Computing $F$-index, coindex and Zagreb polynomials of the $k$th generalized transformation graphs

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**Abstract**

In chemical graph theory, forgotten topological index or $F$-index plays a crucial role to collect information about the properties of chemical compounds. The 4th generalized transformation graphs of a molecular graph preserve the entire information on the molecular topology contained in the relevant molecular graph. In this paper, some exact expressions of the $F$-index and its co-index for the 4th generalized transformation graphs are obtained. Also, the Zagreb polynomials, Zagreb co-polynomials and their complements are computed.

1. Introduction

In theoretical chemistry, chemical compounds are often used to model different molecular structures which are graphically represented as molecular graphs in which atoms as nodes and chemical bonds as edges. Throughout this paper, we consider only molecular graphs that are simple. Let $X = (n,m)$ be such a graph of order $n$ and size $m$ with vertex set $V(X)$ and edge set $E(X)$ such that $|V(X)| = n$ and $|E(X)| = m$. Also, for any vertex $p \in V(X)$, $d(p/X)$ denotes the degree of that vertex in $X$. The graph $\overline{X}$ be the complement of $X$ with the same vertex set $V(X)$ and for any edge, $pq \in E(\overline{X})$ exists if and only if $pq \notin E(X)$. So, it is clear that $E(X) \cup E(\overline{X}) = E(K_n)$ and $|E(\overline{X})| = \left(\binom{n}{2}\right) - |E(X)|$. Therefore, the degree of $p \in V(\overline{X})$ is given by $d(p/\overline{X}) = |V(X)| - 1 - d(p/X)$.

We will follow reference [1] for undefined notation and terminology. Graph theory [2] provides a link between mathematics and chemistry by an important tool named topological index. Forty eight years ago the two oldest graph invariants namely first and second Zagreb indices are introduced by Gutman and Trinajestic [3]. The first Zagreb index is denoted as $M_1(X)$ and is defined by $M_1(X) = \sum_{p \in E(X)} d^2(p/X) = \sum_{p \in E(X)} [d(p/X) + d(q/X)]$. Doscic [4] defined the first Zagreb coindex as $M_1^c(X) = \sum_{p \in E(X)} [d(p/X) + d(q/X)]$. Analogously to another topological index in [3] is calculated as the sum of the power three of degrees of the vertices of a graph. It is further found in Furtula et al. in [5]. This index is named as forgotten topological index or shortly, $F$-index which also influences the total $\pi$-electron energy ($\epsilon$). This index is symbolically expressed as $F(X) = \sum_{p \in E(X)} d^3(p/X) = \sum_{p \in E(X)} [d^2(p/X) + d^2(q/X)]$. In 2016, De [6] introduced a new graph invariant, the $F$-coindex as follows $\overline{F}(X) = \sum_{p \in E(\overline{X})} (d^2(p/\overline{X}) + d^2(q/\overline{X}))$. Transformation graphs preserve the entire information from the original graph into new transformed structure. For details see [7]. The basic properties of transformation graphs can be followed in [8]. For more on transformation graphs refer to [9, 10]. We refer our readers to [11] for recent study.

Analogous to the Zagreb indices, Fath-Tabar [12] defined the first, second and third Zagreb polynomials as

$$M_1(X, x) = \sum_{p \in E(X)} x^{d(p/X) + d(q/X)}$$

$$M_2(X, x) = \sum_{p \in E(X)} x^{d(p/X) + d(q/X)}$$

and

$$M_3(X, x) = \sum_{p \in E(X)} x^{d(p/X) - d(q/X)}$$

respectively.

On the base of Zagreb coindices, Basavanagoud and Jakkannavar [13] defined three new graph polynomials, namely the first, second and third Zagreb co-polynomials. They are as follows

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\[ M_1(X, x) = \sum_{p \in V(X)} x^d(p/X) \]

\[ M_2(X, x) = \sum_{p \in E(X)} x^{d_2}(p) \]

\[ M_3(X, x) = \sum_{p \in E(X)} x^{d_3}(p) \]

respectively.

Additionally, Shuxian [14] presented two new polynomials related to the first Zagreb index like as

\[ M_1^s(X, x) = \sum_{p \in V(X)} x^d(p/X) \]

and

\[ M_2^s(X, x) = \sum_{p \in E(X)} x^{d_2}(p) \]

Further, Bindasree et al. [15] introduced the following polynomials

\[ M_{a,b}(X, x) = \sum_{p \in E(X)} x^{d(a)p + b} \]

and

\[ M'_{a,b}(X, x) = \sum_{p \in E(X)} x^{d(a)p + b} \]

Similarly, Basavanagoud et al. [13] also defined

\[ M_{a,b}(X, x) = \sum_{p \in E(X)} x^{d(a)p + b} \]

and

\[ M'_{a,b}(X, x) = \sum_{p \in E(X)} x^{d(a)p + b} \]

where \( x \) is to be chosen as a variable.

For different recent study of \( F \)-index and its co-index, we refer to [8, 16, 17]. In order to know more about Zagreb polynomials and its co-polynomials for various transformation graphs see [15, 18, 19]. The following Propositions are instrumental in proving for the present considerations.

