n has the maximum Sum-Balaban index and

$$SJ(K_n) = \frac{\binom{n}{2}}{\binom{n}{2}-n+2} \binom{n}{2} \frac{1}{\sqrt{2(n-1)}}.$$

However, the minimum value among n-vertex graphs is not known.

Let $e = uv \in E$. Define three sets as follows:

$$N_u(e) = \{w \in V(G) : d_G(u,w) < d_G(v,w)\},$$

$$N_v(e) = \{w \in V(G) : d_G(v,w) < d_G(u,w)\},$$

$$N_0(e) = \{w \in V(G) : d_G(u,w) = d_G(v,w)\}.$$

Obviously, $N_u(e), N_v(e), N_0(e)$ constitutes a partition of $V(G)$. And set $|N_u(e)| = n_u(e)$, $|N_v(e)| = n_v(e)$ and $|N_0(e)| = n_0(e)$. Gutman [28] presented a graph invariant named as *Szeged index*, defined by

$$S_z = \sum_{e=uv\in E} n_u(e)n_v(e).$$

The above index is based on counting of vertices of the underlying graph. Also the edge-invariant is considered, say "edge-Szeged index" [18, 44]. Randić [56] found the Szeged index does not count the contributions of the vertices at equal distances to the two endpoints of an edge and then proposed the *revised Szeged index* as follows

$$S_z^* = \sum_{e=uv\in E} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

In [7], Aouchiche and Hansen proved the upper bound of the connected graph with n vertices and m edges is $\frac{n^2m}{4}$. Then Xing and Zhou [57] determined the maximum and minimum revised Szeged index of unicyclic graphs with $n \geq 5$ and the unicyclic graph with the unique cycle is of length $r(3 \leq r \leq n)$. Several properties and applications of two indices have been presented in [8, 16, 17].

Denote by K_n, P_n and C_n the complete graph, path graph and cycle graph with n vertices, respectively. Among graphs on n vertices, Balaban index attains its maximum for the complete graph K_n and $J(K_n) = \frac{n^3-n^2}{2(n^2-3n+2)}$, which is slightly more than $n/2$. However, its minimum value among n-vertex graphs is not known. Recently, Knor et al. [42] prove that if G is an n-vertex r-regular graph, then $J(G)$ tends to 0 as n tends to ∞. In other words, zero is also an accumulation point for Balaban index.

Theorem 1. *Let G be an r-regular graph on n vertices with* $r \geq 3$. *Then*

$$J(G) \leq \frac{r^2(r-1)^2}{2(r-2)^2 \left\lfloor \log_{r-1} \frac{(r-2)n+2}{r} \right\rfloor},$$

which implies that $\lim_{n\to\infty} J(G) = 0$.

The upper bound of fullerene graphs was also determined. Fullerenes [40] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces, and their corresponding graphs, fullerene graphs, are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces.

Theorem 2. *Let G be a fullerene graph on $n \geq 60$ vertices. Then $J(G) \leq \frac{25}{\sqrt{n}}$.*

At the end of [42], Knor et al. suggested exploring similar bounds for other indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index. Following the result of Knor et al., we will give bounds for the Sum-Balaban index and the (revised) Szeged index of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively.

2. Regular graphs

In this section, we will concentrate the bounds on r-regular graphs.

Theorem 3. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$SJ(G) \leq \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}}\sqrt{2\lfloor \log_{r-1}(\frac{(r-2)n+2}{r})\rfloor}}.$$

Proof. Let $u \in V(G)$ and n_i be the number of vertices at distance i from u. Thus,

$$w(u) = \sum_i i \cdot n_i, \quad \sum_i n_i = n.$$

Since the graph is r-regular, we have $n_i \leq r(r-1)^{i-1}$. Let s and c satisfy that

$$n = 1 + r + r(r-1) + \ldots + r(r-1)^{s-1} + c, \;\; 0 \leq c < r(r-1)^s.$$

Thus we can bound $w(u)$ in the following way:

$$w(u) = \sum_{i=0}^{s+1} i \cdot n_i \geq 1r + 2r(r-1) + \ldots + sr(r-1)^{s-1} + (s+1)c.$$

