Research Article

The a and (a, b)-Analogs of Zagreb Indices and Coindices of Graphs

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The first and second Zagreb indices were first introduced by Gutman and Trinajstić (1972). It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in elsewhere. Recently, the first and second Zagreb coindices, a new pair of invariants, were introduced in Došlić (2008). In this paper we introduce the a and (a, b)-analogs of the above Zagreb indices and coindices and investigate the relationship between the enhanced versions to get a unified theory.

1. Introduction

Like in many other branches of mathematics, one tries to find in graph theory certain invariants of graphs which depend only on the graph G itself (or in other cases, in addition to, an embedding into the plane or some other manifold), see, for example, [1] and the references given therein. A graph invariant is any function on a graph that does not depend on a labeling of its vertices. A big number of different invariants have been employed to date in graphs structural studies as well as through a broad range of applications including molecular biology, organic chemistry, nuclear physics, neurology, psychology, linguistics, logistics, and economics, see [2]. Here we are interested in the theory of Zagreb indices and Zagreb coindices. The first and second kinds of Zagreb indices were first introduced in [3] (see also [4]). It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in other practical aspects. Recently, the first and second Zagreb coindices, a new pair of invariants, were introduced in [5]. In this paper we introduce the a and (a, b)-analogs of the above Zagreb indices and coindices and investigate

the relationship between the enhanced versions to get a unified theory. Insightfully, this theory will have its place and influence in the territory of mathematical chemistry.

Throughout this work we consider only simple and finite graphs, that is, finite graphs without multiedges or loops. For terms and concepts not mentioned here we refer, for instance, the readers to [6–8]. Let G be a finite simple graph on n vertices and m edges. We denote the set of vertices of G by $V(G)$ and the set of edges of G by $E(G)$. The *complement* of G, denoted by $\overline{G}$, is a simple graph on the set of vertices $V(G)$ in which two vertices are adjacent if and only if they are not adjacent in G. Thus, $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$. Clearly, $|E(G)| + |E(\overline{G})| = |E(K_n)| = \binom{n}{2}$, which implies that $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$. We denote the degree of a vertex u in a graph G by $d_G(u)$. It is easy to see that $d_{\overline{G}}(u) = n - 1 - d_G(u)$ for all $u \in V(G)$. We will omit the subscript G in the degree and other notation if the graph is clear from the context.

Definition 1.1. The first and second Zagreb indices are defined to be

$$M_1(G) = \sum_{u \in V(G)} d(u)^2, \tag{1.1}$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v), \tag{1.2}$$

respectively.

Note that the first Zagreb index may also written as

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)), \tag{1.3}$$

see [9]. The first and second Zagreb indices, first appeared in a topological formula for the total π-energy of conjugated molecules, were introduced by Gutman and Trinajstić in 1972 [3]. Since then these indices have been used as branching indices [10]. The Zagreb indices are found to have applications in QSPR and QSAR studies as well (see [11], e.g.).

The first and second Zagreb coindices were formally introduced in [12] to take account of the contributions of pairs of nonadjacent vertices, with regard to due properties of chemical molecules.

Definition 1.2. The first and second Zagreb coindices are defined to be

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} (d(u) + d(v)), \tag{1.4}$$

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d(u)d(v), \tag{1.5}$$

respectively.

Note that the Zagreb coindices of G are not Zagreb indices of $\overline{G}$: while the defining sums are over the set of edges of $\overline{G}$, the degrees are still with respect to G. So in general $\overline{M}_i(G) \neq M_i(\overline{G})$, $i = 1, 2$.

Now we introduce three a-analogs of the first Zagreb index.

Definition 1.3. The first kind *vertex a-Zagreb index*, *edge a-Zagreb index*, and *a-Zagreb coindex* are defined in order as follows

$$N_a(G) = \sum_{u \in V(G)} d(u)^a,$$

$$Z_a(G) = \sum_{uv \in E(G)} (d(u)^a + d(v)^a), \tag{1.6}$$

$$\overline{Z}_a(G) = \sum_{uv \notin E(G)} (d(u)^a + d(v)^a).$$

It is not hard to see that $N_0(G) = n$, $N_1(G) = Z_0(G) = 2m$ and $\overline{Z}_0(G) = 2\binom{n}{2} - 2m$. Also, $N_2(G) = Z_1(G) = M_1(G)$, $\overline{Z}_1(G) = \overline{M}_1(G)$.

