

ZAGREB INDICES OF GENERALIZED TRANSFORMATION GRAPHS AND THEIR COMPLEMENTS

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ABSTRACT. We consider the generalized transformation graphs G^{ab} and obtain expressions for their first and second Zagreb indices and coindices. Analogous expressions are obtained also for the complements of G^{ab} .

1 Introduction: Transformation graphs and their chemical applications

It is nowadays well known, and established almost a century ago, that graphs provide a natural representation of the structure of covalently bond molecules, thus of practically all organic molecules [2, 9, 14]. The standard and most direct way how a graph representation of a molecule is constructed is that each atom is replaced by a vertex and each (covalent) chemical bond by an edge between the respective

two vertices. Such a “*molecular graph*” in an obvious manner reflects the relevant details of molecular structure, the so-called “*molecular topology*”. Molecular graphs constructed in the above described manner found countless chemical applications and have been considered in many thousands of papers. Such molecular graphs are the object of study in the vast majority of currently produced papers in mathematical chemistry.

However, there exist other, less immediate, ways in which molecular topology can be represented by a graph. Namely, if G is a molecular graph, and if it can be transformed in some way into another graph G^* , so that the correspondence between G and G^* is one-to-one, then the transformation $G \rightarrow G^*$ preserves the entire information on molecular topology contained in G . Consequently, the transformed graph G^* could be used as an equally valid, yet less transparent, representation of molecular structure.

In the chemical literature, there have been a few earlier attempts to shift from ordinary molecular graphs to their transforms. The line graph and the iterated line graphs were used in [15–17, 27]. Attempts to use graph complements were recently reported [25].

The evident advantage of using transformation graphs instead of ordinary molecular graphs lies in the applicability of their topological indices. A topological index of the transformation graph will necessarily reflect other structural features than the same topological index of the ordinary molecular graph. By this, using one and the same class of topological indices, a variety of different structural properties of the underlying molecules could be modeled. For a concrete application of this idea see [15–17, 27].

Zagreb indices belong among the best investigated topological indices, but their properties and chemical applications were always studied for the case of ordinary molecular graphs [3, 10–12, 21]. Recently, we focused our attention to the Zagreb indices (and coindices) of certain transformation graphs [13, 20]. The present work is the continuation of research along the same lines, and is concerned with additional types of transformation graphs.

2 Introduction: Notation and definitions

Let $G = (V, E)$ be a simple graph. The number of vertices and edges of G are denoted by n and m respectively. As usual, n is said to be order and m the size of G . A graph of order n and size m will be, for short, referred to as an (n, m) -graph.

If u and v are two adjacent vertices of G , then the edge connecting them will be denoted by uv . The degree of a vertex $v \in V(G)$ is the number of vertices adjacent to v and is denoted by $d_G(v)$. The complement of G , denoted by \overline{G} , is a graph having the same vertex set as G , in which two vertices are adjacent if and only if they are not adjacent in G . Thus, the size of \overline{G} is $\binom{n}{2} - m$ and $d_{\overline{G}}(v) = n - 1 - d_G(v)$ holds for all $v \in V(G)$.

For terminology not defined here we refer the reader to [19].

In this paper, we are concerned with two degree-based invariants, called first Zagreb index M_1 and second Zagreb index M_2 . These are defined as

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

respectively. Their mathematical theory and chemical applications are nowadays well elaborated; for details see [3, 12, 13, 21]. For historical data on the Zagreb indices see [11]. For surveys on degree-based topological indices see [7, 10].

The first Zagreb index can be written also as [4, 5]

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)] .$$

Došlić [4] defined the first and second Zagreb coindices as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v)$$

respectively.

The following earlier established results will be needed for the present considerations.

