

FIRST ENTIRE ZAGREB INDICES OF TRANSFORMATION OF PATH GRAPH

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Abstract

The First Entire Zagreb Index (FEZI) of a (molecular) graph is defined as the sum of the squares of degree of all the vertices and edges in the specified graph. The exact formulae for the FEZI of various forms of transformations of path graph are established in this paper.

1. Introduction

Chemical graph theory is a field of mathematical chemistry that applies graph theory to create and analyze chemical structures and networks. The structure of a chemical compound or network is represented in this context by a graph, in which points represent atoms and connecting lines reflect chemical structural bonds. A topological parameter for a structure is a numeric quantity obtained from the graphical representation of that structure. It is used to investigate the relative structure's physical and chemical qualities. According to graph theory, this numeric parameter is graph invariant, which implies it is unaffected by how the structure is represented graphically. TIs are used to predict relationships between molecules, such as quantitative structure-property relationships (QSPR), quantitative structure-activity relationships (QSAR), and biological activity. As a result, assessing the lower/upper bounds of these invariants could have a substantial impact on mathematics and bioactivity modeling. We direct

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readers to refer [2], [3] for a full literature assessment. Molecular graphs are connected graphs with nodes (vertices) and edges (edges) that represent atoms and chemical bonds, respectively. The node and edge sets of a graph Xare denoted by the notations V(X) and E(X), respectively. The degree of a vertex a is denoted by d(a) (the degree of an edge is denoted by d(e), the minimum and maximum degrees are denoted by $\delta(X)$ and $\Delta(X)$, respectively, and the open neighbourhood of a in X is denoted by N(a/X). We direct readers to [10] for any concepts or notations not covered here. The first and second Zagreb indices [7] are determined by the following formulas:

$$M_1(X) = \sum_{a \in V(X)} d^2(a/X) = \sum_{ab \in E(X)} [d(a/X) + d(b/X)]$$
(1)

$$M_2(X) = \sum_{ab \in E(X)} d(a/X)d(b/X).$$
⁽²⁾

The Zagreb indices are well-known TIs which have already been studied extensively.

There have been several versions of these TIs published and their properties and uses were examined in the recent study. For example, vertex degree based topological index was introduced in [6] and is defined as

$$F(X) = \sum_{a \in V(X)} d^3(a/X) = \sum_{ab \in E(X)} [d^2(a/X) + d^2(b/X)].$$
 (3)

It was studied in detail by Furtula et al. [4] and named as F-index (forgotten topological index). Milicevic et al. [9] presented an edge-based topological index called the first reformulated Zagreb index, which is defined as:

$$EM_1(X) = \sum_{e \in E(X)} d^2(e/X) = \sum_{e=ab \in E(X)} (d(a/X) + d(b/X) - 2)^2$$
(4)

where d(e/X) = d(a/X) + d(b/X) - 2 denotes the degree of the edge e = ab. Alwardi et al. [1] introduced the First Entire Zagreb Index (FEZI) as FIRST

$$M_1^e(X) = \sum_{a \in V(X) \cup E(X)} d^2(a/X)$$
(5)

where the degree of a vertex/edge u in X is denoted by d(a/X). See [8], [12], [13] for more information on topological descriptors and their applications. Ghalavand [5] developed the relationship between the reformulated Zagreb indices and the original Zagreb indices. In addition, numerous inequalities associated to these indices involving various graphs have been demonstrated.

2. Results and Discussions

Using new graphical transformations, we have several explicit expressions of the FEZI of path graphs and we will refer to X as a graph throughout this section. The graph whose vertex set is $V(X) \cup E(X)$ and in which two vertices are adjacent if and only if they are adjacent or incident in X is called the total graph T(X) of X. Wu and Meng [11] introduced some new graphical transformations that widen the total graph concept. Let X = (V, E) be a graph, and a, b are two elements $V(X) \cup E(X)$. The associativity of p and q is defined as + if they are adjacent or incident, and - if they are not. Assume that xyz is a three-permutation of the set $\{+, -\}$. If both p and q are in V(X) (resp. both p and q are in E(X), or one of p and q is V(X) while the other is E(X), we say that p and q correspond to the first term x (resp. the second term y or the third term z) of X. As a result, one can generate eight graphical transformations because there are eight distinct 3permutations of +, -. Figure 1. shows the eight distinct transformations of path P_4 . It should be noted that X^{+++} is just total graph T(X), and X^{---} is the complement of T(X). For computing the FEZI, we initially present certain lemmas as necessary preliminaries in order to derive our major results. These two lemmas are straightforward but fundamental from the definitions of $M_1(X)$, $M_2(X)$ and F(X).



