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ORIGINAL PAPER

Sum-connectivity index of molecular trees

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Abstract We report lower and upper bounds for the sum-connectivity indices of molecular trees with fixed numbers of vertices and pendant vertices.

Keywords Randić connectivity index · Sum-connectivity index · Product-connectivity index · Molecular trees · Lower and upper bounds

1 Introduction

Let G be a simple graph with vertex-set $V(G)$ and edge-set $E(G)$ [1]. For $v \in V(G)$, $d_G(v)$ or d_v denotes the degree of v in G. The Randić connectivity index of G is defined as [2]

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}.$$

It is one of the most successful molecular descriptors in structure-property and structure-activity relationships studies [3–7]. Mathematical properties of this descriptor as summarized in [8,9] and its generalizations/variants [10–12] have also been studied extensively. We also call the $R(G)$ index as the product-connectivity index of G.

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Motivated by Randić's definition of the product-connectivity index, the sum-connectivity index was recently proposed in [13]. The sum-connectivity index of the graph G is defined as

$$\chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}.$$

It is interesting to note that various kinds of variants and extension of the product-connectivity index have been reported, but there is not a single one on the additive version of the connectivity index before the sum-connectivity index was proposed.

The product-connectivity index and the sum-connectivity index are highly inter-correlated quantities. For example, the correlation coefficient between the product-connectivity index and the sum-connectivity index for 137 alkane-trees [14] is 0.9996.

In [15], we also used both the product-connectivity index and the sum-connectivity index to approximate rather accurately the π-electron energy (E_π) of benzenoid hyrocarbons; the correlation coefficients between $\chi(G)$ and E_π, and $R(G)$ and E_π being 0.9999 and 0.9992, respectively. Some basic mathematical properties of the sum-connectivity index have been established in [13,16,17].

A molecular tree is a tree of maximum degree at most four. It models the skeleton of an acyclic molecule [1]. In [13], the n-vertex molecular trees with the minimum, the second minimum and the third minimum as well as the maximum, the second maximum and the third maximum sum-connectivity indices have been determined for sufficiently large n.

In the present report, we give lower and upper bounds for the sum-connectivity indices of molecular trees with fixed numbers of vertices and pendant vertices. The reason why we report the lower and upper bounds of sum-connectivity indices of molecualr trees is related to our efforts to establish the range of optimal descriptor values for their use in the structure-property-activity modeling. In this, we parallel the results for the closely related product-connectivity index reported by Hansen and Mélot [18].

2 Preliminaries

Let T be an n-vertex molecular tree. Denote by n_i the number of vertices with degree i for $i = 1, 2, 3, 4$, and denote by x_{ij} the number of edges of T that connect vertices of degree i and j, where $1 \le i \le j \le 4$. Then

$$\left.\begin{array}{c} n_1 + n_2 + n_3 + n_4 = n \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1) \\ x_{12} + x_{13} + x_{14} = n_1 \\ x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2 \\ x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \\ x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4. \end{array}\right\} \qquad (1)$$

Obviously, n_1 is the number of pendant vertices.

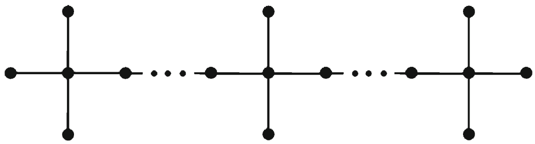

Fig. 1 The structure of $L_e(n, p)$

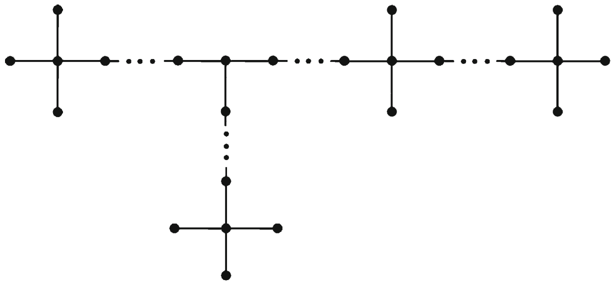

Fig. 2 The structure of $L_o(n, p)$

3 Lower bound for sum-connectivity index of molecular trees

Let $S_{n,p}$ be the tree formed by attaching $p-1$ pendant vertices to a terminal vertex of the $(n-p+1)$-vertex path P_{n-p+1}.