Recently, the index $N_a(G)$ was defined and studied by Zhou and Trinajstić [13], which proved to be a good language in the study of several topological indices.

Next is the analog theory of the second Zagreb index and coindex. For these invariants involving sums of products, we need two parameters to take account of both parties. we define the second kind (a, b)-Zagreb index and (a, b)-Zagreb coindex.

Definition 1.4. The second kind (a, b)-*Zagreb index* and (a, b)-*Zagreb coindex* are, respectively,

$$Z'_{a,b}(G) = \frac{1}{2} \sum_{uv \in E(G)} \left(d(u)^a d(v)^b + d(u)^b d(v)^a \right),$$

$$\overline{Z}'_{a,b}(G) = \frac{1}{2} \sum_{uv \notin E(G)} \left(d(u)^a d(v)^b + d(u)^b d(v)^a \right). \tag{1.7}$$

Clearly,

$$Z'_{1,1}(G) = M_2(G),$$

$$\overline{Z}'_{1,1}(G) = \overline{M}_2(G),$$

$$Z'_{a,b}(G) = Z'_{b,a}(G), \tag{1.8}$$

$$\overline{Z}'_{a,b}(G) = \overline{Z}'_{b,a}(G).$$

Remark 1.5. The Randić [14, 15] index $R_1(G) = \sum_{uv \in E}(1/\sqrt{d(u)d(v)})(= Z'_{-1/2,-1/2}(G))$ of a graph G was first introduced in 1975 by computational chemist Milan Randić. In 1998, Bollobás and Erdös extended into the general Randić index: $R_\alpha(G) = \sum_{uv \in E}(d(u)d(v))^\alpha$ [16]. This graph invariant, sometimes referred to as connectivity index, has been related to a

variety of physical, chemical, and pharmacological properties of organic molecules and has become one of the most popular molecular-structure descriptors (see in particular [14, 17–20]). Note that the second kind (a, b)-Zagreb index actually exists as a double-variable version of the general Randić index:

$$Z'_{\alpha, \alpha}(G) = R_\alpha(G). \tag{1.9}$$

Hence, by applying our general results above we may find a relationship between $R_\alpha(G)$ and $R_\alpha(\overline{G})$.

The main goal of the second section of this paper is to establish relationship between the three a-analogs of the first Zagreb index and coindex. And in the last section we will investigate the second (a, b)-Zagreb index and coindex.

2. The First a-Zagreb Index and Coindex

Next we show how to express the first kind vertex a-Zagreb index and a-Zagreb coindex in terms of the first kind edge a-Zagreb index.

We start by stating a basic relation between the vertex and edge versions of first kind a-Zagreb indices.

Proposition 2.1. *Let G be a simple graph. For all $a \geq 0$, $N_{a+1}(G) = Z_a(G)$.*

Proof. By the definition of $Z_a(G)$, each vertex $u \in V(G)$ contributes to the sum $Z_a(G)$ exactly $d(u) \cdot d(u)^a$. Therefore, $Z_a(G) = \sum_{u \in V(G)} d(u) d(u)^a = N_{a+1}(G)$, as required. $\qquad\square$

Next we explore $Z_a(\overline{G})$, which looks amazingly close to $\overline{Z}_a(G)$. (Later in the proof of Theorem 2.3, we will see the connection between the two.)

