MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 313-328

ISSN 0340 - 6253

Comparing Zagreb Indices for 2-Walk Linear Graphs

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(Received July, 16, 2020)

Abstract

It was conjectured that inequality $M_2(G)/m - M_1(G)/n \geq 0$ holds for all simple connected graphs with n vertices and m edges, where $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb indices of a graph G, respectively. Performing detailed investigations, it was proved that the conjecture does not hold for all general connected graphs, counterexamples were presented in some families of acyclic graphs. The 2-walk (a,b) linear graphs belong to the family of connected non-regular graphs having exactly two main eigenvalues. In this study, we show that $M_2(G)/m - M_1(G)/n \geq 0$ is also true for 2-walk linear graphs.

1 Introduction

We consider connected simple graphs without loops and multiple edges. For a connected graph G, V(G) and E(G) denote the set of vertices and edges, n and m the numbers of vertices and edges, respectively. Denote by d(u) the degree of a vertex u. Let $\Delta=\Delta(G)$ and $\delta=\delta(G)$ be the maximum and the minimum degrees, respectively, of vertices of G. A universal vertex of

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an n-vertex graph is a vertex adjacent to all other vertices, consequently Δ=n-1 holds. An edge of G connecting vertices u and v is denoted by uv.

Using the standard terminology [1, 2, 3, 4], let A=A(G) be the adjacency matrix of a graph G. The adjacency spectrum of a G is the set of graph eigenvalues of A(G) with their multiplicities. For a graph G, we denote by ρ(G) the largest eigenvalue of A(G) and call it the spectral radius of G. The Laplacian matrix of graph G is defined by L(G)= D(G) – A(G), where D(G) is the diagonal matrix of the vertex degrees. The Laplacian spectrum of graph G is the set of the Laplacian eigenvalues of G. Graphs with the same spectrum with respect to matrices A(G) and L(G) are called A-cospectal and L-cospectral, respectively.

A cone over a connected graph G is obtained by adding a vertex to G that is adjacent to all vertices of G. Cone graphs are non-bipartite graphs, they contain triangles and exactly one universal vertex, their diameter is equal to 2.

A graph is called R-regular if all its vertices have the same degree R. A connected graph is called irregular if it contains at least two vertices with different degrees. A bidegreed graph is an irregular graph whose vertices have exactly two different degrees, δ and Δ. A connected bipartite bidegreed graph G is *semiregular* if every edge of G joins a vertex of degree δ to a vertex of degree Δ [5].
A bipartite graph G is called *pseudo-semiregular* [2, 5] if each vertex in the same part of bipartition has the same average degree. From these definitions it follows that any semiregular graph is a bipartite pseudo-semiregular graph. The converse of this statement is not true.

A connected graph G is called *harmonic* (pseudo-regular) [5-24] if there exists a positive integer p(G) such that each vertex u of G has the same average neighbor degree number equal to p(G). For the spectral radius of a harmonic graph G, the equality ρ(G)=p(G) holds. A harmonic graphs with ρ(G)=p(G) is said to be a p-harmonic graph.
From the definition it follows that any regular graph is a harmonic graph. Irregular harmonic graphs are called *strictly harmonic* graphs. It is easy to see that there exist infinitely many bipartite and non-bipartite harmonic graphs.

Recently, the so-called *complete split-like graphs* have been introduced in [25, 26]. By definition a complete split-like graph KSL(n, q, ε) is an n-vertex bidegreed graph with $q \geq 1$ vertices of degree n-1 and n-q vertices of degree ε, where $q \leq \varepsilon < n-1$.

Traditional *complete split graphs* KS(n, q) form a particular subclass of complete split-like graphs, where q=ε holds. Complete split-like graphs KSL(n, q, ε) represent a subset of 2-walk (a,b) linear graphs [2, 25, 26].

For the topological characterization of a molecular graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ were proposed by Gutman and Trinajstić [27].

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of products of the degrees of pairs of adjacent vertices of the graph G. They are defined by

$$M_1(G) = \sum_{u \in V(G)} d^2(u) \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v) .$$

The relations between Zagreb indices and different topological indices used in mathematical chemistry have intensively been studied in the last four decades. Readers are referred to the literature sources given in the reference list [28 - 37].