In other words, a lower bound on $w(u)$ is attained if the breadth-search tree, rooted at u, is an almost complete tree with all leaves at distance s and maybe $s+1$ from u, and every non-leaf vertex is of degree r. So, we have

$$1 + (r-1) + \ldots + (r-1)^{s-1} = \frac{n-1-c}{r},$$

and hence

$$\frac{(r-1)^s - 1}{r-2} = \frac{n-1-c}{r},$$

which gives

$$s = \log_{r-1}\left(\frac{(r-2)n+2-c(r-2)}{r}\right). \tag{1}$$

From (1) and from $c < r(r-1)^s$ we get

$$\frac{(r-2)n+2}{r} = (r-1)^s + \frac{c(r-2)}{r} < (r-1)^s + (r-1)^s(r-2) = (r-1)^{s+1},$$

which means that $\log_{r-1}(\frac{(r-2)n+2}{r}) < s+1$. Since $\log_{r-1}(\frac{(r-2)n+2}{r}) \geq s$ by (1), we have $s = \lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor$. Consequently,

$$\begin{aligned} w(u) \geq sr(r-1)^{s-1} &= \lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor \cdot r \cdot (r-1)^{\lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor - 1} \\ &\geq \lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor r \frac{(r-2)n+2}{r} \frac{1}{(r-1)^2} \\ &= \lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor \frac{(r-2)n+2}{(r-1)^2}. \end{aligned}$$

Thus,

$$\begin{aligned} SJ(G) &\leq \frac{m}{m-n+2} m \frac{1}{\sqrt{2w(u)}} \\ &\leq \frac{\frac{rn}{2}}{\frac{rn}{2} - n + 2} \frac{rn}{2} \frac{1}{2\sqrt{\lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor \frac{(r-2)n+2}{(r-1)^2}}} \\ &< \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}} \sqrt{2\lfloor \log_{r-1}(\frac{(r-2)n+2}{r}) \rfloor}}. \end{aligned}$$

∎

Next, we consider the Szeged index of r-regular graphs.

Theorem 4. *Let G be an r-regular connected graph on n vertices, where n is even and $r \leq \frac{n}{2}$. Then*

$$S_z(G) \leq \frac{rn^3}{8}.$$

And this bound is tight.

Proof. By the definition, we know that $n_u(e)+n_v(e) \leq n$ and $n_0(e) \geq 0$. So the smaller the $n_0(e)$ is and the closer $n_u(e)$ and $n_v(e)$ are, and then the larger the Szeged index is. Hence,

$$S_z(G) = \sum_{e=uv\in E} n_u(e)n_v(e) \leq m\frac{n}{2}\frac{n}{2} \leq \frac{rn^3}{8}.$$

We say this bound is tight, namely, for given n and r, there exist a graph G satisfying that $S_z(G) = \frac{rn^3}{8}$. We construct such a graph as follows. Constitute a bipartite graph $B_{\frac{n}{2},r}$ with vertex classes $X = \{u_i : 1 \leq i \leq \frac{n}{2}\}$ and $Y = \{u_i' : 1 \leq i \leq \frac{n}{2}\}$ in which u_i join to the corresponding vertices u_i' , $u_{i+1}', \dots, u_{i+r-1}'$, where the subscripts are taken modulo $\frac{n}{2}$. See Figure 1 for $B_{6,3}$.

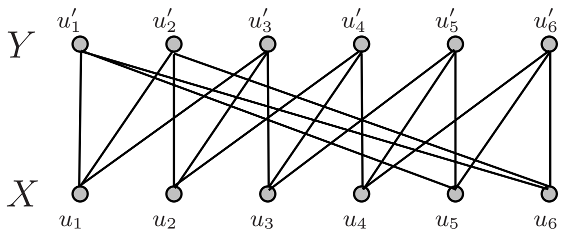

Figure 1: The graph $B_{6,3}$.

By some elementary calculations, we get $n_u(e) = n_u(e) = \frac{n}{2}$ for an arbitrary edge $e = uv$. Therefore,

$$S_z(B_{\frac{n}{2},r}) = \frac{rn^3}{8}.$$

The result is proved. ∎

Theorem 5. *Let G be an r-regular connected graph on n vertices. Then*

$$S_z^*(G) \leq \frac{rn^3}{8}.$$

And this bound is tight.