**Proposition 1.** [20] Let \( X \) be a graph with \( n \) vertices and \( m \) edges and \( \overline{X} \) be the complement of \( X \). Then

(i) \( M_1(\overline{X}) = \frac{n(n-1)}{2} - 6m(n-1) + M_1(X) \),

(ii) \( M_2(\overline{X}) = 2m(n-1) - M_2(X) \),

(iii) \( M_3(\overline{X}) = 2m^2 + \frac{1}{2} M_1(X) - M_2(X) = 3m(n-1)^2 + M_1(\overline{X}) - (n-1) M_1(\overline{X}) \),

(iv) \( M_4(\overline{X}) = M_1(X) + M_4(\overline{X}) \).

**Proposition 2.** [21] Let \( X \) be an \((n, m)\) graph. Then

(i) \( M_1(X_k^{+}) = (k+1)^2 M_1(X) + 4mk \),

(ii) \( M_2(X_k^{+}) = m^2(kn + 4 - 4k) + (k+1)^2 M_2(X) + (n-2)^2 km \),

(iii) \( M_3(X_k^{+}) = 4m(n-1)(k+1)(k-1)^2 M_3(X) + n(n-1)^2 + 4mk \),

(iv) \( M_4(X_k^{+}) = M_1(X) + km(n-k)(n-1) + (k+1)^2 M_1(X) + km(n-2)^2 \).

**Proposition 3.** [6] Let \( X \) be a graph of order \( n \) and size \( m \). Then

(i) \( F(\overline{X}) = \frac{n(n-1)}{2} - 6m(n-1)^2 + 3(n-1)M_4(X) - F(X) \),

(ii) \( \overline{F}(X) = (n-1)M_1(X) - F(X) = 2m(n-1)^2 + F(\overline{X}) - 2(n-1)M_1(\overline{X}) \),

(iii) \( \overline{F}(X) = 2m(n-1)^2 - (n-1)M_1(X) - \overline{F}(X) \).

2. The \( k \)th generalized transformation graphs \( X_k^{+w} \)

The \( k \)th generalized transformations which was introduced by Jummannaver et al. [21] is the new graphical transformations of generalized transformations [18, 22] of a graph. This concept was developed by using semitotal-point graph which was defined by Sampathkumar and Chikkodimath in [23] and later put forward as the \( k \)th semitotal-point graph which was introduced by Jog in [24] of a graph.

**Definition 1.** [21] Consider \( X(V(X), E(X)) \) be a simple, connected graph and \( u, v \) are the two graph parameters having values \(+\) or \(-\). The \( k \)-th generalized transformation graph (GTG) \( X_k^{+w} \) is a new graph having \( V(X_k^{+w}) = V(X) \cup (E' \cup \sum_{j=1}^k E_j) \) as vertex set and \( p, q \in V(X_k^{+w}) \) such that the vertices \( p \) and \( q \) are adjacent in \( X_k^{+w} \) if and only if the following conditions (i) and (ii) hold:

1. \( p \) and \( q \) are adjacent in \( X \) if \( u = + \) and non adjacent in \( X \) if \( u = - \).
2. \( p \in E(X) \) and \( q \in E_j \), for some \( j \in \beta \) (where \( \beta = 1, 2, \ldots, m \) or \( 0 \)).

Suppose \( e_j \) be the edge of \( X \) and \( E_1, E_2, \ldots, E_m \) be the distinct edge set and each \( E_j \) is corresponding to the edge \( e_j \) in \( X \) such that \( |E_j| = k_j, j = 1(0)m \). The vertex \( p \) and \( e_j \) are incident in \( X \) and are not incident in \( X \) if \( u = - \).

There exist 4-distinguished 2-permutations of \(+, -\). The four graphical transformations in \( X \) like \( X_1^{+w}, X_2^{+w}, X_3^{+w} \) and \( X_4^{+w} \) can be established. Also their complements like \( \overline{X}_1^{+w}, X_1^{+w}, X_2^{+w} \), \( \overline{X}_3^{+w} \) and \( \overline{X}_4^{+w} \) can be obtained. The vertex \( p \) of \( X_k^{+w} \) corresponding to a vertex \( p \) of \( X \) is referred to as a point vertex. Also, the vertex \( e \) of \( X_k^{+w} \) corresponding to an edge \( e \) of \( X \) is referred to as a line vertex. To know more about the transformation graphs we can study in [25, 26].

There are two different types of edge partitions in the \( k \)th GTG \( (X_k^{+w}) \) and its complement \( \overline{X}_k^{+w} \). Firstly in each \( X_k^{+w} \), the edges can be split into two parts like \( E_k^{+w/1} \) and \( E_k^{+w/2} \). Other hand, in each \( \overline{X}_k^{+w} \), the partition of the edge set \( E(\overline{X}_k^{+w}) \) can be separated into three subsets like \( E_1^{+w/1}, E_2^{+w/1}, E_3^{+w/1} \). As an example, the edges of \( E(X_k^{+w}) \) can be split into two parts like \( E_k^{+w/1} = \{ pe \} \) and \( E_k^{+w/2} = \{ pe \} \) the vertex \( p \) and edge \( e \) in \( X \) are incident to each other and the edges of \( E(\overline{X}_k^{+w}) \) can be divided into three parts like \( E_1^{+w/1} = \{ pe \} \) and \( E_2^{+w/2} = \{ pe \} \) the vertex \( p \) and edge \( e \) in \( X \) are not incident to each other and \( E_3^{+w/1} = \{ ef \} \) (see Fig. 1).