Figure 1. Eight distinct transformation of path graph P_4 .

Lemma 2.1 [1] [5]. For any simple graph X.

- 1. $M_1^e(X) = M_1(X) + EM_1(X)$.
- 2. $M_1^e(X) = 4|E(X)| 3M_1(X) + 2M_2(X) + F(X).$

Theorem 2.1. The FEZI of P_n^{+++} is given $M_1^e(P_n^{+++}) = F(P_n^{+++})$ + $EM_1(P_n^{+++}) - rM_1(P_n^{+++}) + qM_2(P_n^{+++}) + r(r^2 + 7r + 36q + 4 - 40n + 2p^2 - 2pq - 2q^2) + qr(q + 2r - 9) - 3p(2p - 5) - 2q^2(q + p) - 4(r + 1)^2.$

Proof. Let $X = P_n^{+++}$ be a (2n-1, 4n-5) graph with the degree sequence (r, q, p) where $r = \Delta$, $p = \delta$ and q = 3. Here |V(X)| = 2n - 1 and |E(X)| = 4n - 5. Using definition (5), we have

$$M_1^e(X) = \sum_{a \in V(X) \cup E(X)} d^2(a/X)$$

$$= \sum_{ab \in E(X)} (d(a/X) + d(b/X)) + \sum_{ab \in E(X)} (d(a/X) + d(b/X) - 2)^2$$
$$= D_1 + D_2$$

where D_1 and D_2 are the sums of the terms that come next to them in that order. Edge partitions can be classified into four types depending on the degrees of the end vertices of each edge in X. E_1 , E_2 , E_3 and E_4 . The first type is such that $d_a = p$, $d_b = q$ for $e = ab \in E(X)$, the second type is such that $d_a = p$, $d_b = r$ for $e = ab \in E(X)$, the third type is such that $d_a = p$, $d_b = r$ for $e = ab \in E(X)$, and the fourth type is such that $d_a = d_b = r$ for $e = ab \in E(X)$. There are p edges in the first and second types, r edges in the third type, and 4n - 3q - r edges in the fourth type, as indicated in Table [1].

Table 1. Edge partition of P_n^{+++} .

(d_a, d_b) where $ab \in E(X)$	Number of edges
(p,q)	р
(p, r)	р
(q, r)	r
(r, r)	4n - 3q - r

Now
$$D_1 = \sum_{ab \in E_1} (d(a) + d(b)) + \sum_{ab \in E_2} (d(a) + d(b)) + \sum_{ab \in E_3} (d(a) + (d(b)))$$

$$+\sum_{ab\in E_4} (d(a) + d(b))$$

= $p(p+q) + p(p+r) + r(q+r) + (4n - 3q - r)(2r).$
Also $D_2 = \sum_{i=1}^{4} \left[\sum_{ab\in E_i} (d(a) + d(b) - 2)^2 \right]$
= $p(p+q-2)^2 + p(p+r-2)^2 + r(q+r-2)^2 + (4n - 3q - r)(2r - 2)^2$