Proposition 2.2. *Let G be a simple graph on n vertices and m edges. For all $a \geq 1$,*

$$Z_a\left(\overline{G}\right) = n(n-1)^{a+1} - \sum_{j=0}^{a} \binom{a+1}{j+1} (-1)^j (n-1)^{a-j} Z_j(G). \tag{2.1}$$

Proof. Noting that

$$
\begin{aligned}
N_{a+1}\left(\overline{G}\right) &= \sum_{u \in V(\overline{G})} d_{\overline{G}}(u)^{a+1} \\
&= \sum_{u \in V(G)} (n - 1 - d_G(u))^{a+1} \\
&= \sum_{i=0}^{a+1} \binom{a+1}{i} (-1)^i (n-1)^{a+1-i} \sum_{u \in V(G)} d_G(u)^i \\
&= \sum_{i=0}^{a+1} \binom{a+1}{i} (-1)^i (n-1)^{a+1-i} N_i(G).
\end{aligned}
\tag{2.2}
$$

Hence by Proposition 2.1,

$$Z_a\left(\overline{G}\right) = n(n-1)^{a+1} - \sum_{j=0}^{a} \binom{a+1}{j+1}(-1)^j(n-1)^{a-j}Z_j(G), \tag{2.3}$$

completing the proof. □

Theorem 2.3. *Let G be a simple graph on n vertices and m edges. For $a \geq 1$,*

$$\overline{Z}_a(G) = (n-1)Z_{a-1}(G) - Z_a(G). \tag{2.4}$$

Proof. From the definitions,

$$\begin{aligned}
\overline{Z}_a(G) &= \sum_{uv \notin E(G)} d(u)^a + d(v)^a \\
&= \sum_{uv \in E(\overline{G})} \left(n-1-d_{\overline{G}}(u)\right)^a + \left(n-1-d_{\overline{G}}(v)\right)^a \\
&= \sum_{j=0}^{a} \binom{a}{j} \sum_{uv \in E(\overline{G})} (-1)^j(n-1)^{a-j}\left(d_{\overline{G}}(u)^j + d_{\overline{G}}(v)^j\right) \\
&= \sum_{j=0}^{a} (-1)^j(n-1)^{a-j}\binom{a}{j}Z_j\left(\overline{G}\right).
\end{aligned} \tag{2.5}$$

Thus, by Proposition 2.2,

$$\overline{Z}_a(G) = \sum_{j=0}^{a}(-1)^j(n-1)^{a-j}\binom{a}{j}\left[n(n-1)^{j+1} - \sum_{i=0}^{j}\binom{j+1}{i+1}(-1)^i(n-1)^{j-i}Z_i(G)\right]. \tag{2.6}$$

When taking off the bracket in the above expression, the first sum obtained is equivalent to zero. So we have

$$\begin{aligned}
\overline{Z}_a(G) &= -\sum_{j=0}^{a}\sum_{i=0}^{j}(-1)^j(n-1)^{a-j}\binom{a}{j}\binom{j+1}{i+1}(-1)^i(n-1)^{j-i}Z_i(G) \\
&= -\sum_{i=0}^{a}\left((-1)^i(n-1)^{a-i}Z_i(G)\sum_{j=i}^{a}(-1)^j\binom{a}{j}\binom{j+1}{i+1}\right).
\end{aligned} \tag{2.7}$$

Using the identity (after a little careful analysis),

$$\sum_{j=i}^{a}(-1)^j\binom{a}{j}\binom{j+1}{i+1} = \begin{cases} (-1)^i, & i = a \\ (-1)^{i+1}, & i = a-1 \\ 0, & i \leq a-2, \end{cases} \tag{2.8}$$

we obtain that $\overline{Z}_a(G) = (n-1)Z_{a-1}(G) - Z_a(G)$, as claimed. $\qquad\qquad\square$

Example 2.4. Let $a = 1$, Theorem 2.3 implies that $\overline{M}_1(G) = 2(n-1)m - M_1(G)$. This is the result shown at [5, Proposition 2].

Rewriting Theorem 2.3 for the complement graph of G, one can see the following result about "co-complement."