Theorem 2.1. [13, 26] *For any (n, m) -graph G ,*

$$M_1(\overline{G}) = M_1(G) + n(n-1)^2 - 4m(n-1) .$$

Theorem 2.2. [1, 13] *Let G be any (n, m) -graph. Then*

$$M_1(G) + \overline{M}_1(G) = 2m(n - 1) .$$

Theorem 2.3. [1, 13] *Let G be a simple graph. Then*

$$\overline{M}_1(G) = \overline{M}_1(\overline{G}) .$$

Theorem 2.4. [1, 13] *Let G be a simple (n, m) -graph. Then*

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G) .$$

Theorem 2.5. [1, 13] *Let G be a simple (n, m) -graph. Then*

$$\overline{M}_2(G) = M_2(\overline{G}) - (n - 1)M_1(\overline{G}) + \overline{m}(n - 1)^2 .$$

3 Generalized transformation graphs G^{ab}

Sampathkumar and Chikkodimath [22] defined the *semitotal-point graph* $T_2(G)$ as the graph whose vertex set is $V(G) \cup E(G)$, and where two vertices are adjacent if and only if (i) they are adjacent vertices of G or (ii) one is a vertex of G and other is an edge of G incident with it. Many papers are devoted to semitotal-point graphs [20, 22–24]. Inspired by this definition, we now introduce some new graphical transformations. These generalize the concept of semitotal-point graph.

Let $G = (V, E)$ be a graph, and let α, β be two elements of $V(G) \cup E(G)$. We say that the associativity of α and β is $+$ if they are adjacent or incident in G , otherwise is $-$. Let ab be a 2-permutation of the set $\{+, -\}$. We say that α and β correspond to the first term a of ab if both α and β are in $V(G)$, whereas α and β correspond to the second term b of ab if one of α and β is in $V(G)$ and the other is in $E(G)$. The generalized transformation graph G^{ab} of G is defined on the vertex set $V(G) \cup E(G)$. Two vertices α and β of G^{ab} are joined by an edge if and only if their associativity in G is consistent with the corresponding term of ab .

We denote the complement of the generalized transformation graph G^{ab} by $\overline{G^{ab}}$.

In view of above, one can obtain four graphical transformations of graphs, since there are four distinct 2-permutations of $\{+, -\}$. Note that G^{++} is just the semitotal-point graph $T_2(G)$ of G , whereas the other generalized transformation graphs are G^{+-} , G^{-+} and G^{--} .

In other words, the generalized transformation graph G^{ab} is a graph whose vertex set is $V(G) \cup E(G)$, and $\alpha, \beta \in V(G^{ab})$. α and β are adjacent in G^{ab} if and only if either (*) and (**) holds:

(*) $\alpha, \beta \in V(G)$, α, β are adjacent in G if $a = +$ and α, β are not adjacent in G if $a = -$.

(**) $\alpha \in V(G)$ and $\beta \in E(G)$, α, β are incident in G if $b = +$ and α, β are not incident in G if $b = -$.

The vertex v_i of G^{ab} corresponding to a vertex v_i of G is referred to as a *point vertex*. The vertex e_i of G^{ab} corresponding to an edge e_i of G is referred to as a *line vertex*.

In this paper, we obtain expressions for the first and second Zagreb indices and coindices of the above defined generalized transformation graphs G^{ab} and their complements $\overline{G^{ab}}$.

4 Results

We start by stating the following propositions, needed for the proving our main results.

Proposition 4.1. *Let G be an (n, m) -graph. Then the degrees of point and line vertices in G^{ab} are*

- (i) $d_{G^{++}}(v_i) = 2d_G(v_i)$ and $d_{G^{++}}(e_i) = 2$.
- (ii) $d_{G^{+-}}(v_i) = m$ and $d_{G^{+-}}(e_i) = n - 2$.
- (iii) $d_{G^{-+}}(v_i) = n - 1$ and $d_{G^{-+}}(e_i) = 2$.
- (iv) $d_{G^{--}}(v_i) = n + m - 1 - 2d_G(v_i)$ and $d_{G^{--}}(e_i) = n - 2$.