3. The results on the \( F \)-index and its co-index of \( X_k^{+w} \)

The following theorems can be used to compute the results on \( F \)-index and its co-index of the \( k \)th GTG \( X_k^{+w} \).

**Theorem 1.** Let \( X \) be a graph with \( n \) vertices and \( m \) edges. Then the \( F \)-index and its co-index of \( X_k^{+w} \) are calculated as

(i) \( F(X_k^{+w}) = (k+1)^2 F(X) + 8k m \),

(ii) \( \overline{F}(X_k^{+w}) = (n+km-1)(k+1)^2 M_1(X) - (k+1)^3 F(X) + 4km(n+km-3) \).

**Proof.** (i) From the definition of \( F \)-index, we have

\[
F(X_k^{+w}) = \sum_{p \in V(X_k^{+w})} d^1(p/X_k^{+w})
= \sum_{p \in V(X_k^{+w} \setminus V(X))} d^1(p/X_k^{+w}) + \sum_{p \in V(X_k^{+w} \cap V(X))} d^1(p/X_k^{+w})
\]

With the help of Table 1
Theorem 1. Let $X$ be a graph of order $n$ and size $m$. Then

(i) $F(X) = (n^* + (n + k)m)^2 - (n + k)(n + k + 1)F(X) - km(n + k - 1)^3 - 8km(n + k - 1)$.

(ii) $F(X) = (n + k)(n + k + 1)^2(M_k(X) + 4km(n + k - 1) - 8km).

Proof. (i) Using the Propositions 2 and 3, Table 1 and Theorem 1, we have

$$F(X^{+\perp}) = n^* - 3 - 6n^* + 3M_k(X) - (k + 1)^3 F(X) + 4km(n + k - 1)^3 - 8km(n + k - 1).$$

Table 1. [21] The degree distributions of the point vertices and line vertices in $X^{+\perp}$ and $X^{-\perp}$ are corresponding to that vertices and edges in $X$.

| Degrees of point vertices | Degrees of line vertices | Orders | Sizes |
|---------------------------|--------------------------|--------|-------|
| $d(p/X^{+\perp}) = (k + 1)d(p/X)$ | $d(e/X^{+\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{-\perp}) = (k + 1)d(p/X)$ | $d(e/X^{-\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{+\perp}) = (k + 1)d(p/X)$ | $d(e/X^{+\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{-\perp}) = (k + 1)d(p/X)$ | $d(e/X^{-\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{+\perp}) = (k + 1)d(p/X)$ | $d(e/X^{+\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{-\perp}) = (k + 1)d(p/X)$ | $d(e/X^{-\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{+\perp}) = (k + 1)d(p/X)$ | $d(e/X^{+\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |
| $d(p/X^{-\perp}) = (k + 1)d(p/X)$ | $d(e/X^{-\perp}) = 2$ | $(km + n)$ | $(2k + 1)$ |

Fig. 1. An example of $X^{+\perp}$: $X^{+\perp}$ of a graph $X(5,6)$ and its complement $X^{-\perp}$.
(ii) \( F(X_k^{+-}) = (k-1)^3 F(X) + (n-2km-1)(k-1)^2 M_1(X) + 6m^3k^2(k-1) \) \( - nm^3k^3 - km(n-2)^3 + km(n+k-1)\) \( nmk + 4m - 4km + (n-2)^2 \).

**Proof.** (i) The \( F \)-index of \( X_k^{+-} \) can be revealed as

\[
F(X_k^{+-}) = \sum_{p \in V(X_k^{+-})} d^3(p/X_k^{+-}) = \sum_{p \in V(X_k^{+-}) \cap V(X)} d^3(p/X_k^{+-}) + \sum_{p \in V(X_k^{+-}) \cap V'(X)} d^3(p/X_k^{+-}) = \sum_{p \in V(X)} \left( k(m-d(X)) + d(X) \right)^3 + \sum_{p \in V(X)} (n-2)^3 + 3km(k-1)^2d^2(p/X) + 3m^2k^2(1-k)d(p/X) + m^3k^3 \) \( (n-2)^3 km \) \( = (1-k)^3 F(X) + 3km(k-1)^2 M_1(X) \) \( -6m^3k^2(k-1) + m^3k^3 n + (n-2)^3 mk. \)

(ii) With the help of Propositions 1, 2 and 3, we can prove it in a similar way. \( \square \)

**Corollary 2.** Consider \( X(n,m) \) be a graph and \( X_k^{+-} \) be the complement of \( X_k^{+-} \). Then

(i) \( F(X_k^{+-}) = (k-1)^3 F(X) + (n-1)(k-1)^2 M_1(X) + (n + km)(n + km - 1)^3 - nm^3k^3 - km(n-2)^3 + km(n-2)(k+1) \) \( n + km - 1)^2 + 3km \) \( nmk + 4m - 4km + (n-2)^2 \) \( (n + km - 1) + 6m^3k^2(k-1). \)

(ii) \( F(X_k^{+-}) = (k-1)^3 (km - 2n + 2) M_1(X) - (k-1)^3 F(X) - (n + 2km)(n-2)^2 km + 2m(n-2)(k+1) \) \( n + km - 1)^2 - 2m^2(kn - 4k + 4)(n + km - 1) + nm^3k^3 - 6m^3k^2(k-1). \)

In the following, we obtain the \( F \)-index of the \( k \)th GTG \( X_k^{-+} \) (see Fig. 3).