Proof. We know the sum of $n_u(e) + \frac{n_0(e)}{2}$ and $n_v(e) + \frac{n_0(e)}{2}$ is n. Therefore, the closer the above two values are, the larger the product is. So, if $n_u(e) + \frac{n_0(e)}{2} = n_v(e) + \frac{n_0(e)}{2} = \frac{n}{2}$, then the product is largest obviously. At this time,

$$S_z^*(G) \leq \frac{rn^3}{8}.$$

If for arbitrary n and r satisfying that nr is even, we can find a graph with the required conditions and the revised Szeged index is $\frac{rn^3}{8}$, then the theorem is proved obviously.

In the following, we will characterize such an r-regular graph $C_{n,r}$ with n vertices. First, we start from a cycle with n vertices, i.e., C_n. Since at least one of r and n is even, we consider two situations.

Case 1. One of r and n is odd.

For each vertex u in C_n, u is adjacent to every vertex of a path P_{r-2} which lies on C_n, satisfying that the distances in C_n between u and two endpoints of P_{r-2} are equal. Then we get an r-regular graph. As examples, see Figure 2 for $C_{8,5}$ and $C_{9,4}$.

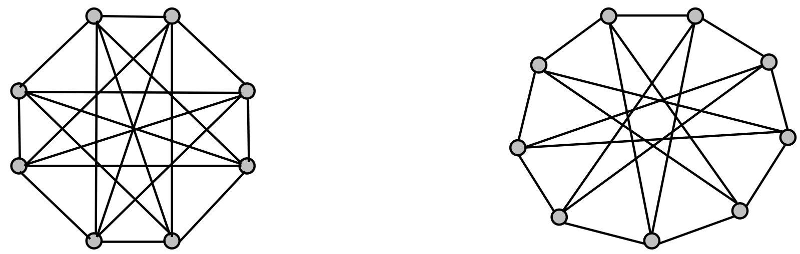

Figure 2: The graph $C_{8,5}$ (left) and $C_{9,4}$ (right).

Case 2. Both of r and n are even.

For each vertex u in C_n, find the symmetrical vertex v of u on C_n and join u to $\frac{r-2}{2}$ consecutive vertices on the left and right sides of v on C_n, respectively. Then we get an r-regular graph. See Figure 3 for $C_{6,4}$.

It is easy to calculate the values of $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ for each edge of $C_{n,r}$. ∎

Next, we will give a lower bound of the revised Szeged index.

Theorem 6. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$S_z^*(G) \geq \frac{n(r^2+2r)(2n-r-2)}{8}.$$

Proof. From the above proof, we know the larger the difference value of $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ is, the lower the product is. Therefore, we need to find the

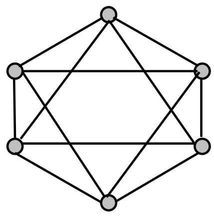

Figure 3: The graph $C_{6,4}$.

largest difference. For some edge $e(=uv)$ of G, we know that $r-1$ neighbors of u are either in $N_u(e)$ or $N_0(e)$. Obviously, the difference between $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ is largest when the graph satisfies the following conditions: u and v have $r-2$ common neighbors which form a complete subgraph K_{r-2}; the other neighbor x of u is adjacent to all neighbors of v. See Figure 4. In this case, $n_u(e)=2$, $n_v(e)=n-r$ and $n_0(e)=r-2$. So we get the conclusion

$$S_z^*(G)\geq\frac{rn}{2}(2+\frac{r-2}{2})(n-r+\frac{r-2}{2})\geq\frac{n(r^2+2r)(2n-r-2)}{8}.$$

∎

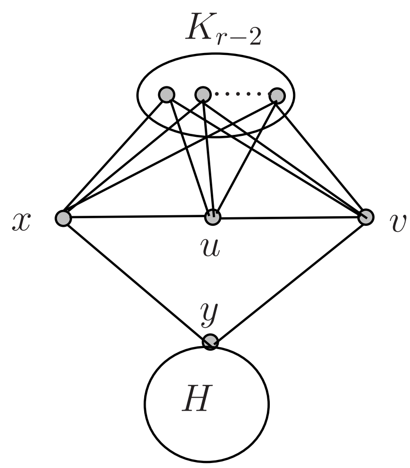

Figure 4: The graph G.