For comparing Zagreb indices of a graph G with n vertices and m edges the following topological invariant was proposed:

$$Z(G) = \frac{M_2(G)}{m} - \frac{M_1(G)}{n} . \qquad (1)$$

It was conjectured that $Z(G) \geq 0$ is valid for all connected simple graphs [38, 39]. In the literature the inequality $Z(G) \geq 0$ is referred to as the Zagreb indices inequality. Performing detailed investigations for checking the validity of inequality $Z(G) \geq 0$, it has been revealed that $Z(G) \geq 0$ is fulfilled for several particular graph families, but it does not hold for all general connected graphs [31, 32].

It is important to note that among connected graphs the validity of the Zagreb indices inequality has been proved for trees, unicyclic graphs, connected bidegreed graphs and molecular graphs with Δ≤4 [19, 31, 32, 34]. However, it was demonstrated by counterexamples that there exist bicyclic and tricyclic graphs not satisfying the Zagreb indices inequality [31, 32, 34, 36]. Recently, it has been proved that for almost all connected graphs Z(G)≥0 is fulfilled [35].

The so-called *2-walk (a,b) linear graphs* represent a broad class of connected irrregular graphs. In this study it will be shown that 2-walk (a,b) linear graphs satisfy the Zagreb indices inequality.

2 Preliminaries

A connected irregular graph G is called 2-walk linear (more precisely, 2-walk (a,b)–linear) if there exists a unique rational number pair (in fact, integers pair) (a,b) such that

$$S(u) = d(u)t(u) = ad(u) + b \qquad (2)$$

holds for every vertex u of G, where S(u) is the sum of the degrees of all vertices adjacent to u, and t(u) stands for the average of degrees of vertices adjacent to u [14]. As an example, consider the 12-vertex and 20-edge connected graph with degree set (3, 4, 5) depicted in Fig.1. This triangle-free graph having chromatic number 4 is known as the Grötzsch graph. From Eq. (2) it follows that this 2-walk (a, b) linear graph has parameters a=1 and b=10.

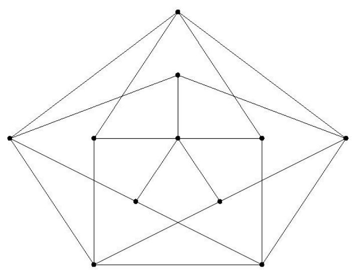


Figure 1. A 11-vertex 2-walk (a,b) regular graph.

Lemma 1 [19]: If G is a 2-walk (a,b) linear graph, then a and b are integers, and a ≥0.

Lemma 2 [10, 14, 18]: A connected irregular graph has exactly two main eigenvalues $\rho > \mu$ if and only if it is 2-walk linear.

Lemma 3 [10, 14]: Let G be a connected 2-walk (a,b) linear graph with two main eigenvalues ρ and μ, where ρ is the spectral radius of G, and $\rho > \mu$. Then

$$\rho, \mu = \frac{1}{2}\left(a \pm \sqrt{a^2 + 4b}\right),$$

consequently $\rho + \mu = a$ and $\rho\mu = -b$.

Lemma 4 [10]: Let G be a connected graph with spectral radius ρ. Then G is semiregular graph if and only if G has two main eigenvalues ρ and μ, and $\mu = -\rho$. In other words, G is semi-regular if and only if G is 2-walk (0,b) linear graph, that is a=0 holds.

Lemma 5 [5, 12]: A connected irregular graph G with spectral radius $\rho(G)$ is *strictly harmonic (harmonic and irregular)* if and only if G has exactly two main eigenvalues ρ and 0. This means that G must be a 2-walk (a, 0) linear graph, where $a = \rho(G)$ and $b = 0$.

Lemma 6 [26]: Complete split-like graphs KSL(n, q, ε) form a subset of 2-walk (a, b) linear graphs.

3 Some properties of 2-walk (a,b) linear graphs

Some fundamental properties of 2-walk linear graphs are summarized in Refs. [14-25].

Lemma 7 [5]: Let G be a connected n-vertex graph with spectral radius $\rho(G)$. Then

$$\rho(G) \geq \sqrt{\frac{M_1(G)}{n}},$$

and equality holds if and only if G is regular or semiregular.