**Theorem 3.** Let \( X \) be an \((n,m)\) graph. Then \( F \)-index and its co-index for \( X_k^{-+} \) are given by

(i) \( F(X_k^{-+}) = (k-1)^3 F(X) + 3(k-1)^2 M_1(X) + (n-1)^3 + 6m(n-1)^2(k-1) + 8km. \)

(ii) \( F(X_k^{-+}) = (km - 2n + 2)(k-1)^2 M_1(X) - (k-1)^3 F(X) + 2m(n-1)(k-1) \) \( 2(2km - n+1) + km(n-2)^2 + 4km + 5n-12). \)

**Proof.** (i) We get from the definition of \( F \)-index

\[
F(X_k^{-+}) = \sum_{p \in V(X_k^{-+})} d^3(p/X_k^{-+}) = \sum_{p \in V(X_k^{-+}) \cap V(X)} d^3(p/X_k^{-+}) + \sum_{p \in V(X_k^{-+}) \cap V'(X)} d^3(p/X_k^{-+}) = \sum_{p \in V(X)} \left( (k-1)d(p/X) + (n-1)^3 \right) + \sum_{p \in V(X)} 2^3 \) \( + 3(n-1)^2(k-1)d(p/X) \) \( + 8km \) \( = (k-1)^3 F(X) + n(n-1)^3 + 3(k-1)^2(n-1) M_1(X) \) \( + 6m(n-1)^2(k-1) + 8km. \)

(ii) From Theorem 3, Table 1 and Propositions 1, 2, 3 we can get the required expression. \( \square \)

**Corollary 3.** Let us consider \( X \) be a graph with \( n \) vertices and \( m \) edges and \( X_k^{-+} \) be the complement of the graph \( X_k^{-+} \). Then

(i) \( F(X_k^{-+}) = 3km(k-1)^2 M_1(X) - (k-1)^3 F(X) + (n + km)(n + km - 1)^3 - 6m(n-1)^2(k-1) - 3m^3 + 4km - 2m(n + km - 1)^2 + 12mkn + 1) + km(n - 1)^2(2n + 3km - 2) - 8km. \)
(ii) $F(X_k^-) = (k+1)^3F(X) - 2m(k+1)(n+km-1)(2kn+2n-5) + km(km+1)(n-2)^2 - 2(n+km-1)(k+1)^2 M_1(X)$.

**Proof.** (i) From the definition of $F$-index, we get

$$F(X_k^-) = \sum_{pq \notin E(X^-)} \left( d^2(p/X_k^-) + d^2(q/X_k^-) \right)$$

$$= \sum_{pq \notin E(X)} \left[ \left( (n+km-1) - (k+1)d(p/X) \right)^2 + \left( (n+km-1) - (k+1)d(q/X) \right)^2 ight]$$

$$+ \sum_{p \in V(X)} k(m - \bar{d}(p/X))((n+km-1))$$

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Proof. (i) Let \( M_1(X, x^{(k+1)}) \) be the polynomial for the graph \( X^{k+1} \) of degree \( k \) for any vertex \( x \). Then the edges of \( E(X^{k+1}) \) can be divided into two parts like \( E_{1}^{k+1} = \{pq \in E(X)\mid p \notin E_X\} \) and \( E_{2}^{k+1} = \{pq \in E(X)\mid p \in E_X\} \). The vertex \( x \) is incident to each other such that \( |E_{1}^{k+1}| = m \) and \( |E_{2}^{k+1}| = 2k \), respectively.

\[
\begin{align*}
&= \sum_{pq \in E_{1}^{k+1}} x^{k+1}(d(p/X)+d(q/X)) + \sum_{pq \in E_{2}^{k+1}} x^{k+1}(d(p/X)+d(q/X)+2) \\
&= M_1(X, x^{(k+1)}) + x^k \sum_{pq \in E(X)} d(p/X)x^{(k+1)}d(q/X) \\
&= M_1(X, x^{(k+1)}) + x^k M_1'(X, x^{(k+1)}),
\end{align*}
\]

(ii) Now,

\[
M_2(X_k, x) = \sum_{pq \in E(X)} x^{\delta(p/X)+\delta(q/X)} \\
= \sum_{pq \in E_{1}^{k+1}} x^{k+1}(d(p/X)+d(q/X)) + \sum_{pq \in E_{2}^{k+1}} x^{k+1}(d(p/X)+d(q/X)+2) \\
= M_2(X, x^{(k+1)}) + x^k \sum_{pq \in E(X)} d(p/X)x^{(k+1)}d(q/X) \\
= M_2(X, x^{(k+1)}) + x^k M_1'(X, x^{(k+1)}),
\]