Lemma 1 *Zhou and Trinajstić* [13] *Let T be a tree with n vertices and p pendant vertices, where $3 \le p \le n-2$. Then*

$$\chi(T) \ge \frac{1}{\sqrt{p+2}} + \frac{p-1}{\sqrt{p+1}} + \frac{1}{\sqrt{3}} + \frac{n-p-2}{2}$$

with equality if and only if $T = S_{n,p}$.

From the previous lemma, among the molecular trees with n vertices and p pendant vertices, if $p \le 4$, then $S_{n,p}$ is the unique graph with the minimum sum-connectivity index, while if $p \ge 5$, then $S_{n,p}$ is no longer a molecular tree.

Let S_n be the n-vertex star. We define two types of n-vertex molecular trees.

The first type is denoted by $L_e(n, p)$ for even p with $6 \le p \le \lfloor \frac{n+3}{2} \rfloor$, see Fig. 1. Such trees are composed by $\frac{p-2}{2}$ stars S_5, which are connected by paths whose lengths may be zero. Note that $n_1 = p$, $n_2 = n - \frac{3p}{2} + 1$, $n_3 = 0$, $n_4 = \frac{p}{2} - 1$, $x_{14} = p$, $x_{24} = p-4$, and $x_{22} = n - 2p + 3$ for all such trees. It is easily seen that for given n and p, any such tree has the same sum-connectivity index, equal to

$$\frac{p}{\sqrt{5}} + \frac{p-4}{\sqrt{6}} + \frac{n-2p+3}{2} = \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right)p + \frac{3}{2} - \frac{4}{\sqrt{6}}.$$

The second type is denoted by $L_o(n, p)$ for odd p with $9 \le p \le \lfloor \frac{n+2}{2} \rfloor$, see Fig. 2. The structure of $L_o(n, p)$ is similar to $L_e(n, p)$, but, in this case, such trees are composed by $\frac{p-3}{2}$ stars S_5 and one star S_4, which are connected by paths whose lengths may be zero, and the unique star S_4 is connected by three paths to stars S_5. Note that $n_1 = p, \quad n_2 = n - \frac{3p+1}{2} + 1, \quad n_3 = 1, \quad n_4 = \frac{p-1}{2} - 1, \quad x_{14} = p, \quad x_{24} = p - 6, \quad x_{23} = 3$, and $x_{22} = n - 2p + 2$ for all such trees. It is easily seen that for given n and p, any such tree has the same sum-connectivity index, equal to

$$\frac{p}{\sqrt{5}} + \frac{p-6}{\sqrt{6}} + \frac{3}{\sqrt{5}} + \frac{n-2p+2}{2} = \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right) p + 1 - \sqrt{6} + \frac{3}{\sqrt{5}}.$$

Proposition 1 *Let T be a molecular tree with n vertices and $p \geq 5$ pendant vertices. Then*

$$\chi(T) \geq \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right) p + \frac{3}{2} - \frac{4}{\sqrt{6}}$$

with equality if and only if T is of the type $L_e(n, p)$ for even p with $6 \leq p \leq \lfloor \frac{n+3}{2} \rfloor$. Moreover, if p is odd and $9 \leq p \leq \lfloor \frac{n+2}{2} \rfloor$, then

$$\chi(T) \geq \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right) p + 1 - \sqrt{6} + \frac{3}{\sqrt{5}}$$

with equality if and only if T is of the type $L_o(n, p)$.

Proof We consider (1) as a system of six linear equations in the unknowns $x_{14}, x_{22}, x_{24}, n_2, n_3, n_4$, and solve it. Then the solutions depend on the remaining parameters, namely on $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}, p$ and n. Using the abbreviations

$$\begin{aligned} f_1 &= p - x_{12} - x_{13} \\ f_2 &= x_{12} + x_{23} \\ f_3 &= x_{13} + x_{23} + 2x_{33} + x_{34} \\ f_4 &= x_{34} + 2x_{44}, \end{aligned}$$

we have

$$\begin{aligned} x_{14} &= f_1 \\ x_{22} &= n - \frac{5}{2}p + \frac{1}{2}f_1 - \frac{1}{2}f_2 + \frac{1}{6}f_3 + \frac{1}{2}f_4 + 3 \\ x_{24} &= 2p - f_1 - \frac{2}{3}f_3 - f_4 - 4 \\ n_2 &= n - \frac{3}{2}p - \frac{1}{6}f_3 + 1 \\ n_3 &= \frac{1}{3}f_3 \\ n_4 &= \frac{1}{2}p - \frac{1}{6}f_3 - 1. \end{aligned}$$