Lemma 8 [40]: Das verified that for a simple connected graph G

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

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) = \frac{1}{2} \sum_{u \in V(G)} d^2(u)t(u).$$

Lemma 9 [30]: Let G be a connected n-vertex graph and let ρ(G) be the spectral radius of G. Then

$$\rho(G) \geq \frac{2M_2(G)}{M_1(G)} = \frac{\sum_{u \in V(G)} d^2(u)t(u)}{\sum_{u \in V(G)} d(u)t(u)},$$

and equality holds if and only if G is regular or strictly harmonic.

Lemma 10 [24]: Let G be a p-harmonic graph with spectral radius ρ(G). Then Zagreb indices $M_1(G)$ and $M_2(G)$ can be calculated as $M_1(G)=2mp(G)=2m\rho(G)$ and $M_2(G)=mp^2(G)=m\rho^2(G)$.

Lemma 11 [26]: It has been proved that if G is a complete split-like graph KSL(n, q, ε) then

$$\rho, \mu = \frac{1}{2}\left(\varepsilon - 1 \pm \sqrt{(\varepsilon+1)^2 + 4q(n-\varepsilon-1)}\right).$$

As an example, some different types of 2-walk linear graphs are illustrated in Fig. 2.

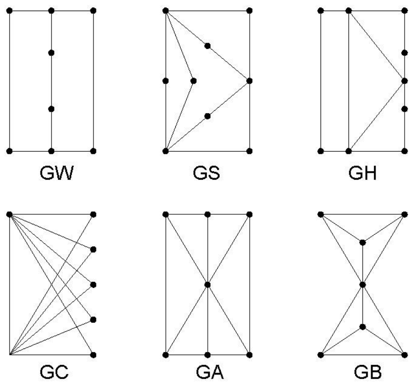


Figure 2. Bidegreed 2-walk (a,b) linear graphs.

As can be observed,

GW is an ordinary 2-wall linear graph, with parameters a=1 and b=3,

GS is a semiregular graph with a=0 and b=8,

GH is a strictly harmonic graph with a=3 an b=0,

GC is a complete split graph KS(7, 2) with a=1, and b=10,

Non-isomorphic graphs GA and GB have identical parameters a=2 and b=6. They belong to the class of complete split-like graphs of type KSL(7,1, 3).

Since graphs in Fig.2 are connected bidegreed graphs, based on previous considerations, the Zagreb indices inequality holds for them.

Remark 1 A 2-walk linear graph can simply be constructed from connected regular graphs. If G_R is an n-vertex connected ($R \geq 2$)-regular graph differing from the complete graph K_n, then the cone over G_R will be a 2-walk (a,b) linear graph identical to the complete split-like graph KSL(n+1, 1, R+1). It is easy to construct infinitely many values of (a, b) such that a 2-walk (a, b) linear graph exists, using the cone over regular graphs.

Remark 2 It has been proved that for every integer $k \geq 1$, there exists a 2-walk (a, b) linear graph G having at least k different degrees [15]. In other words, the number of distinct degrees of certain 2-walk linear graphs can be arbitrary large. In Fig. 3 this observation is demonstrated by the 34 vertex 3-harmonic graph with a degree set (1, 2, 3, 4, 5, 6) [41].

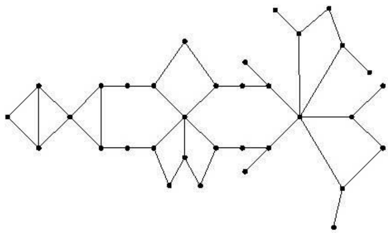


Figure 3. A 3-harmonic graph with degree set (1, 2, 3, 4, 5, 6).

As it is known, if a graph G does not share its spectrum with other graphs, then G is uniquely determined by its spectrum [42]. An important observation is that the spectrum does not unambiguously characterize the combinatorial structure of 2-walk linear graphs.

For two graphs J_1 and J_2 with disjoint vertex sets, J_1 U J_2 denotes the disjoint union of graphs J_1 and J_2. The join J_1 V J_2 of graphs J_1 and J_2 is the graph obtained from J_1 U J_2 by joining every vertex of J_1 with every vertex of J_2.