(iii) From the definition of \( M_3(X, x) \) and putting \( X = X_k \), we have

\[
M_3(X_k, x) = \sum_{pq \in E(X)} x^{\delta(p/X)+\delta(q/X)} \\
= \sum_{pq \in E_{1}^{k+1}} x^{k+1}(d(p/X)+d(q/X)) + \sum_{pq \in E_{2}^{k+1}} x^{k+1}(d(p/X)+d(q/X)+2) \\
= M_3(X, x^{(k+1)}) + \sum_{pq \in E(X)} d(p/X)x^{(k+1)}d(q/X) + \left(\frac{km}{2}\right)
\]

\[
= M_3(X, x^{(k+1)}) + \frac{k}{x^2} M_0(X, x^{(k+1)}) - \frac{k}{x^2} M_1'(X, x^{(k+1)}) + \left(\frac{km}{2}\right).
\]

Corollary 5. The Zagreb polynomials for the graph \( X_k^{k+1} \) are expressed as

\[
\begin{align*}
&\text{(i) } M_1(X_k^{k+1}, X) = x^{k+1}(X, x^{(k+1)}) + \operatorname{km} x^{k+1}(X, x^{(k+1)}) M_0(X, x^{(k+1)}) \\
&\quad - \frac{km}{2} M_1'(X, x^{(k+1)}) + \left(\frac{km}{2}\right), \\
&\text{(ii) } M_2(X_k^{k+1}, X) = \frac{k}{x^2} M_0(X, x^{(k+1)}) - \frac{k}{x^2} M_1'(X, x^{(k+1)}) + \left(\frac{km}{2}\right), \\
&\text{(iii) } M_3(X_k^{k+1}, X) = \frac{k}{x^2} M_0(X, x^{(k+1)}) - \frac{k}{x^2} M_1'(X, x^{(k+1)}) + (\sqrt{\frac{km}{2}}).
\end{align*}
\]
\( M_1(\overline{X^+}^k, x) = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} \cdot d(q/\overline{X^+}^k) \)
\[ = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} + \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} \cdot d(q/\overline{X^+}^k) \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{d(c/\overline{X^+}^k)} \cdot d(f/\overline{X^+}^k) \]
\[ = \sum_{p \in E(X)} x^{(n+4k-1)(-k+1+1)d(p/X)+d(q/X)} \]
\[ + k \sum_{p \in E(X)} x^{2(n+4k-2)(-k+1+1)d(p/X)} \]
\[ + \left( \frac{km}{2} \right) x^{2(n+4k-3)} \]
\( = \overline{M_0}(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^{2(n+4k-3)} \)

(iii) Now,
\[ M_1(\overline{X^+}^k, x) = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} \cdot d(q/\overline{X^+}^k) \]
\[ = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} + \sum_{p \in E(\overline{X^+}^k)} x^{d(p/\overline{X^+}^k)} \cdot d(q/\overline{X^+}^k) \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{d(c/\overline{X^+}^k)} \cdot d(f/\overline{X^+}^k) \]
\[ = \sum_{p \in E(X)} x^{(n+4k-1)(-k+1+1)d(p/X)+d(q/X)} \]
\[ + k \sum_{p \in E(X)} x^{2(n+4k-2)(-k+1+1)d(p/X)} \]
\[ + \left( \frac{km}{2} \right) x^{2(n+4k-3)} \]
\( = \overline{M_0}(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^{2(n+4k-3)} \)

Corollary 6.

(i) \( \overline{M_1}(X^+^k, x) = \overline{M_1}(X, x^{(k+1)}) + kmx^2M_0(X, x^{(k+1)}) - x^2kM_1^+(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^4 \)

(ii) \( \overline{M_2}(X^+^k, x) = \overline{M_2}(X, x^{(k+1)}) + mkM_0(X, x^{(k+1)}) - kM_1^+(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^4 \)

The partition of the edge set \( E(\overline{X^+}^k) \) follows as Corollary 5

\[ = \sum_{p \in E(X)} x^{(k+1+1)d(p/X)+d(q/X)} \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{(n+4k-1)(-k+1+1)d(p/X)+d(q/X)} \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{2(n+4k-2)(-k+1+1)d(p/X)} \]
\[ = \overline{M_0}(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^4 \]

(ii) \( \overline{M_2}(X^+^k, x) = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/X^+^k)+d(q/X^+^k)} \]
\[ = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/X^+^k)} + \sum_{p \in E(\overline{X^+}^k)} x^{d(p/X^+^k)} + \sum_{c \in E(\overline{X^+}^k)} x^{d(c/X^+^k)} \]
\[ = \sum_{p \in E(X)} x^{(k+1+1)d(p/X)+d(q/X)} \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{(n+4k-1)(-k+1+1)d(p/X)+d(q/X)} \]
\[ + \sum_{c \in E(\overline{X^+}^k)} x^{2(n+4k-2)(-k+1+1)d(p/X)} \]
\[ = \overline{M_0}(X, x^{(k+1)}) + \left( \frac{km}{2} \right) x^4 \]