3. Fullerene graphs

Here we consider the chemical structure–fullerene.

Theorem 7. *Let G be a fullerene graph on $n \geq 60$ vertices. Then*

$$SJ(G) \leq \frac{9n}{\sqrt{n\sqrt{n}}}.$$

Proof. Let $u \in V(G)$ and n_i be the number of vertices at distance i from u. Then $n_0 = 1$ and $n_1 = 3$. Moreover, it is shown that $n_{i+1} \leq n_i + 3$ for $i \geq 1$. This immediately gives the bound $n_i \leq 3i$ for $i \geq 1$. We obtain a lower bound of $w(u)$ by assuming each $n_i = 3i$ for $i \geq 1$, as in this way we have fewer vertices at higher distance. So

$$w(u) = \sum_i i \cdot n_i \geq 1 * 3 + 2 * 6 + \ldots + s * 3s + (s+1)c,$$

for some s and c, where $0 \leq c < 3s+3$ and $1 + 3 + \cdots + 3s + c = n$. Hence,

$$3(1 + 2 + \cdots + s + (s+1)) \geq n,$$

and so

$$s^2 + 3s + 2 \geq \frac{2n}{3}.$$

Since $n \geq 60$, we have $s \geq 5$, and hence $s^2 \geq 3s + 2$, which gives $s \geq \sqrt{\frac{n}{3}}$. Since s is integer, we obtain

$$s \geq \left\lceil \sqrt{\frac{n}{3}} \right\rceil.$$

Consequently,

$$w(u) \geq 1 * 3 + 2 * 6 + \cdots + 3\lceil\sqrt{\frac{n}{3}}\rceil^2 + c(\lceil\sqrt{\frac{n}{3}}\rceil + 1) \geq 3 \sum_{j=1}^{\lceil\sqrt{\frac{n}{3}}\rceil} j^2 > \frac{n}{3}\sqrt{\frac{n}{3}}.$$

Thus,

$$SJ(G) \leq \frac{m}{m-n+2} m \frac{1}{\sqrt{2w(u)}} \leq \frac{\frac{rn}{2}}{\frac{rn}{2} - n + 2} \frac{rn}{2} \frac{1}{\sqrt{2\frac{n}{3}\sqrt{\frac{n}{3}}}} \leq \frac{9\sqrt{3\sqrt{3}}n}{2\sqrt{2n\sqrt{n}}} < \frac{9n}{\sqrt{n\sqrt{n}}}.$$

$\blacksquare$

We know that the smallest fullerene graph is the dodecahedral C_{20}. Other fullerenes are denoted by $C_{2n}, n = 12, 13, \ldots$. For each edge $e(= uv)$ of one fullerene, there are at least 2 vertices at the same distance to u and v. Particularly, for the five edges of the outer pentagonal or hexagonal faces, there are at least 4 such vertices. Then we can get Theorem 8 directly.

Theorem 8. *Let G be a fullerene graph on n vertices. Then*

$$S_z(G) < \frac{3n(n-2)^2}{8} - 5(n-3).$$

The following result can be obtained directly from Theorems 2.2 and 2.3.

Theorem 9. *Let G be a fullerene graph on $n \geq 60$ vertices. Then*

$$\frac{15n(2n-5)}{8} < S_z^*(G) \leq \frac{3n^3}{8}.$$

4. Cubic graphs

In [42], Knor et al. consider a special cubic graph H_n. In this section, we consider the Sum-Balaban and the (revised) Szeged index value of H_n.

Let $4|n$, and H_n be such a graph which has the cycle of length $3\frac{n}{4}$, in which every third vertex is doubled, see Figure 5 for H_{12}. In other words, H_n is obtained from $n/4$ copies of $K_4 - e$ joined by $n/4$ extra edges. Obviously, H_n is a cubic connected graph. And we can get the following conclusion.