We need only x_{14}, x_{22} and x_{24}, which are

$$x_{14} = p - x_{12} - x_{13}$$
$$x_{22} = n - 2p - x_{12} - \frac{1}{3}x_{13} - \frac{1}{3}x_{23} + \frac{1}{3}x_{33} + \frac{2}{3}x_{34} + x_{44} + 3$$
$$x_{24} = p + x_{12} + \frac{1}{3}x_{13} - \frac{2}{3}x_{23} - \frac{4}{3}x_{33} - \frac{5}{3}x_{34} - 2x_{44} - 4.$$

Substituting them back into the formula

$$\chi(T) = \frac{x_{12}}{\sqrt{3}} + \frac{x_{13}}{2} + \frac{x_{14}}{\sqrt{5}} + \frac{x_{22}}{2} + \frac{x_{23}}{\sqrt{5}} + \frac{x_{24}}{\sqrt{6}} + \frac{x_{33}}{\sqrt{6}} + \frac{x_{34}}{\sqrt{7}} + \frac{x_{44}}{2\sqrt{2}},$$

we have

$$\begin{aligned}\chi(T) = {} & \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right)p + \frac{3}{2} - \frac{4}{\sqrt{6}} \\ & + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}} - \frac{1}{2} + \frac{1}{\sqrt{6}}\right)x_{12} + \left(\frac{1}{3} - \frac{1}{\sqrt{5}} + \frac{1}{3\sqrt{6}}\right)x_{13} \\ & + \left(-\frac{1}{6} + \frac{1}{\sqrt{5}} - \frac{2}{3\sqrt{6}}\right)x_{23} + \left(\frac{1}{6} - \frac{1}{3\sqrt{6}}\right)x_{33} \\ & + \left(\frac{1}{3} - \frac{5}{3\sqrt{6}} + \frac{1}{\sqrt{7}}\right)x_{34} + \left(\frac{1}{2} - \frac{2}{\sqrt{6}} + \frac{1}{2\sqrt{2}}\right)x_{44},\end{aligned}$$

i.e.,

$$\begin{aligned}\chi(T) = {} & \frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right)p + \frac{3}{2} - \frac{4}{\sqrt{6}} \\ & + 0.0384x_{12} + 0.0222x_{13} + 0.0084x_{23} + 0.0306x_{33} + 0.0309x_{34} \\ & + 0.0371x_{44}\end{aligned}$$

with positive coefficients for $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}$. Thus it is clear that for fixed n and p, $\chi(T)$ will be minimum if and only if the parameters $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}$ are all equal to zero (provided it is possible). If so, then $x_{14} = p$, $x_{22} = n - 2p + 3$, $x_{24} = p - 4$, $n_2 = n - \frac{3p}{2} + 1$, $n_3 = 0$, and $n_4 = \frac{p}{2} - 1$, implying that p is even and T is of the type $L_e(n, p)$.

Suppose that not all of $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}$ in $\chi(T)$ are zero. Let

$$\begin{aligned}F = F(T) = \chi(T) - \left[\frac{n}{2} + \left(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - 1\right)p + \frac{3}{2} - \frac{4}{\sqrt{6}}\right] \\ = 0.0384x_{12} + 0.0222x_{13} + 0.0084x_{23} + 0.0306x_{33} + 0.0309x_{34} \\ + 0.0371x_{44}.\end{aligned}$$