(iii) \( \overline{M_3}(X^+^k, x) = \sum_{p \in E(\overline{X^+}^k)} x^{d(p/X^+^k)+d(q/X^+^k)} \)
\[ M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) + d(q/X_k^{+\pm})) \right|} + \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) - d(q/X_k^{+\pm})) \right|} + \sum_{e \in \Gamma_k} x^{\left| (d(p/X_k^{+\pm}) + d(f/X_k^{+\pm})) \right|} = \sum_{p \in E(X_k)} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k)} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]

**Corollary 7.**

(i) \( M_t(X_k^{+\pm}, x) = 2^{n+4m-1} M_t(X_k, x^{(k+1)}) + kx^{2n+4m-2} M_t^+(X_k, x^{(k+1)}) \).

(ii) \( M_t(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + kx^{4n+6m-3} M_t^+(X_k, x^{(k+1)}) \).

(iii) \( M_t(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) \).

**Proof.** (i) With the help of the definition \( M_t(X, x) \) and putting \( X = X_k^{+\pm} \), we get

\[ M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) + d(q/X_k^{+\pm})) \right|} = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]

(ii) \( M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) - d(q/X_k^{+\pm})) \right|} + \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) + d(q/X_k^{+\pm})) \right|} + \sum_{e \in \Gamma_k} x^{\left| (d(p/X_k^{+\pm}) + d(f/X_k^{+\pm})) \right|} = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]

(iii) \( M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) + d(q/X_k^{+\pm})) \right|} = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]

**5. The Zagreb polynomials on \( X_k^{+\pm} \)**

The expressions for the Zagreb polynomials of the \( k \)th GTG \( X_k^{+\pm} \) are obtained as follows here.

**Theorem 6.** For the \( k \)th GTG \( X_k^{+\pm} \), the Zagreb polynomials are

\[ M_1(X_k^{+\pm}, x) = x^{2km} M_t(X_k, x^{(k+1)}) + kmx^{(n+km-2)} M_t(X_k, x^{(k+1)}) - kx^{(n+km-2)} M_t^+(X_k, x^{(k+1)}). \]

\[ M_2(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + kmx^{(n-2km)} M_t(X_k, x^{(k+1)}) - kx^{(n-2km)} M_t^+(X_k, x^{(k+1)}). \]

\[ M_3(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + kmx^{(n-2km)} M_t(X_k, x^{(k+1)}) - kx^{(n-2km)} M_t^+(X_k, x^{(k+1)}). \]

**Proof.** (i) The edges of \( E(X_k^{+\pm}) \) can be separated into two parts like \( E_1^{+\pm} = \{pq \in E(X_k^{+\pm}) \mid p \neq e \text{ and edge } e \text{ is not incident to either other in } X \} \) such that \( |E_1^{+\pm}| = m \) and \( |E_2^{+\pm}| = km(n-2) \), respectively.

By the definition of \( M_t(X, x) \) and putting \( X = X_k^{+\pm} \), we have

\[ M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) + d(q/X_k^{+\pm})) \right|} + \sum_{p \in E(X_k^{+\pm})} x^{\left| (d(p/X_k^{+\pm}) - d(q/X_k^{+\pm})) \right|} + \sum_{e \in \Gamma_k} x^{\left| (d(p/X_k^{+\pm}) + d(f/X_k^{+\pm})) \right|} = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]

The rest part of the theorem can be established in a similar way.

**Corollary 8.**

(i) \( M_1(X_k^{+\pm}, x) = x^{2km} M_t(X_k, x^{(k+1)}) + kmx^{(n+km-2)} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \)

(ii) \( M_2(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + kmx^{(n-2km)} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \)

(iii) \( M_3(X_k^{+\pm}, x) = M_t(X_k, x^{(k+1)}) + kmx^{(n-2km)} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \)

**Proof.** (i) The edges of \( E(X_k^{+\pm}) \) can be divided into three parts such as \( E_1^{+\pm} = \{pq \in E(X_k^{+\pm}) \mid p \neq e \text{ and edge } e \text{ is incident to } X \} \) and \( E_2^{+\pm} = \{pq \in E(X_k^{+\pm}) \mid p \neq e \} \), respectively such that \( |E_1^{+\pm}| = (\frac{n}{2}) - m \), \( |E_2^{+\pm}| = 2km \) and \( |E_3^{+\pm}| = (\frac{n}{2}) \), respectively.

By the definition of the polynomial \( M_t(X, x) \) and setting \( X = X_k^{+\pm} \), we get

\[ M_t(X_k^{+\pm}, x) = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = \sum_{p \in E(X_k^{+\pm})} x^{\left( (k+1)d(p/X_k) - (k+1)d(q/X_k) \right)} + \frac{k}{x^2} \sum_{g \in E(X_k^{+\pm})} d(p/X_k) x^{(k+1)d(p/X_k)} = M_t(X_k, x^{(k+1)}) + \frac{k}{x^2} M_t^+(X_k, x^{(k+1)}) + \left( \frac{km}{2} \right). \]
Corollary 9.