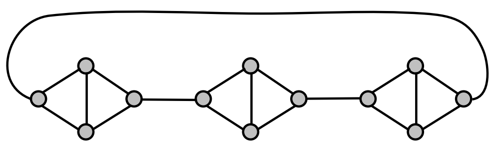

Figure 5: The graph H_{12}.

Theorem 10. *For positive n is divisible by 4, it holds*

$$SJ(H_n) \leq 6\sqrt{2}.$$

Proof. Let $\ell = \frac{3n}{4}$. First we give a lower bound for $w(u), u \in V(H_n)$. In order to do so, we find the total distance $cw(u)$ from u to the vertices of the original cycle. If l is even, then

$$cw(u) = 1+2+\cdots+\frac{\ell}{2}+1+2+\cdots+(\frac{\ell}{2}-1) = \frac{\ell^2}{4}.$$

Similarly, if ℓ is odd, then

$$cw(u) = 2(1+2+\cdots+\frac{\ell-1}{2}) = \frac{\ell^2-1}{4}.$$

As there is at least one vertex in H_n not on the original cycle and different from u, and as the distance of this vertex to u is at least one, for both the above cases we get

$$w(u) \geq cw(u)+1 > \frac{\ell^2}{4} = \frac{9n^2}{64}.$$

Hence,

$$SJ(H_n) \leq \frac{\frac{3n}{2}}{\frac{3n}{2}-n+2}\frac{3n}{2}\frac{1}{\sqrt{2\frac{9n^2}{64}}} = \frac{12n}{\sqrt{2}(n+4)} < 6\sqrt{2}.$$

∎

From the properties of this graph, we can get the following results easily.

Theorem 11. *For positive n divisible by 4, it holds*

$$S_z(H_n) = \begin{cases} \frac{5n(n-2)^2+4n}{16} & \text{if } \frac{n}{4} \text{ is odd,} \\ \frac{5n^3-8n^2+4n}{16} & \text{if } \frac{n}{4} \text{ is even.} \end{cases}$$

Theorem 12. *For positive n divisible by 4, it holds*

$$S_z^*(H_n) = \begin{cases} \frac{3n^3}{8} & \text{if } \frac{n}{4} \text{ is odd,} \\ \frac{3n^3-2n}{8} & \text{if } \frac{n}{4} \text{ is even.} \end{cases}$$

5. Summary and Conclusion

Knor et al. gave an upper bound for the Balaban index of r-regular graphs on n vertices and a better upper bound for fullerene graphs. They also suggested exploring similar bounds for other indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index, and give bounds for these three indices of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively. As a future work, it would be interesting to consider other topological indices for regular graphs.

Acknowledgments

The authors would like to thank the two referees for their valuable suggestions. This work was supported by NSFC and PCSIRT.

References

[1] S. Alikhani, M.A. Iranmanesh, H. Taheri, Harary index of dendrimer nanostar NS2[n], *MATCH Commum. Math. Comput. Chem.* **71**(2014) 383–394.

[2] T. Al-Fozan, P. Manuel, I. Rajasingh, and R.S. Rajan. Computing Szeged index of certain nanosheets using partition technique. *MATCH Commun. Math. Comput. Chem.* **72**(2014), 339–353.

[3] M. Arezoomand, B. Taeri, Zagreb Indices of the Generalized Hierarchical Product of Graphs, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 131-140.

[4] A.R. Ashrafi, H. Shabani, and M.V. Diudea. Balaban index of dendrimers. *MATCH Commun. Math. Comput. Chem.* **69**(2013), 151–158.

[5] M. Azari, A. Iranmanesh, Chemical Graphs Constructed from Rooted Product and Their Zagreb Indices, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 901–919.

[6] M. Azari and A. Iranmanesh. Harary index of some nano-structures. *MATCH Commum. Math. Comput. Chem.* **71**(2014), 373–382.

[7] A.T. Balaban, Highly discriming distance-based topological index, *Chem. Phys. Lett.* **89** (1982) 399–404.

[8] A.T. Balaban, Topological indices based on topological distance in molecular graphs, *Pure Appl. Chem.* **55** (1983) 199–206.