Proposition 4.2. *Let G be an (n, m) -graph. Then the order of G^{ab} is $(n + m)$.*

- (i) *The size of G^{++} is $3m$.*
- (ii) *The size of G^{+-} is $m(n - 1)$.*

(iii) The size of G^{-+} is $m + \frac{1}{2}n(n-1)$.

(iv) The size of G^{--} is $\frac{1}{2}n(n-1) + m(n-3)$.

In the recent paper [20], the following two relations have been established.

Lemma 4.3. [20] *Let G be an (n, m) -graph. Then*

$$M_1(G^{++}) = M_1(T_2(G)) = 4[m + M_1(G)] .$$

Lemma 4.4. [20] *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(G^{++}) = 2m(3m + 3n - 5) - 4M_1(G) .$$

We are now prepared to state and prove our main results.

Theorem 4.5. *Let G be an (n, m) -graph. Then*

$$M_1(\overline{G^{++}}) = 4[M_1(G) + m] + (n + m - 1)[(n + m)(n + m - 1) - 12m] . \quad (1)$$

Proof. From Theorem 2.1, it follows

$$M_1(\overline{G^{++}}) = M_1(G^{++}) + n_1(n_1 - 1)^2 - 4m_1(n_1 - 1)$$

where n_1 and m_1 are the number of vertices and edges of G^{++} . Eq. (1) is now obtained by applying Lemma 4.3 and Proposition 4.2. \square

Theorem 4.6. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(\overline{G^{++}}) = 2m(3m + 3n - 5) - 4M_1(G) .$$

Proof. Apply Theorem 2.3 and Lemma 4.4. \square

Theorem 4.7. *Let G be an (n, m) -graph. Then*

$$M_1(G^{+-}) = nm^2 + m(n-2)^2 .$$

Proof. Since G^{+-} has $n + m$ vertices,

$$M_1(G^{+-}) = \sum_{u \in V(G^{+-})} d_{G^{+-}}(u)^2 = \sum_{u \in V(G^{+-}) \cap V(G)} d_{G^{+-}}(u)^2 + \sum_{u \in V(G^{+-}) \cap E(G)} d_{G^{+-}}(u)^2 .$$

From Proposition 4.1, we have

$$M_1(G^{+-}) = \sum_{u \in V(G)} (m)^2 + \sum_{u \in E(G)} (n-2)^2 = nm^2 + m(n-2)^2 .$$

\square

Corollary 4.8. *Let G be an (n, m) -graph. Then*

$$M_1(\overline{G^{+-}}) = n(n-1)^2 + m(m+1)^2 . \quad (2)$$

Proof. From Theorem 2.1, $M_1(\overline{G^{+-}}) = M_1(G^{+-}) + n_1(n_1-1)^2 - 4m_1(n_1-1)$, where n_1 and m_1 are number of vertices and edges of G^{+-} . Eq. (2) follows now from Theorem 4.7 and Proposition 4.2. \square

Corollary 4.9. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(G^{+-}) = m [2(n-1)(m+n-1) - nm - (n-2)^2] . \quad (3)$$

Proof. By Theorem 2.2, $\overline{M}_1(G^{+-}) = 2m_1(n_1-1) - M_1(G^{+-})$, where n_1 and m_1 are number of vertices and edges in G^{+-} . Eq. (3) follows now from Proposition 4.2 and Theorem 4.7. \square

Corollary 4.10. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(\overline{G^{+-}}) = m [2(n-1)(n+m-1) - nm - (n-2)^2] .$$

Proof. Apply Theorem 2.3 and Corollary 4.9. \square

Theorem 4.11. *Let G be an (n, m) -graph. Then*

$$M_1(G^{-+}) = n(n-1)^2 + 4m .$$

Proof. Since G^{-+} has $n+m$ vertices,

$$M_1(G^{-+}) = \sum_{u \in V(G^{-+})} d_{G^{-+}}(u)^2 = \sum_{u \in V(G^{-+}) \cap V(G)} d_{G^{-+}}(u)^2 + \sum_{u \in V(G^{-+}) \cap E(G)} d_{G^{-+}}(u)^2 .$$