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We acquire the desired result by adding D_1 and D_2 together. After simplification, we get $M_1^e(P_n^{+++}) = F(P_n^{+++}) + EM_1(P_n^{+++}) - rM_1(P_n^{+++})$ $+ qM_2(P_n^{+++}) + r(r^2 + 7r + 36q + 4 - 40n + 2p^2 - 2pq - 2q^2) + qr(q + 2r - 9)$ $- 3p(2q - 5) - 2q^2(q + p) - 4(r + 1)^2$ where $M_1(P_n^{+++}) = \sum_{u \in V(X)} d_a^2 = 2(p^2 + q^2) + (2n - 5)r^2$, $M_2(P_n^{+++}) = 2(pq + 2qr + pr) + (4n - 3q - r)r^2$, $F(P_n^{+++}) = 2(p^3 + q^3) + (2n - 5)r^3$ and $EM_2(P_n^{+++}) = 2[q^2 + r^2) + 4(r + 1)^2 + (4n - 3q - r)(r + 2)^2$. Theorem 2.2. The FEZI of P_n^{---} , $n \ge 5$ is given by $M_1^e(P_n^{---})$ $= 5M_1(P_n^{---}) + 4M_2(P_n^{---}) + \frac{2}{2}F(P_n^{---}) + EM_1(P_n^{---}) - 4r^2[(n - 4)(n - 3)]$

$$= 5t M_1(T_n^{-1}) + 4t M_2(T_n^{-1}) + \frac{1}{s} F(T_n^{-1}) + Et M_1(T_n^{-1}) - 4T_1(n-4)(n-3) + \sum_{k=4}^{n-1} (n-k) + \sum_{m=5}^{n-1} (n-m) - 2r(r+s-2)^2 - 16s^2 - 12t^2 - 16(n-3)rt - 8st + 2rs^2 - 8r^2 + 8r - 8r^2s - 4\frac{t^3}{s}.$$

Proof. Let $X = P_n^{---}$ be a $(2n - 1, 2n^2 - 7n + 6)$ graph with the degree sequence (t, s, r) where r = 2n - 6, s = 2n - 5 and t = 2n - 4. Here |V(X)| = 2n - 1 and $|E(X)| = 2n^2 - 7n + 6$. Using definition (5), we have

$$M_1^e(X) = \sum_{a \in V(X) \cup E(X)} d^2(a/X)$$
$$= \sum_{ab \in E(X)} (d(a/X) + d(b/X)) + \sum_{ab \in E(X)} (d(a/X) + d(b/X) - 2)^2$$
$$= D_1 + D_2$$

where D_1 and D_2 are the sums of the terms that come next to them in that order. There are three different forms of vertex partitions based on the degrees of the end vertices of each edge in $X : V_1, V_2$ and V_3 . The first type

is such that $d_a = r$ for $u \in V(X)$; the second type is such that $d_a = s$ for $u \in V(X)$ and the third type is such that $d_a = t$ for $u \in V(X)$. Similarly, edge partitions can be classified into six types depending on the degrees of the end vertices of each edge in $X : E_1, E_2, E_3$, and E_4, E_5, E_6 . The first type is such that $d_a = d_b = r$ for $e = ab \in E(X)$; the second type is such that $d_a = r, d_b = r$ for $e = ab \in E(X)$; the second type is such that $d_a = r, d_b = t$ for $e = ab \in E(X)$; the fourth type is such that $d_a = d_b = s$ for $e = ab \in E(X)$; the fifth type is such that $d_a = s, d_b = t$ for $e = ab \in E(X)$ and the sixth type is such that $d_a = d_b = t$ for $e = ab \in E(X)$. There are $[(n-4)(n-3) + \sum_{k=4}^{n-1} (n-k) + \sum_{m=5}^{n-1} (n-m)]$ edges in the first type, (4n-14) edges in the second type, (4n-12) edges in the third type, and one edge in the fourth type is indicated in Table [2].

Now
$$D_1 = \sum_{u \in V_1} d(a)^2 + \sum_{u \in V_2} d(a)^2 + \sum_{u \in V_3} d(a)^2$$

= $sr^2 + 2s^2 + 2t^2 = M_1(X)$

and

$$D_{2} = [(n-4)(n-3) + \sum_{k=4}^{n-1} (n-k) + \sum_{m=5}^{n-1} (n-m)](2r-2)^{2} + (4n-14)$$
$$(r+s-2)^{2} + (4n-12)(r+t-2)^{2} + (2s-2)^{2} + 2(s+t-2)^{2} + (2t-2)^{2}$$
$$= EM_{1}(X).$$

(d_a, d_b) where $ab \epsilon E(X)$	Number of Edges
(r, r)	$(n-4)(n-3) + \sum_{k=4}^{n-1} (n-k)$
	$+\sum_{m=5}^{n-1}(n-m)$
(r, s)	4n - 14

Table 2. Edge partition of P_n^{---} .