(i) \( \overline{M}_1(X_k^{k+}, x) = x^{-2km}M_1(X, x^{-k(k-1)}) + kx^{(n+k)m-2}M^*_1(X, x^{-k(k-1)}) + \left(\frac{kn}{2}\right)\delta_n(x^{-2}) \)

(ii) \( \overline{M}_2(X_k^{k+}, x) = \overline{M}_2 \left( x^{-k-2(k-1)} \right) + kx^{(n-k)m}M^*_1(X, x^{-k(k-1)}) + \left(\frac{kn}{2}\right)x^{-2(k-1)} \)

(iii) \( \overline{M}_3(X_k^{k+}, x) = \overline{M}_3(X, x^{-k}) + kx^{[n-km]}M^*_1(X, x^{-k}) + \left(\frac{kn}{2}\right) \)

Corollary 10.

(i) \( \overline{M}_1(X_k^{-}, x) = x^{2n-1}M_1(X, x^{-k(k-1)}) + kmx^{(n+k)m}M_0(X, x^{-k(k-1)}) - kx^{(n+k)m}M^*_1(X, x^{-k}) \)

(ii) \( \overline{M}_2(X_k^{-}, x) = \overline{M}_2 \left( x^{-k+2(k-1)} \right) + kmx^{(n-1)(k+1)m}M_0(X, x^{-k(k-1)}) - kx^{(n-1)(k+1)m}M^*_1(X, x^{-k(k-1)}) \)

(iii) \( \overline{M}_3(X_k^{-}, x) = \overline{M}_3(X, x^{-k}) + kx^{[n-km]}M^*_1(X, x^{-k}) \)

6. The Zagreb polynomials on \( X_k^{k+} \)

The \( X_k^{k+} \) is one kind of the 4th GTG of \( X \). The F-index and its co-index and also the Zagreb polynomials for the \( X_k^{k+} \) and its complement are obtained in the following theorems.

The two parts of the edges \( E(X_k^{k+}) \) are \( E_1^{k+} = \{(pq) \not\in E(X)\} \) and \( E_2^{k+} = \{(pq) \in E(X)\} \) such that \( |E_1^{k+}| = \left(\begin{array}{c} n \\ k \end{array}\right) \) and \( |E_2^{k+}| = 2km \), respectively. Analogously, \( E(X_k^{-}) = E_1^{-k-} \cup E_2^{-k-} \cup E_3^{-k-} \).

Also, \( |E_1^{-k-}| = m, |E_2^{-k-}| = km(n-2) \) and \( |E_3^{-k-}| = \left(\frac{kn}{2}\right) \)

Theorem 7. The Zagreb polynomials of \( X_k^{-k} \) are given by

(i) \( M_1(X_k^{-k}, x) = x^{2n-1}M_1(X, x^{-k(k-1)}) + kx^{(n+k)m}M_0(X, x^{-k(k-1)}) - kx^{(n+k)m}M^*_1(X, x^{-k}) \)

(ii) \( M_2(X_k^{-k}, x) = \overline{M}_2 \left( x^{-k+2(k-1)} \right) + kmx^{(n-k)(k+1)m} \times M_0(X, x^{-k(k-1)}) - kx^{(n-k)(k+1)m}M^*_1(X, x^{-k(k-1)}) \)

(iii) \( M_3(X_k^{-k}, x) = \overline{M}_3(X, x^{-k}) + kx^{[n-km]}M_0(X, x^{-k}) - kx^{[n-km]} \times M^*_1(X, x^{-k}) \)

Corollary 11.

(i) \( M_1(X_k^{k+}, x) = x^{2n-1}M_1(X, x^{-k(k-1)}) + kmx^{(n+2)(k-3)m}M_0(X, x^{-k(k-1)}) \)

(ii) \( M_2(X_k^{k+}, x) = \overline{M}_2 \left( x^{-k+2(k-1)} \right) + kmx^{(n+k)(k-3)m}M_0(X, x^{-k(k-1)}) \)

(iii) \( M_3(X_k^{k+}, x) = \overline{M}_3(X, x^{-k}) + kx^{(n+3)(k-1)m}M_0(X, x^{-k}) - kx^{(n+3)(k-1)m} \times M^*_1(X, x^{-k}) \)

Corollary 12.

(i) \( M_1(X_k^{-k}, x) = x^{2n-1}M_1(X, x^{-k(k-1)}) - kx^{(n+1)(k-1)m}M_0(X, x^{-k}) + \left(\frac{kn}{2}\right)x^{-k} \)

(ii) \( M_2(X_k^{-k}, x) = \overline{M}_2 \left( x^{-k+2(k-1)} \right) + kmx^{(n-k)(k+1)m}M_0(X, x^{-k}) - kx^{(n-k)(k+1)m}M^*_1(X, x^{-k}) \)

(iii) \( M_3(X_k^{-k}, x) = \overline{M}_3(X, x^{-k}) + kx^{(n+2)(k-1)m}M_0(X, x^{-k}) \)

7. The Zagreb polynomials on \( X_k^{++} \)

There exist four \( k \) th GTG of a graph for the 2-permutation of \( (+, -) \). The \( X_k^{++} \) is one kind of that four graphical transformations of the graph \( X \).