By Proposition 4.1,

$$M_1(G^{-+}) = \sum_{u \in V(G)} (n-1)^2 + \sum_{u \in E(G)} (2)^2 = n(n-1)^2 + 4m .$$

\square

Corollary 4.12. *Let G be an (n, m) -graph. Then*

$$M_1(\overline{G^{-+}}) = m^3 + 3nm^2 + n^2m - 6m^2 - 6nm + 9m . \quad (4)$$

Proof. Theorem 2.1 implies

$$M_1(\overline{G^{-+}}) = M_1(G^{-+}) + n_1(n_1 - 1)^2 - 4m_1(n_1 - 1)$$

where n_1 and m_1 are number of vertices and edges of G^{-+} . Eq. (4) follows now from Theorem 4.11 and Proposition 4.2. \square

The next two corollaries are deduced in a fully analogous manner.

Corollary 4.13. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(G^{-+}) = 2m^2 - 6m + n^2m + nm .$$

Corollary 4.14. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(\overline{G^{-+}}) = 2m^2 - 6m + n^2m + nm .$$

Theorem 4.15. *Let G be an (n, m) -graph. Then*

$$M_1(G^{--}) = 4M_1(G) + m(n - 2)^2 + (n + m - 1)[n(n + m - 1) - 8m] . \quad (5)$$

Proof. Since G^{--} has $n + m$ vertices,

$$M_1(G^{--}) = \sum_{u \in V(G^{--})} d_{G^{--}}(u)^2 = \sum_{u \in V(G^{--}) \cap V(G)} d_{G^{--}}(u)^2 + \sum_{u \in V(G^{--}) \cap E(G)} d_{G^{--}}(u)^2 .$$

In view of Proposition 4.1,

$$\begin{aligned} M_1(G^{--}) &= \sum_{u \in V(G)} [n + m - 1 - 2d_G(u)]^2 + \sum_{u \in E(G)} (n - 2)^2 \\ &= n(n + m - 1)^2 + M_1(G) - 4(n + m - 1) \cdot 2m + m(n - 2)^2 \end{aligned}$$

and Eq. (5) follows. \square

Corollary 4.16. *Let G be an (n, m) -graph. Then*

$$M_1(\overline{G^{--}}) = 4M_1(G) + m^3 + 2m^2 + m . \quad (6)$$

Proof. Theorem 2.1 results in

$$M_1(\overline{G^{--}}) = M_1(G^{--}) + n_1(n_1 - 1)^2 - 4m_1(n_1 - 1)$$

where n_1 and m_1 are number of vertices and edges of G^{--} . Eq. (6) is then obtained by bearing in mind Theorem 4.15 and Proposition 4.2. \square

The next two corollaries are deduced in a fully analogous manner.

Corollary 4.17. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(G^{--}) = m(n + 2)(n + m - 1) - 4M_1(G) - m(n - 2)^2 .$$

Corollary 4.18. *Let G be an (n, m) -graph. Then*

$$\overline{M}_1(\overline{G^{--}}) = m(n + 2)(n + m - 1) - 4M_1(G) - m(n - 2)^2 .$$

Theorem 4.19. *Let G be an (n, m) -graph. Then*

$$M_2(G^{++}) = M_2(T_2(G)) = 4[M_1(G) + M_2(G)] .$$

Proof. Since G^{++} has $n + m$ vertices and $3m$ edges,

$$\begin{aligned} M_2(G^{++}) &= \sum_{uv \in E(G^{++})} d_{G^{++}}(u) d_{G^{++}}(v) = \sum_{uv \in E(G^{++}) \cap E(G)} d_{G^{++}}(u) d_{G^{++}}(v) \\ &+ \sum_{uv \in E(G^{++}) - E(G)} d_{G^{++}}(u) d_{G^{++}}(v) . \end{aligned}$$