Proposition 2.5. *Let $a \geq 0$ and let G be any simple graph. Then*

$$\overline{Z}_a(\overline{G}) = \sum_{j=0}^{a}\binom{a}{j}(-1)^j(n-1)^{a-j}Z_j(G). \tag{2.9}$$

Proof. By Theorem 2.3 we have $\overline{Z}_a(\overline{G}) = (n-1)Z_{a-1}(\overline{G}) - Z_a(\overline{G})$. Then according to Proposition 2.2,

$$\begin{aligned}\overline{Z}_a(\overline{G}) &= \sum_{j=0}^{a}\left(\binom{a+1}{j+1} - \binom{a}{j+1}\right)(-1)^j(n-1)^{a-j}Z_j(G) \\ &= \sum_{j=0}^{a}\binom{a}{j}(-1)^j(n-1)^{a-j}Z_j(G),\end{aligned} \tag{2.10}$$

as desired. $\qquad\qquad\square$

Remark 2.6. To conclude, the first kind vertex a-Zagreb index $N_a(G)$, the a-Zagreb coindex $\overline{Z}_a(G)$, and their operations on complement graphs $N_a(\overline{G})$ and $\overline{Z}_a(\overline{G})$ may all be expressed explicitly via the first kind edge j-Zagreb indices $Z_j(G)$. Hence, from now on we will rename the the edge a-Zagreb index $Z_a(G)$ to the "first kind a-Zagreb index."

Example 2.7. The following are the first kind a-Zagreb index and coindex for complete graphs, paths, and cycles on n vertices by direct calculations:

$$Z_a(K_n) = n(n-1)^{a+1}, \qquad \overline{Z}_a(K_n) = 0,$$

$$Z_a(P_n) = 2 + (n-2)2^{a+1}, \qquad \overline{Z}_a(P_n) = 2(n-2) + \binom{n-2}{2}2^{a+1},$$

$$Z_a(\overline{P_n}) = 2(n-2)^{a+1} + (n-2)(n-3)^{a+1}, \qquad \overline{Z}_a(\overline{P_n}) = 2(n-2)^a + 2(n-2)(n-3)^a,$$

$$Z_a(C_n) = n2^{a+1}, \qquad \overline{Z}_a(C_n) = n(n-3)2^a,$$

$$Z_a(\overline{C_n}) = n(n-3)^{a+1}, \qquad \overline{Z}_a(\overline{C_n}) = 2n(n-3)^a.$$

$$\tag{2.11}$$

3. The Second (a,b)-Zagreb Index and Coindex

Let G be any simple graph with m edges, then from the definition we have $Z'_{0,0}(G) = m$ and $Z'_{a,0}(G) = Z'_{0,a}(G) = N_{a+1}(G)$.

The second kind (a,b)-Zagreb index and coindex are about complementary to each other, but not commutable. Specifically, if we think of the coindex as an operation "co" conducted on the second kind (a,b)-Zagreb index $Z'_{a,b}(G)$ and the graph complement $Z'_{a,b}(\overline{G})$ as another operation on the second kind (a,b)-Zagreb index $Z'_{a,b}(G)$, then the order of the two operations does matter. Actually even for the special cases of $Z_a(\overline{G})$ versus $\overline{Z}_a(G)$ and of $\overline{M}_i(G)$ versus $M_i(\overline{G})$ ($i = 1, 2$), there is no exchangeability. Nonetheless we demonstrate a convolution theorem of the two operations mentioned.

Theorem 3.1. *Let G be a simple graph. For all $a, b \geq 0$,*

$$Z'_{a,b}(\overline{G}) = \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}\overline{Z}'_{i,j}(G), \tag{3.1}$$

$$\overline{Z}'_{a,b}(G) = \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}Z'_{i,j}(\overline{G}). \tag{3.2}$$

Proof. For (3.1), from the definitions,

$$
\begin{aligned}
Z'_{a,b}(\overline{G}) &= \frac{1}{2}\sum_{uv\in E(\overline{G})}\left(d_{\overline{G}}(u)^a d_{\overline{G}}(v)^b + d_{\overline{G}}(u)^b d_{\overline{G}}(v)^a\right) \\
&= \frac{1}{2}\sum_{uv\notin E(G)}\left((n-1-d_G(u))^a(n-1-d_G(v))^b + (n-1-d_G(u))^b(n-1-d_G(v))^a\right) \\
&= \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}\frac{1}{2}\sum_{uv\notin E(G)}d_G(u)^i d_G(v)^j + d_G(u)^j d_G(v)^i \\
&= \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}\overline{Z}'_{i,j}(G),
\end{aligned}
\tag{3.3}
$$

as claimed.