[9] A.T. Balaban, P.V. Khadikar, S. Aziz, Comparison of topological indices based on iterated 'sum' versus 'product' operations, *Iranian J. Math. Chem.* **1** (2010) 43–67.

[10] S. B. Bozkurt and D. Bozkurt. On incidence energy. *MATCH Commun. Math. Comput. Chem.* **72**(2014), 215–225.

[11] L. Chen, Y. Shi, The maximal matching energy of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 105–120.

[12] Z. Chen, M. Dehmer, Y. Shi, H. Yang, Sharp upper bounds for the Balaban index of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.*, accepted for publication.

[13] K. C. Das, I. Gutman, A. S. Cevik, B. Zhou, On Laplacian energy. *MATCH Commun. Math. Comput. Chem.* **70**(2013) 689–696.

[15] K. C. Das, S. Sorgun, On Randić energy of graphs, *MATCH Commun. Math. Comput. Chem.* **72**(2014) 227–238.

[15] M. Dehmer, Y. Shi, The uniqueness of D_{MAX}-matrix graph invariants, *PLOS ONE* **9**(1)(2014), e83868.

[16] H. Deng, On the Balaban index of trees, *MATCH Commum. Math. Comput. Chem.* **66** (2011) 253–260.

[17] H. Deng, On the Sum-Balaban index, *MATCH Commum. Math. Comput. Chem.* **66** (2011) 273–284.

[18] A. Dolati, I. Motevalian, A. Ehyaee, Szeged index, edge Szeged index, and semi-star trees, *Discrete Appl. Math.* **158** (2010) 876–881.

[19] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 235–244.

[20] M. Eliasi, D. Vukicevic, Comparing the Multiplicative Zagreb Indices, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 765-773

[21] L. Feng, W. Liu, A. Ilić, G. Yu, The degree distance of unicyclic graphs with given matching number, *Graphs Combin.* **29** (2013) 449–462.

[22] L. Feng, W. Liu, G. Yu, S. Li, The hyper-wiener index of graphs with given bipartition, *Utilitas Math.* **95** (2014) 23–32.

[23] L. Feng, G. Yu, W. Liu, Further resuts regarding the degree Kirchhoff index of a graph, *Miskolc Math. Notes* **15** (2014) 97–108.

[24] L. Feng, G. Yu, K. Xu, Z. Jiang, A note on the Kirchhoff index of bicyclic graphs, *Ars Combin.* **114** (2014) 33–40.

[25] C. M. da Fonseca, M. Ghebleh, A. Kanso, D. Stevanovic, Counterexamples to a conjecture on Wiener index of common neighborhood graphs, *MATCH Commun. Math. Comput. Chem.* **72(1)**(2014) 333–338.

[26] C.M. da Fonseca and D. Stevanovic. Further properties of the second Zagreb index. *MATCH Commum. Math. Comput. Chem.* **72**(2014), 655–668.

[27] M. Ghorbani, M. Faghani, A.R. Ashrafi, R.S. Heidari, and A. Graovac. An upper bound for energy of matrices associated to an infinite class of fullerenes. *MATCH Commun. Math. Comput. Chem.* **71**(2014), 341–354.

[28] I. Gutman, A formula for the Wiener number of trees and its extension to graphs con- taining cycles, *Graph Theory Notes of New York* **27** (1994) 9–15.

[29] I. Gutman, An exceptional property of first Zagreb index, *MATCH Commum. Math. Comput. Chem.* **72** (2014) 733–740.

[30] I. Gutman, X. Li, Y. Shi, J. Zhang, Hypoenergetic trees, *MATCH Commun. Math. Comput. Chem.* **60**(2008) 415–426.

[31] F. Harary, *Graph Theory*, Addison Wesley Publishing Company, Reading, MA, USA, 1969.

[32] S.A. Hosseini, M.B. Ahmadi, and I. Gutman. Kragujevac trees with minimal atom-bond connectivity index. *MATCH Commun. Math. Comput. Chem.* **71** (2014) 5–20.

[33] K. Hrinakova, M. Knor, R. Skrekovski, A. Tepeh, A congruence relation for the Wiener index of graphs with a tree-like structure, *MATCH Commun. Math. Comput. Chem.* **72(3)**(2014) 791–806.