In view of Proposition 4.1, we have

$$\begin{aligned} M_2(G^{++}) &= \sum_{uv \in E(G)} [2d_G(u) \cdot 2d_G(v)] + \sum_{uv \in E(G^{++}) - E(G)} 2 \cdot 2d_G(v) \\ &= 4M_2(G) + 4 \sum_{v \in V(G)} d_G(v)^2 . \end{aligned}$$

\square

Corollary 4.20. *Let G be an (n, m) -graph. Then*

$$\overline{M}_2(G^{++}) = 2m(9m - 1) - 6M_1(G) - 4M_2(G) . \quad (7)$$

Proof. From Theorem 2.4, $\overline{M}_2(G^{++}) = 2m_1^2 - M_2(G^{++}) - \frac{1}{2}M_1(G^{++})$, where m_1 is number of edges in G^{++} . Eq. (7) follows by applying Proposition 4.2, Theorem 4.19, and Lemma 4.3. \square

The next two corollaries are deduced in a fully analogous manner.

Corollary 4.21. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} M_2(\overline{G^{++}}) &= 2m[11m + 2n - 3] + 2(2n + 2m - 5)M_1(G) - 4M_2(G) \\ &\quad + (n + m - 1)^2 \left[\binom{n + m}{2} - 9m \right]. \end{aligned}$$

Corollary 4.22. *Let G be an (n, m) -graph. Then*

$$\overline{M}_2(\overline{G^{++}}) = 4M_2(G) - 4(n + m - 2)M_1(G) + m(3m^2 - 10m + 3n^2 + 6nm - 10n + 7) .$$

Theorem 4.23. *Let G be an (n, m) -graph. Then*

$$M_2(G^{+-}) = m^3 + m^2(n - 2)^2 .$$

Proof. Since G^{+-} has $n + m$ vertices and $m(n - 1)$ edges,

$$\begin{aligned} M_2(G^{+-}) &= \sum_{uv \in E(G^{+-})} d_{G^{+-}}(u) d_{G^{+-}}(v) = \sum_{uv \in E(G^{+-}) \cap E(G)} d_{G^{+-}}(u) d_{G^{+-}}(v) \\ &\quad + \sum_{uv \in E(G^{+-}) - E(G)} d_{G^{+-}}(u) d_{G^{+-}}(v) . \end{aligned}$$

Proposition 4.1 implies

$$M_2(G^{+-}) = \sum_{uv \in E(G)} m \cdot m + \sum_{uv \in E(G^{+-}) - E(G)} m(n - 2) = m^3 + m^2(n - 2)^2 .$$

\square

Corollary 4.24. *Let G be an (n, m) -graph. Then*

$$\overline{M}_2(G^{+-}) = \frac{m}{2} [m(2n^2 - 2m - 4 - n) - (n - 2)^2] .$$

Corollary 4.25. *Let G be an (n, m) -graph. Then*

$$M_2(\overline{G^{+-}}) = \frac{1}{2} [n^4 + m^4 - 3n^3 + m^3 + 4nm^2 - 2n^2m + 8nm + 3n^2 - 5m^2 - 7m - n] .$$

Corollary 4.26. *Let G be an (n, m) -graph. Then*

$$\overline{M}_2(\overline{G^{+-}}) = m [n^2m + 2n^2 - 3mn + 2m - 5n + 3] .$$

Theorem 4.27. *Let G be an (n, m) -graph. Then*

$$M_2(G^{-+}) = \frac{n-1}{2} [n(n-1)^2 - 2m(n-1) + 8m] .$$

Proof. Since G^{-+} has $n+m$ vertices and $\frac{1}{2}n(n-1) + m$ edges,

$$\begin{aligned} M_2(G^{-+}) &= \sum_{uv \in E(G^{-+})} d_{G^{-+}}(u) d_{G^{-+}}(v) = \sum_{uv \in E(G^{-+}) \cap E(\overline{G})} d_{G^{-+}}(u) d_{G^{-+}}(v) \\ &+ \sum_{uv \in E(G^{-+}) - E(\overline{G})} d_{G^{-+}}(u) d_{G^{-+}}(v) . \end{aligned}$$