If one of $x_{12}, x_{33}, x_{34}, x_{44}$ is not equal to zero, then $F > 0.026$. If $x_{13} \geq 1$, then $x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3 \geq 3$, implying that either $x_{13} = 1$ and thus one of x_{23}, x_{33}, x_{34} is at least 1 or $x_{13} \geq 2$, from which we have $F > 0.026$. Similarly, if $x_{23} = 1, 2$, or is at least 4, then $F > 0.026$. Thus the only possible combination of $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}$, for which $F \leq 0.026$ is $x_{12} = x_{13} = x_{33} = x_{34} = x_{44} = 0, x_{23} = 3$ with $n_3 = 1$. If so, then $x_{14} = p, \quad x_{22} = n - 2p + 2, \quad x_{24} = p - 6, \quad n_2 = n - \frac{3p+1}{2} + 1, \quad n_3 = 1$, and $n_4 = \frac{p-1}{2} - 1$, implying that p is odd and T is of the type $L_o(n, p)$. It follows that if not all of $x_{12}, x_{13}, x_{23}, x_{33}, x_{34}, x_{44}$ in $\chi(T)$ are zero, then $\chi(T)$ achieves the minimum value if and only if p is odd and T is of the type $L_o(n, p)$. The result follows. □

4 Upper bound for sum-connectivity index of molecular trees

The ramification subgraph of a tree is the subgraph induced by the vertices of degree greater than or equal to three.

Lemma 2 *Let T be a molecular tree with n vertices and $p \geq 3$ pendant vertices. Then the ramification subgraph of T is a tree if $\chi(T)$ is maximum.*

Proof If $p = 3$, then T has only one vertex of degree three, forming the ramification subgraph, which is a tree.

Let T be a molecular tree with the maximum sum-connectivity index among the molecular trees with n vertices and $p \geq 4$ pendant vertices. Suppose that the ramification subgraph of T is not a tree. Then there are two vertices, say u and v of degree three or four, which are connected by a path $ux_0x_1 \ldots x_s v$ of length $s + 2 \geq 2$, where $x_0, x_1, \ldots, x_s$ are all of degree two. Let T' be the tree obtained from T by deleting the edges ux_0 and $x_s v$, adding edges uv and zx_0, where z is a pendant vertex, whose neighbour in T is denoted by w. Let $d_y = d_T(y)$ for $y \in V(T)$. Note that $d_w \geq 2$ and $d_u, d_v = 3, 4$. It is easily seen that

$$\begin{aligned}
&\chi(T') - \chi(T) \\
&\quad = \frac{1}{\sqrt{d_u + d_v}} + \frac{1}{\sqrt{2 + d_w}} + \frac{1}{\sqrt{3}} - \left(\frac{1}{\sqrt{1 + d_w}} + \frac{1}{\sqrt{2 + d_u}} + \frac{1}{\sqrt{2 + d_v}} \right) \\
&\quad = \frac{1}{\sqrt{2 + d_w}} - \frac{1}{\sqrt{1 + d_w}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{d_u + d_v}} - \frac{1}{\sqrt{2 + d_u}} - \frac{1}{\sqrt{2 + d_v}} \\
&\quad \geq \frac{1}{\sqrt{2 + 2}} - \frac{1}{\sqrt{1 + 2}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{d_u + d_v}} - \frac{1}{\sqrt{2 + d_u}} - \frac{1}{\sqrt{2 + d_v}} \\
&\quad \geq \frac{1}{2} + \frac{1}{\sqrt{3 + 3}} - \frac{1}{\sqrt{2 + 3}} - \frac{1}{\sqrt{2 + 3}} > 0,
\end{aligned}$$

which is a contradiction to the choice of T. The result follows. □

Define a type $U(n, p)$ of n-vertex molecular trees. For each of such trees, there are $p-2$ vertices of maximal degree three, which induce a tree (its ramification subgraph)

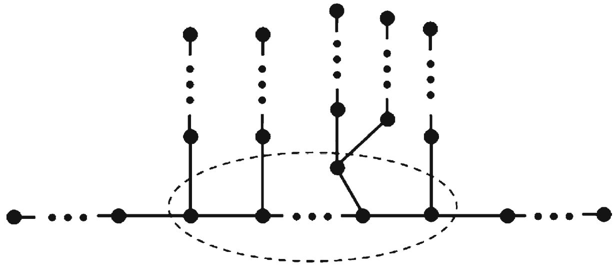

Fig. 3 The structure of $U(n, p)$

and any of these vertices is adjacent to either another vertex of degree three or a vertex of degree two. Note that $x_{12} = p, x_{22} = n - 3p + 2, x_{13} = 0, x_{23} = p, x_{33} = p - 3, n_2 = n - 2p + 2, n_3 = p - 2$, and $n_4 = 0$ for all such trees. Such trees exist if $3 \le p \le \left\lfloor \frac{n+2}{3} \right\rfloor$. An example is shown in Fig. 3, where we note that the ramification subgraph (marked with a dotted circle) may be different. One can see that for given n and p, any such tree has the same sum-connectivity index, equal to