Lemma 12 [43]**:** Consider simple connected regular graphs G_R and G_S. Let G_R be an R-regular graphs with n(R) vertices and G_S an S-regular graph with n(S) vertices with adjacency eigenvalues denoted by $\alpha_1, \alpha_2, \ldots, \alpha_{n(R)-1}, \alpha_{n(R)}=R$ and $\beta_1, \beta_2, \ldots, \beta_{n(S)-1}, \beta_{n(S)} = S$, respectively. Then the corresponding adjacency eigenvalues of join graph G_R V G_S will be

$$\alpha_1,\alpha_2,...,\alpha_{n(R)-1},\beta_1,\beta_2,...,\beta_{n(S)-1},\ \ \frac{1}{2}\left[R+S\pm\sqrt{(R-S)^2+4n(R)n(S)}\right].$$

Proposition 1 There exist A-cospectral 2-walk linear graphs belonging to the family of complete split-like graphs.

Proof. Consider the two non-isomorphic 10-vertex, A-cospectral 4-regular graphs depicted in Fig. 4 [3].

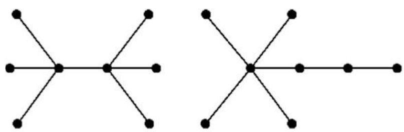
G_A G_B

Figure 4. Four-regular A-cospectral graphs with 10 vertices.

Denote by $GC_A = K_1 \vee G_A$ and $GC_B = K_1 \vee G_B$ the corresponding 11-vertex cone graphs of 4-regular graphs G_A and G_B depicted in Fig. 4. Based on Remark 1, it is easy to see that non-isomorphic cone graphs GC_A and GC_B are 2-walk (a,b) linear graphs with identical parameters a=4 and b=10. More exactly, they belong to the family of complete split-like graphs of type KSL(11,1,5). By Lemma 12 it follows that 11-vertex bidegreed cone graphs GC_A and GC_B are A-cospectral. From above considerations it can be concluded that 2-walk linear graphs (including complete split-like graphs) are not determined by their adjacency spectra.

Proposition 2 [42]: There exist non-isomorphic A-cospectral tree graphs T_A and T_B which are characterized by the same adjacency spectrum, and T_A is a 2-walk linear graph while T_B does not belong to the family of 2-walk linear graphs.

Proof. In Fig. 5 two A-cospectral 8-vertex trees are depicted [42].



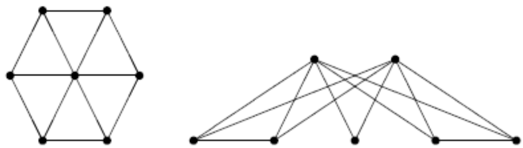
T_A T_B

Figure 5. A-cospectral 8-vertex trees.

It is easy to check that the tree shown on the left is a 2-walk (a,b) linear graph with parameters a=1 and b=3, but the graph demonstrated on the right is not a 2-walk linear graph.

Proposition 3 [44]: There exist connected Laplacian cospectral graphs L_A and L_B characterized by the same Laplacian spectrum, and between them only L_A is a 2-walk linear graph.

Proof. In Fig. 6 two 7-vertex connected graphs are depicted [44].



L_A L_B

Figure 6. Laplacian cospectral 7-vertex graphs.

Graph L_A isomorphic to the 7-vertex wheel graph is a 2-walk linear graph with parameter a= 2 and b=6, while L_B is not a 2-walk linear graph.

It has been proved in [44] that graph L_A and graph L_B are Laplacian cospectral graphs having the same integral Laplacian spectrum (7, 5, 4, 4, 2, 2, 0). It follows that the 2-walk linear graph L_A is not determined by its Laplacian spectrum.

4 Zagreb indices inequality for 2-walk (a,b) linear graphs

Proposition 4 [45]: Let G be a connected n-vertex graph. Then

$$\sum_{u\in V(G)} S^2(u) \geq \frac{M_1^2(G)}{n} \tag{3}$$

$$\sum_{u\in V(G)} S^2(u) \geq \frac{4M_2^2(G)}{M_1(G)} \tag{4}$$

In Eq.(3) equality holds if G is regular or semiregular graph, while in Eq.(4) equality holds if G is a harmonic graph.