[34] Y. Hu, X. Li, Y. Shi, T. Xu, Connected (n,m)-graphs with minimum and maximum zeroth-order general Randić index, *Discrete Appl. Math.* **155**(8)(2007) 1044–1054.

[35] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* **54**(2)(2005) 425–434.

[36] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, *Linear Algebra Appl.* **434** (2011) 1370–1377.

[37] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of unicyclic graphs, *European J. Combin.* **32** (2011) 662–673.

[38] S. Ji, X. Li, Y. Shi, The extremal matching energy of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **70**(2) (2013), 697–706.

[39] A. Khosravanirad. A lower bound for Laplacian Estrada index of a graph. *MATCH Commum. Math. Comput. Chem.* **70** (2013) 175–180.

[40] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, R.E. Smalley, C60: Buckmin- sterfullerene, *Nature* **318** (1985) 162–163.

[41] M. Knor, B. Lužar, R. Škrekovski, and I. Gutman. On Wiener index of common neighborhood graphs. *MATCH Commum. Math. Comput. Chem.* **72** (2014) 321–332.

[42] M. Knor, R. Škrekovski, and A. Tepeh. Balaban index of cubic graphs. *MATCH Commum. Math. Comput. Chem.* **73** (2015) 519–528.

[43] H. Li, Y. Zhou, L. Su, Graphs with extremal matching energies and prescribed parameters, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 239–248.

[44] J. Li, A relation between the edge Szeged index and the ordinary Szeged index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 621–625.

[45] S. Li, B. Zhou, On the Balaban index of trees, *Ars Combin.* **100** (2011) 503–512.

[46] X. Li, Y. Li, Y. Shi, I. Gutman, Note on the HOMO-LUMO index of graphs, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 85–96.

[47] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[48] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, 2012.

[49] X. Li, Y. Shi, M. Wei, and J. Li, On a conjecture about tricyclic graphs with maximal energy, *MATCH Commun. Math. Comput. Chem.* **72**(1)(2014), 183–214.

[50] H. Lin. Extremal Wiener index of trees with given number of vertices of even degree. *MATCH Commum. Math. Comput. Chem.* **72** (2014) 311–320.

[51] H. Lin. On the Wiener index of trees with given number of branching vertices. *MATCH Commum. Math. Comput. Chem.* **72** (2014) 301–310.

[52] J. Ma, Y. Shi, J. Yue, The Wiener polarity index of graph products, *Ars Combin.* **116** (2014) 235–244.

[53] I. Z. Milovanovic, E. I. Milovanovic, A. Zakic, A short note on graph energy, *MATCH Commun. Math. Comput. Chem.* **72(1)**(2014) 179–182.

[54] J.L. Palacios. A resistive upper bound for the ABC index. *MATCH Commun. Math. Comput. Chem.* **72** (2014) 709–713.

[55] J. Rada, R. Cruz, Vertex-Degree-Based Topological Indices Over Graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 603–616.

[56] M. Randić, On generalization of Wiener index for cyclic structures, *Acta Chim. Slov.* **49**(2002) 483–496.

[57] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2010.

[58] A. Vasilyev, R. Darda, D. Stevanovic, Trees of given order and independence number with minimal first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 775–782.

[59] R. Xing, B. Zhou, A. Grovac, On Sum-Balaban index, *Ars Combin.* **104** (2012) 211–223.

[60] K. Xu, S. Klavzar, K. Das, J. Wang, Extremal (n,m)-graphs with respect to distance-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 865–880.

[61] K. Xu, M. Liu, K. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.

[62] G. Yu, L. Feng, On connective eccentricity index of graphs, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 611–628.

[63] G. Yu, H. Qu, L. Tang, L. Feng, On the connective eccentricity index of trees and unicyclic graphs with given diameter, *J. Math. Anal. Appl.* **420** (2014) 1776–1786.

[64] G. Yu, X. Zhang, L. Feng, The inertia of weighted unicyclic graphs, *Linear Algebra Appl.* **448** (2014) 130–152.

[65] B. Zhou, N. Trinajstic, Bounds on the Balaban index, *Groat. Chem. Acta.* **81** (2008) 319–323.