$$\frac{p}{\sqrt{3}} + \frac{p}{\sqrt{5}} + \frac{p-3}{\sqrt{6}} + \frac{n-3p+2}{2} = \frac{n}{2} + \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - \frac{3}{2}\right) p + 1 - \frac{3}{\sqrt{6}}.$$

Proposition 2 *Let T be a molecular tree with n vertices and $p \ge 3$ pendant vertices. Then*

$$\chi(T) \le \frac{n}{2} + \left(\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}} - \frac{3}{2}\right) p + 1 - \frac{3}{\sqrt{6}}$$

with equality if and only if T is of the type $U(n, p)$ with $3 \le p \le \left\lfloor \frac{n+2}{3} \right\rfloor$.

Proof In a similar manner as in the proof of Proposition 1, we consider (1) as a system of six linear equations in the unknowns $x_{12}, x_{22}, x_{33}, n_2, n_3, n_4$. Then

$$\begin{aligned}
x_{12} &= p - x_{13} - x_{14} \\
x_{22} &= n - \frac{5}{2}p + \frac{1}{2}x_{13} + \frac{3}{4}x_{14} - \frac{1}{2}x_{23} - \frac{1}{4}x_{24} + \frac{1}{4}x_{34} + \frac{1}{2}x_{44} + 2 \\
x_{33} &= \frac{3}{2}p - \frac{1}{2}x_{13} - \frac{3}{4}x_{14} - \frac{1}{2}x_{23} - \frac{3}{4}x_{24} - \frac{5}{4}x_{34} - \frac{3}{2}x_{44} - 3.
\end{aligned}$$

Substituting them back into the formula for $\chi(T)$, we have

$$\begin{aligned}
\chi(T) = &\frac{n}{2} + \left(\frac{1}{\sqrt{3}} + \frac{3}{2\sqrt{6}} - \frac{5}{4}\right) p + 1 - \frac{3}{\sqrt{6}} \\
&+ \left(-\frac{1}{\sqrt{3}} + \frac{3}{4} - \frac{1}{2\sqrt{6}}\right) x_{13} + \left(-\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{5}} + \frac{3}{8} - \frac{3}{4\sqrt{6}}\right) x_{14}
\end{aligned}$$

$$+\left(-\frac{1}{4}+\frac{1}{\sqrt{5}}-\frac{1}{2\sqrt{6}}\right)x_{23}+\left(-\frac{1}{8}+\frac{1}{4\sqrt{6}}\right)x_{24}$$
$$+\left(\frac{1}{8}-\frac{5}{4\sqrt{6}}+\frac{1}{\sqrt{7}}\right)x_{34}+\left(\frac{1}{4}-\frac{3}{2\sqrt{6}}+\frac{1}{2\sqrt{2}}\right)x_{44}. \quad (2)$$

Suppose that $\chi(T)$ is maximum among the n-vertex molecular trees with p pendant vertices. Then by Lemma 2, $x_{33}+x_{34}+x_{44}=n_3+n_4-1$. Since $x_{13}+x_{23}+2x_{33}+x_{34}=3n_3$ and $x_{14}+x_{24}+x_{34}+2x_{44}=4n_4$, we have $x_{13}+x_{14}+x_{23}+x_{24}=n_3+2n_4+2$. From $p+n_2+n_3+n_4=n$ and $p+2n_2+3n_3+4n_4=2(n-1)$, we have $n_3+2n_4=p-2$, and thus $x_{13}+x_{14}+x_{23}+x_{24}=p$, i.e., $x_{23}=p-x_{13}-x_{14}-x_{24}$. Now it follows from (2) that