(r, t)	4n - 12
(s, s)	1
(s, t)	2
(<i>t</i> , <i>t</i>)	1

We acquire the desired result by adding D_1 and D_2 together. After simplification, we get $M_e^1(P_n^{---}) = 5M_1(P_n^{---}) + 4M_2(P_n^{---}) + \frac{2}{s}F(P_n^{---}) + EM_1(P_n^{---}) - 4r^2[(n-4)(n-3) + \sum_{k=4}^{n-1}(n-k) + \sum_{m=5}^{n-1}(n-m)] - 2r(r+s-2)^2 - 16s^2 - 12t^2 - 16(n-3)rt - 8st + 2rs^2 - 8r^2 + 8r - 8r^2s - 4\frac{t^3}{s}$ where $M_1(P_n^{---}) = \sum_{u \in V(X)} d_a^2 = sr^2 + 2s^2 + 2t^2$,

$$M_2(P_n^{---}) = \left[(n-4)(n-3) + \sum_{k=4}^{n-1} (n-k) + \sum_{m=5}^{n-1} (n-m) \right] r^2 + (4n-14)rs$$
$$+ (4n-12)rt + s^2 + 2st + t^2,$$

 $F(P_n^{---}) = sr^3 + 2s^3 + 2t^3$ and

$$EM_{1}(P_{n}^{---}) = \left[(n-4)(n-3) + \sum_{k=4}^{n-1}(n-k) + \sum_{n=5}^{n-1}(n-m) + n - \frac{13}{2} \right]$$
$$-8r \left[(n-4)(n-3) + \sum_{k=4}^{n-1}(n-k) + \sum_{n=5}^{n-1}(n-m) + 4n - 13 \right]$$
$$+ 4 \left[(n-4)(n-3) + \sum_{k=4}^{n-1}(n-k) + \sum_{n=5}^{n-1}(n-m) + 8n - 22 \right]$$
$$-8s[2n-5] - 16t[n-2] + 8rt[n-3] + 4st + 4rs[2n-7] + 4s^{2}[n-2]$$
$$+ 2t^{2}[2n-3].$$

Theorem 2.3. The FEZI of
$$P_n^{++-}$$
 is given by $M_1^e(P_n^{++-}) = M_1(P_n^{++-})$
+ $\frac{F(P_n^{++-})}{y} + 4M_2(P_n^{++-}) + (n^2 - 5n + 8)[x^2 + y^2 + 4 - 4y - 4x - 2xy]$
+ $(3n - 5)(4 - 8x) + (n - 4)(4 - 8y) - (n - 3)y^2 - (n + 2)\frac{x^3}{y}$.

Proof. Let P_n^{++-} be a graph with the degree sequence (x, y) where x = n - 1 and y = n. Here $|V(P_n^{++-})| = (2n - 1)$ and $|E(P_n^{++-})| = n^2 - n - 1$. Edge partitions are classified into three types based on the degrees of the end vertices of each edge in $P_n^{++-} : E_1, E_2$ and E_3 are indicated in Table [3].

Edge partition (d_a, d_b)	Number of edges
(x, x)	3n - 5
(x, y)	$n^2 - 5n + 8$
(y, y)	n-4

Table 3. Edge partition of P_n^{++-} .