And similarly for (3.2), noting that

$$
\begin{aligned}
\overline{Z}'_{a,b}(G) &= \frac{1}{2}\sum_{uv\notin E(G)}\left(d_G(u)^a d_G(v)^b + d_G(u)^b d_G(v)^a\right) \\
&= \frac{1}{2}\sum_{uv\in E(\overline{G})}\left((n-1-d_{\overline{G}}(u))^a(n-1-d_{\overline{G}}(v))^b + (n-1-d_{\overline{G}}(u))^b(n-1-d_{\overline{G}}(v))^a\right)
\end{aligned}
$$

$$= \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}\frac{1}{2}\sum_{uv\in E(\overline{G})}d_{\overline{G}}(u)^i d_{\overline{G}}(v)^j + d_{\overline{G}}(u)^j d_{\overline{G}}(v)^i$$

$$= \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}Z'_{i,j}\left(\overline{G}\right). \tag{3.4}$$

□

Remark 3.2. Even though the convoluted recurrences between the co-complement operations are established by Theorem 3.1, one can not use induction to prove that $Z'_{a,b}(\overline{G}) = \overline{Z}'_{a,b}(G)$ because that is wrong starting from the basic step.

Theorem 3.3. *Let G be a simple graph. For all $a, b \geq 0$,*

$$Z'_{a,b}(G) = N_a(G)N_b(G) - N_{a+b}(G) - \overline{Z}'_{a,b}(G). \tag{3.5}$$

Proof. From the definitions we have

$$N_a(G)N_b(G) = N_{a+b}(G) + Z'_{a,b}(G) + \overline{Z}'_{a,b}(G),$$

$$N_a\left(\overline{G}\right) = \sum_{i=0}^{a}\binom{a}{i}(-1)^i(n-1)^{a-i}N_i(G). \tag{3.6}$$

Thus, by Theorem 3.1 we obtain

$$Z'_{a,b}\left(\overline{G}\right) = \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}\left(N_i(G)N_j(G) - N_{i+j}(G) - Z'_{i,j}(G)\right),$$

$$\overline{Z}'_{a,b}\left(\overline{G}\right) = \sum_{i=0}^{a}\sum_{j=0}^{b}\binom{a}{i}\binom{b}{j}(-1)^{i+j}(n-1)^{a+b-i-j}Z'_{i,j}(G), \tag{3.7}$$

which implies that

$$Z'_{a,b}\left(\overline{G}\right) = N_a\left(\overline{G}\right)N_b\left(\overline{G}\right) - Z'_{a,b}\left(\overline{G}\right) - \sum_{j=0}^{a+b}(-1)^j(n-1)^{a+b-j}N_j(G)\sum_{i=0}^{a}\binom{a}{i}\binom{b}{j-i}. \tag{3.8}$$

Using the fact that $\sum_{i=0}^{a}\binom{a}{i}\binom{b}{j-i} = \binom{a+b}{j}$, we obtain

$$Z'_{a,b}\left(\overline{G}\right) = N_a\left(\overline{G}\right)N_b\left(\overline{G}\right) - \overline{Z}'_{a,b}\left(\overline{G}\right) - \sum_{j=0}^{a+b}\binom{a+b}{j}(-1)^j(n-1)^{a+b-j}N_j(G), \tag{3.9}$$

which implies that

$$Z'_{a,b}\left(\overline{G}\right) = N_a\left(\overline{G}\right)N_b\left(\overline{G}\right) - N_{a+b}\left(\overline{G}\right) - \overline{Z}'_{a,b}\left(\overline{G}\right), \tag{3.10}$$

which implies our claim. $\square$

Example 3.4. The (a, b)-Zagreb for complete graphs, paths, and cycles on n vertices are calculated:

$$Z'_{a,b}(K_n) = \binom{n}{2}(n-1)^{a+b}, \qquad \overline{Z}'_{a,b}(K_n) = 0,$$

$$Z'_{a,b}(P_n) = 2^a + 2^b + (n-3)2^{a+b}, \qquad \overline{Z}'_{a,b}(P_n) = 1 + (n-3)\left(2^a + 2^b\right) + \binom{n-3}{2}2^{a+b},$$

$$Z'_{a,b}(C_n) = n2^{a+b}, \qquad \overline{Z}'_{a,b}(C_n) = n(n-3)2^{a+b-1}. \tag{3.11}$$