The two subset of the edge set \( E(X_k^{++}) \) are \( E_{1}^{++} = \{(pq) \not\in E(X)\} \) and \( E_{2}^{++} = \{(pq) \in E(X)\} \) such that \( |E_1^{++}| = \left(\begin{array}{c} n \\ k \end{array}\right) \) and \( |E_2^{++}| = km(n-2) \), respectively. Similarly, \( E(X_k^{++}) = E_1^{++} \cup E_2^{++} \cup E_3^{++} \).

Also, \( |E_1^{++}| = m, |E_2^{++}| = km(n-2) \) and \( |E_3^{++}| = \left(\frac{kn}{2}\right) \)

Theorem 8.

(i) \( M_1(X_k^{-k}, x) = x^{2n+2(k-1)m}M_1(X, x^{-k(k-1)}) + kmx^{(n+2)(k-3)m}M_0(X, x^{-k(k-1)}) \)

(ii) \( M_2(X_k^{-k}, x) = \overline{M}_2 \left( x^{-k+2(k-1)} \right) + kmx^{(n-k)(k+1)m} \times M_0(X, x^{-k(k-1)}) - kx^{(n-k)(k+1)m}M^*_1(X, x^{-k(k-1)}) \)

(iii) \( M_3(X_k^{-k}, x) = \overline{M}_3(X, x^{-k}) + kx^{(n+3)(k-1)m}M_0(X, x^{-k}) - kx^{(n+3)(k-1)m} \times M^*_1(X, x^{-k}) \)
Corollary 14.

(i) \( M_1 \left( \overrightarrow{X_k^c}, x \right) = M_1 \left( X, x^{(k+1)} \right) + k x \left( 2k+1 \right) M_1 \left( X, x^{(k+1)} \right) + (k^2) x^{2(k+1)} \).

(ii) \( M_2 \left( \overrightarrow{X_k^c}, x \right) = M_2 \left( X, x^{(k+1)^2} \right) + k M_1 \left( X, x^{(k+1)(k+1)} \right) + \frac{k^2}{2} x^{2(k+1)} \).

(iii) \( M_3 \left( \overrightarrow{X_k^c}, x \right) = M_3 \left( X, x^{(k+1)} \right) + k x \left( k+1 \right) M_1 \left( X, x^{(k+1)} \right) + \frac{k^2}{2} x^{2(k+1)} \).

Corollary 15.

(i) \( \overrightarrow{M_1} \left( \overrightarrow{X_k^c}, x \right) = \frac{x^{2(n+4k+1)} M_1 \left( X, x^{(n+1)} \right) + k x \left( 2n+4k-3 \right) M_1 \left( X, x^{(n+1)} \right)}{x^{(2k+1)} + \frac{k^2}{2} x^{2(2k+1)}} \).

(ii) \( \overrightarrow{M_2} \left( \overrightarrow{X_k^c}, x \right) = \frac{M_1 \left( X, x^{(n+1)} \right) + k M_2 \left( X, x^{(n+1)(k+1)} \right)}{x^{(2k+1)} + \frac{k^2}{2} x^{2(2k+1)}} \).

(iii) \( \overrightarrow{M_3} \left( \overrightarrow{X_k^c}, x \right) = \frac{M_3 \left( X, x^{(n+1)} \right) + k x \left( n+1 \right) M_1 \left( X, x^{(n+1)} \right)}{x^{(2k+1)} + \frac{k^2}{2} x^{2(2k+1)}} \).

Corollary 16.

(i) \( \overrightarrow{M_1} \left( \overrightarrow{X_k^c}, x \right) = \overrightarrow{M_1} \left( X, x^{(k+1)} \right) + k m x^{(k+1)} M_0 \left( X, x^{(k+1)} \right) - k x^{(2k+1)} \).

(ii) \( \overrightarrow{M_2} \left( \overrightarrow{X_k^c}, x \right) = \frac{M_2 \left( X, x^{(k+1)^2} \right) + k m M_1 \left( X, x^{(k+1)(k+1)} \right) - k M_1 \left( X, x^{(k+1)(k+1)} \right) \)}{x^{(k+1)(k+1)}} \).

(iii) \( \overrightarrow{M_3} \left( \overrightarrow{X_k^c}, x \right) = \overrightarrow{M_3} \left( X, x^{(k+1)} \right) + k m x^{(k+1)} M_0 \left( X, x^{(k+1)} \right) - k x^{(k+1)(k+1)} M_1 \left( X, x^{(k+1)} \right) \).

8. Conclusion

In this paper, we present some explicit expressions for the \( F \)-index (and co-index) of the \( k \)th generalized transformation graphs of a molecular graph in terms of various graph invariants. Also, some figures are constructed to show their changes under different \( k \)th generalized transformation graphs. The Zagreb polynomials, their co-polynomials and their complements are determined for the same transformation graphs. This work will help researchers working in the field of chemical graph theory that has many applications in chemical engineering. In future, we would like to consider a significant extension of the existing work in the literature for many other topological indices and their corresponding polynomials.

Declarations

Author contribution statement

D. Maji: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data; Wrote the paper.

G. Ghorai: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data.

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