Proposition 5 Let G be a 2-walk (a,b) linear graph. Then the following equalities hold:

(i) $$\sum_{u\in V(G)} \frac{S(u)}{d(u)} = \sum_{u\in V(G)} t(u) = an + b \sum_{u\in V(G)} \frac{1}{d(u)} > 0 \tag{5}$$

(ii) $$\sum_{u\in V(G)} S(u) = \sum_{u\in V(G)} d(u)t(u) = M_1(G) = 2ma + nb \tag{6}$$

(iii) $$\sum_{u\in V(G)} d(u)S(u) = \sum_{u\in V(G)} d^2(u)t(u) = 2M_2(G) = aM_1(G) + 2mb \tag{7}$$

(iv) $$\sum_{u\in V(G)} S^2(u) = a^2 M_1(G) + 4mab + nb^2 \tag{8}$$

Proof. The above equalities can be deduced from Eq. 2 and Lemma 8.

Remark 3 [46]: Let G be a strictly harmonic graph with spectral radius ρ. Because b=0, from Eq.(6), Eq.(7) and Lemma 9 one obtains that

$$\rho = a = \frac{2M_2(G)}{M_1(G)} = \frac{M_1(G)}{2m} = \sqrt{\frac{M_2(G)}{m}} = \frac{1}{n}\sum_{u\in V(G)} t(u) = \frac{1}{n}\sum_{uv\in E(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right).$$

Let G be an irregular connected graph G with n vertices and m edges. Consider the topological index $\alpha_G(n, m)$ defined by

$$\alpha_G(n,m) = \left(\frac{2m}{n}\right)\frac{Z(G)}{Var(G)} \tag{9}$$

where Var(G) is the Bell‘s graph irregularity index formulated as [47]

$$Var(G) = \frac{1}{n}\sum_{u\in V(G)} \left(d(u) - \frac{2m}{n}\right)^2 = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2 .$$

As it is known, Var(G)≥0 and Var(G)=0 if and only if G is a regular graph.

For an irregular graph G, the topological index $\alpha_G(n,m)$ is determined primarily by the actual value of Z(G). It follows that $\alpha_G(n,m)$ can be either a positive number or a negative number or zero.

Proposition 6 Let G be a connected 2-walk (a,b) linear graph, and let $\Omega(G) = M_1^2(G) - 4mM_2(G)$ by definition.

Then

$$a = \left(\frac{2m}{n}\right)\frac{Z(G)}{Var(G)} = \alpha_G(n,m) \geq 0 \quad \text{and} \quad b = \frac{\Omega(G)}{n^2 Var(G)}.$$

Consequently, for a 2-walk (a,b) linear graph G, the Zagreb indices inequality holds.

Proof. If G is a 2-walk (a,b) linear graph, then $a \geq 0$ and $Var(G) > 0$ are fulfilled.
From Eq.(6) and Eq.(7) one obtains that

$$a = \frac{2(nM_2 - mM_1)}{nM_1 - 4m^2} = \frac{2nm\left(\frac{M_2}{m} - \frac{M_1}{n}\right)}{nM_1 - 4m^2} = \left(\frac{2m}{n}\right)\frac{Z(G)}{Var(G)} = \alpha_G(n,m) \qquad (10)$$

and

$$b = \frac{M_1^2 - 4mM_2}{nM_1 - 4m^2} = \frac{\Omega(G)}{n^2 Var(G)}.$$

It is easy to see that $\Omega(G)$ can be either a positive number or a negative number or zero. This implies that for a 2-walk (a,b) linear graph parameter b can be positive or negative numbers or zero.

Remark 4 There exist connected irregular graphs, for which $Z(G) = M_2/(G)/m - M_1/(G)/n$ is equal to 0 or less than 0 [30, 31, 32]. If $Z(G) < 0$ is fulfilled, then G cannot be a 2-walk (a,b) linear graph. For a 2-walk (a,b) linear graph $Z(G) = 0$ holds if and only if G is a semiregular graph with parameter a=0.

In what follows it will be demonstrated that formulas represented by Eqs.10 and 11 can be deduced by using an alternative concept.