Recently, Ashrafi et al. [21] considered the Zagreb coindices of graph operations, such as those of union, sum, Cartesian product, disjunction, symmetric difference, composition, and corona. Similar and interesting treatment is also found in [22]. Being a vividly growing field of mathematical chemistry, many interesting phenomena are under discovery and much work still needs to be done.

References

[1] C. Godsil and G. Royle, *Algebraic Graph Theory*, vol. 207, Springer, New York, NY, USA, 2004.

[2] R. Todeschini and V. Consoni, *Handnook of Molecular Descriptors*, Wiley-VCH, New York, NY, USA, 2002.

[3] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[4] I. Gutman and K. Ch. Das, "The first Zagreb index 30 years after," *Communications in Mathematical and in Computer Chemistry*, no. 50, pp. 83–92, 2004.

[5] A. R. Ashrafi, T. Došlić, and A. Hamzeh, "The Zagreb coindices of graph operations," *Discrete Applied Mathematics*, vol. 158, no. 15, pp. 1571–1578, 2010.

[6] R. Diestel, *Graph Theory*, vol. 173, Springer, New York, NY, USA, 2nd edition, 2000.

[7] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, Fla, USA, 2nd edition, 1992.

[8] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, NJ, USA, 1996.

[9] S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, "The Zagreb indices 30 years after," *Croatica Chemica Acta*, vol. 76, no. 2, pp. 113–124, 2003.

[10] I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The Journal of Chemical Physics*, vol. 62, no. 9, pp. 3399–3405, 1975.

[11] J. Devillers and A. T. Balaban, Eds., *Topological Indices and Related Descriptors in QSAR and QSPR, Gordon & Breach*, Amsterdam, The Netherlands, 1999.

[12] T. Došlić, "Vertex-weighted Wiener polynomials for composite graphs," *Ars Mathematica Contemporanea*, vol. 1, no. 1, pp. 66–80, 2008.

[13] B. Zhou and N. Trinajstić, "Some properties of the reformulated Zagreb indices," *Journal of Mathematical Chemistry*, vol. 48, no. 3, pp. 714–719, 2010.

[14] M. Randić, "On the recognition of identical graphs representing molecular topology," *The Journal of Chemical Physics*, vol. 60, pp. 3920–3928, 1974.

[15] M. Randić, "On characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.

[16] B. Bollobás and P. Erdös, "Graphs of extremal weights," *Ars Combinatoria*, vol. 50, pp. 225–233, 1998.

[17] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, NY, USA, 1976.

[18] L. B. Kier and L. H. Hall, *Molecular Connectivity in Structure: Activity Analysis*, Wiley, New York, NY, USA, 1986.

[19] X. Li and Y. Shi, "A survey on the Randić index," *Communications in Mathematical and in Computer Chemistry*, vol. 59, no. 1, pp. 127–156, 2008.

[20] M. Randić, "On history of the Randić index and emerging hostility toward chemical graph theory," *Communications in Mathematical and in Computer Chemistry*, vol. 59, no. 1, pp. 5–124, 2008.

[21] A. R. Ashrafi, T. Došlić, and A. Hamzeh, "Extremal graphs with respect to the Zagreb coindices," *Communications in Mathematical and in Computer Chemistry*, vol. 65, no. 1, pp. 85–92, 2011.

[22] M. H. Imrich and S. Klavžar, *Product Graphs: Structure and Recognition*, John Wiley & Sons, New York, NY, USA, 2000.