$$\chi(T)=\frac{n}{2}+\left(\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}-\frac{3}{2}\right)p+1-\frac{3}{\sqrt{6}}$$
$$+\left(-\frac{1}{\sqrt{3}}+1-\frac{1}{\sqrt{5}}\right)x_{13}+\left(-\frac{1}{\sqrt{3}}+\frac{5}{8}-\frac{1}{4\sqrt{6}}\right)x_{14}$$
$$+\left(\frac{1}{8}-\frac{1}{\sqrt{5}}+\frac{3}{4\sqrt{6}}\right)x_{24}+\left(\frac{1}{8}-\frac{5}{4\sqrt{6}}+\frac{1}{\sqrt{7}}\right)x_{34}$$
$$+\left(\frac{1}{4}-\frac{3}{2\sqrt{6}}+\frac{1}{2\sqrt{2}}\right)x_{44},$$

i.e.,

$$\chi(T)=\frac{n}{2}+\left(\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}-\frac{3}{2}\right)p+1-\frac{3}{\sqrt{6}}$$
$$-0.0246x_{13}-0.0544x_{14}-0.0160x_{24}-0.0073x_{34}-0.0088x_{44},$$

with negative coefficients for $x_{13}, x_{14}, x_{24}, x_{34}, x_{44}$. Now it is clear that for fixed n and p, $\chi(T)$ will be maximum if and only if the parameters $x_{13}, x_{14}, x_{24}, x_{34}, x_{44}$ are all equal to zero (provided it is possible). If so, then we have $x_{12}=p$, $x_{22}=n-3p+2$, $x_{23}=p$, $x_{33}=p-3$, $n_2=n-2p+2$, $n_3=p-2$, and $n_4=0$. It is easy to see that the solutions describe trees of the type $U(n,p)$. □

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References

1. N. Trinajstić, *Chemical Graph Theory*, 2nd revised edn. (CRC Press, Boca Raton, FL, 1992)
2. M. Randić, On characterization of molecular branching. J. Am. Chem. Soc. **97**, 6609–6615 (1975)
3. L.B. Kier, L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, New York, 1976)
4. L.B. Kier, L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Research Studies Press/Wiley, Letchworth/New York, 1986)

5. J. Devillers, A.T. Balaban (eds.), *Topological Indices and Related Descriptors in QSAR and QSPR* (Gordon and Breach, Amsterdam, 1999)
6. R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors* (Wiley-VCH, Weinheim, 2000)
7. M.V. Diudea (ed.), *QSPR/QSAR Studies by Molecular Descriptors* (Nova, Hungtin, N.Y., 2001)
8. X. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors* (University of Kragujevac, Kragujevac, 2006)
9. I. Gutman, B. Furtula (eds.), *Recent Results in the Theory of Randić Index* (University of Kragujevac, Kragujevac, 2008)
10. L. Pogliani, From molecular connectivity indices to semiempirical connectivity terms: recent trends in graph theoretical descriptors. Chem. Rev. **100**, 3827–3858 (2000)
11. M. Randić, The connectivity index 25 years later. J. Mol. Graph. Model. **20**, 19–35 (2001)
12. R. García-Domenech, J. Gálvez, J.V. Julián-Ortiz, L. Pogliani, Some new trends in chemical graph theory. Chem. Rev. **108**, 1127–1169 (2008)
13. B. Zhou, N. Trinajstić, On a novel connectivity index. J. Math. Chem. **46**, 1252–1270 (2009)
14. B. Lučić, S. Nikolić, N. Trinajstić, B. Zhou, S. Ivaniš Turk, in *Sum-Connectivity index*, ed. by I. Gutman, B. Furtula. Novel Molecular Structure Descriptors—Theory and Applications I. (University of Kragujevac, Kragujevac, 2010), pp. 101–136
15. B. Lučić, N. Trinajstić, B. Zhou, Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons. Chem. Phys. Lett. **475**, 146–148 (2009)
16. Z. Du, B. Zhou, N. Trinajstić, Sum-connectivity indices of trees and unicyclic graphs of fixed maximum degree. (To appear).
17. Z. Du, B. Zhou, N. Trinajstić, Minimum sum-connectivity indices of trees and unicyclic graphs of a given matching number. J. Math. Chem. **47**, 842–855 (2010)
18. P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs. 6. Analyzing bounds for the connectivity index. J. Chem. Inf. Comput. Sci. **43**, 1–14 (2003)