Proposition 4.1 implies

$$\begin{aligned} M_2(G^{-+}) &= \sum_{uv \in E(\overline{G})} (n-1)(n-1) + \sum_{uv \in E(G^{-+}) - E(\overline{G})} (n-1)^2 \\ &= \frac{n-1}{2} [n(n-1)^2 - 2m(n-1) + 8m] . \end{aligned}$$

□

Corollary 4.28. *Let G be an (n, m) -graph. Then*

$$\overline{M}_2(G^{-+}) = 2 \left[\binom{n}{2} + m \right]^2 - (n-1) \left[n \binom{n}{2} + 5m - mn \right] - 2m .$$

Corollary 4.29. *Let G be an (n, m) -graph. Then*

$$M_2(\overline{G^{-+}}) = \frac{1}{2} [4nm^3 + 3n^2m^2 - 18nm^2 - n^2m + 6nm - 9m^3 + m^4 + 27m^2 - 9m] .$$

Corollary 4.30. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} \overline{M}_2(\overline{G^{-+}}) &= \frac{1}{2} [(n+m)(n+m-1) - 2m - n(n-1)^2] \\ &- \frac{1}{2} [4nm^3 + 3n^2m^2 - 15nm^2 - 8m^3 + m^4 + 21m^2] . \end{aligned}$$

Theorem 4.31. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} M_2(G^{--}) &= (n+m-1) \left\{ (n+m-1) \left[\binom{n}{2} - m \right] + m(n-2)^2 - 2\overline{M}_1(G) \right\} \\ &+ 4\overline{M}_2(G) - 2(n-2)[2m^2 - M_1(G)] . \end{aligned} \quad (8)$$

Proof. Since G^{--} has $n+m$ vertices and $\binom{n}{2} + m(n-3)$ edges,

$$\begin{aligned} M_2(G^{--}) &= \sum_{uv \in E(G^{--})} d_{G^{--}}(u) d_{G^{--}}(v) = \sum_{uv \in E(G^{--}) \cap E(\overline{G})} d_{G^{--}}(u) d_{G^{--}}(v) \\ &+ \sum_{uv \in E(G^{--}) - E(\overline{G})} d_{G^{--}}(u) d_{G^{--}}(v) . \end{aligned}$$

Proposition 4.1 implies

$$\begin{aligned} M_2(G^{--}) &= \sum_{uv \in E(\overline{G})} [(n+m-1) - 2d_G(u)] [(n+m-1) - 2d_G(v)] \\ &+ \sum_{uv \in E(G^{--}) - E(\overline{G})} (n-2)[n+m-1 - 2d_G(v)] \end{aligned}$$

from which Eq. (8) straightforwardly follows. \square

Corollary 4.32. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} \overline{M}_2(G^{--}) &= 2(n+m-1)\overline{M}_1(G) - 4\overline{M}_2(G) - 2(n-1)M_1(G) \\ &+ \frac{1}{2} [m^2n^2 + 16m^2 - 4m^2n - 3mn^2 + 4nm - 2m + 2m^3] . \end{aligned}$$

Corollary 4.33. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} M_2(\overline{G^{--}}) &= 2(n+m-1)\overline{M}_1(G) - 4\overline{M}_2(G) + 2M_1(G)(n+2m-1) \\ &+ \frac{m}{2} [23m - 8nm - 8n^2 + 16n - 9 + m^2 + m^3] . \end{aligned}$$

Corollary 4.34. *Let G be an (n, m) -graph. Then*

$$\begin{aligned} \overline{M}_2(\overline{G^{--}}) &= 4\overline{M}_2(G) - 2(n+m-1)\overline{M}_1(G) - 2(n+2m)M_1(G) \\ &+ \frac{1}{2} [8m^3 + 8nm^2 + 8n^2m - 16nm + 8m] . \end{aligned}$$

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