Let G be a connected irregular graph with n vertices and m edges. For arbitrary real numbers A and B consider the two-variable function $Q_G(A,B)$ defined as

$$Q_G(A,B) = \frac{1}{n}\sum_{u\in V}\left(S(u) - Ad(u) - B\right)^2 = \frac{1}{n}\sum_{u\in V}\left(d(u)t(u) - Ad(u) - B\right)^2 . \qquad (11)$$

It is easy to see that there exist a uniquely defined (AL, BL) parameter pair which minimizes the function $Q_G(A,B)$. These parameters (AL, BL) can be determined by solving the following system composed of two linear equations

$$\sum_{u\in V(G)} d^2(u)t(u) = 2M_2(G) = A\sum_{u\in V} d^2(u) + B\sum_{u\in V(G)} d(u) = AM_1(G) + 2mB$$
$$\sum_{u\in V(G)} d(u)t(u) = M_1(G) = A\sum_{u\in V(G)} d(u) + nB = 2mA + nB$$

One obtains that

$$AL = \frac{2\left(nM_2 - mM_1\right)}{nM_1 - 4m^2} = \left(\frac{2m}{n}\right)\frac{Z(G)}{Var(G)} \qquad (12)$$

and

$$BL = \frac{M_1^2 - 4mM_2}{nM_1 - 4m^2} = \frac{\Omega(G)}{n^2 Var(G)} \qquad (13)$$

From previous considerations the following proposition can be obtained.

Proposition 7 Let G be an n-vertex connected irregular graph. Then $Q_G(AL,BL)$ is a topological index for which $Q_G(AL,BL) \geq 0$ holds. If $Q_G(AL,BL) > 0$ is fulfilled then G does not belong to the class of 2-walk linear graphs. If $Q_G(AL,BL) = 0$ holds then G is a 2-walk (a, b) linear graphs with parameters a = AL and b = BL. Consequently, the topological index $Q_G(AL,BL)$ characterizes quantitatively the structural difference between graph G and a possible 2-walk (a,b) linear graph.

5 Additional remarks

Let G be a connected graph with m edges and a spectral radius ρ(G). Graph G is said to be a Z_2 graph if the following identity holds [6, 7]

$$\rho(G) = \sqrt{\frac{M_2(G)}{m}} .$$

There are several 2-walk linear graphs belonging to the family of Z_2 graphs [6, 7]. But there exist infinitely many Z_2 graphs not belonging to the class of 2-walk linear graphs.

Proposition 8 A Z_2 graph satisfies the Zagreb indices inequality.

Proof. Because for a connected Z_2 graph G with n vertices and m edges and a spectral radius ρ, $M_2(G)= m\rho^2$ is valid, then from Lemma 7 one obtains that

$$Z(G) = \frac{M_2(G)}{m} - \frac{M_1(G)}{n} = \rho^2 - \frac{M_1(G)}{n} \geq 0$$

where equality holds if and only if G is a regular or a semiregular graph. As an example, small Z_2 graphs are depicted in Fig. 7. These graphs are not 2-walk linear graphs, yet all of them satisfy the Zagreb indices inequality.

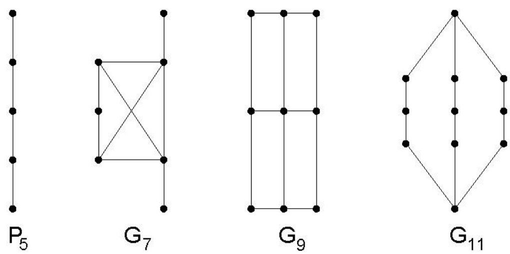


Figure 7. Four Z_2 graphs satisfying the Zagreb indices inequality.

It should be noted that path P_5, and graphs G_9, G_{11} are not semiregular graphs. They belong to the class of bipartite pseudo-semiregular graphs. Graph G_7 with 7 vertices and 9 edges is a non-bipartite sporadic graph. Because for graph G_7, $M_2(G_7)=81$ holds, this implies that $\rho(G_7) = \sqrt{M_2(G_7)/m} = \sqrt{9} = 3$. It should be emphasized that all these graphs are molecular graphs, consequently, they satisfy the Zagreb indices inequality.

Acknowledgement: The authors would like to thank Dr László Horváth for extensive help with computer graphics.

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