Using definition (5) we have

$$M_1^e(P_n^{++-}) = \sum_{a \in V(P_n^{++-}) \cup E(P_n^{++-})} d^2(a/P_n^{++-})$$

$$= \sum_{ab \in E(P_n^{++-})} (d(a/P_n^{++-}) + d(b/P_n^{++-})) + \sum_{ab \in E(P_n^{++-})} (d(a/P_n^{++-}) + d(b/P_n^{++-}) - 2)^2$$

Simplification using Table [2], we get $M_1^e(P_n^{++-}) = M_1(P_n^{++-}) + \frac{F(P_n^{++-})}{y}$ + $4M_2(P_n^{++-}) + (n^2 - 5n + 8)[x^2 + y^2 + 4 - 4y - 4x - 2xy] + (3n - 5)(4 - 8x)$ + $(n - 4)(4 - 8y) - (n - 3)y^2 - (n + 2)\frac{x^3}{y}$ where $M_1(P_n^{++-}) = (n + 2)x^2$ + $(n - 3)y^2$, $M_2(P_n^{++-}) = (3n - 5)x^2 + (n^2 - 5n + 8)xy + (n - 4)y^2$ and $F(P_n^{++-})$ = $(n + 2)x^3 + (n - 3)y^3$.

Theorem 2.4. The FEZI of
$$P_n^{--+}$$
 is given by $M_1^e(P_n^{--+}) = M_1(P_n^{--+})$
+ $\frac{F(P_n^{--+})}{t} + 4M_2(P_n^{--+}) + \frac{1-2t}{(t-1)^2} EM_1(P_n^{--+}) + \sum_{k=2}^{n-1} [(n-k)+5]$
 $\left[\frac{1-2t}{(t-1)^2}(2s-2)^2 + 4 - 8s\right] + (4n-14)[s^2 + t^2 - 4t - 4s - 2st + 4 - \frac{1-2t}{(t-1)^2}$
 $(s+t-2)^2] - \frac{n+2}{t}s^3 - (n-3)t^2.$

Proof. Let P_n^{--+} be a semiregular graph with the degree sequence (s, t) where s = n-1 and t = n-2. Here $|V(P_n^{--+})| = 2n-1$ and $|E(P_n^{--+})| = n^2 - 2n + 2$. Edge partitions are classified into three types based on the degrees of the end vertices of each edge in $P_n^{++-}: E_1, E_2$ and E_3 are indicated in Table [4].

Edge partition (d_a, d_b)	Number of edges
(t, t)	n-5
(s, t)	4n - 14
(s, s)	$\left[\sum_{k=2}^{n-1} (n-k)\right] + 5$

Table 4. Edge partition of P_n^{--+} .

For the graph P_n^{--+} ,

$$M_1(P_n^{--+}) = (n+2)s^2 + (n-3)t^2,$$
(6)

$$M_2(P_n^{-+}) = (n-5)t^2 + (4n-14)st + \left[\sum_{k=2}^{n-1} (n-k) + 5\right]s^2,$$
(7)

$$F(P_n^{--+}) = (n+2)s^3 + (n-3)t^3,$$
(8)

and

$$EM_{1}(P_{n}^{--+}) = t^{2}[8n - 34] + 2s^{2}[2n + 3 + 2\sum_{k=2}^{n-1}(n-k)] + t[96 - 24n] - 8s[2n - 2 + 8\sum_{k=2}^{n-1}(n-k)] + 4[5n - 14 + \sum_{k=2}^{n-1}(n-k)] + 4st(2n - 7)$$
(9)

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Using Definition (5), Table [4] and equations (6)-(9), we get the desired result.

Theorem 2.5. The FEZI of
$$P_n^{+-+}$$
 is given by $M_1^e(P_n^{+-+}) = M_1(P_n^{+-+})$
+ $\frac{F(P_n^{+-+})}{q} + 2M_2(P_n^{+-+}) + EM_1(P_n^{+-+}) - 2(n-3)q^2 - 2\sum_{k=5}^{n-1} (n-k)t^2$
- $2s^2 - 4(n-4)st - (n-2)q^2 - 4rq - 4rs - 4qt(n-3) - 4qs - 2\frac{r^3}{q} - 2\frac{r^3}{q}$
- $\frac{(n-3)}{q}t^3 - \frac{2s^3}{q}$.

Proof. Let P_n^{+-+} be a graph with degree sequence (q, s, t, r) where q = 4, s = n - 1, t = -2 and r = 2. Here $|V(P_n^{+-+})| = 2n - 1$ and $|E(P_n^{+-+})| = \frac{1}{2}[n^2 + n]$. In P_n^{+-+} , there are eight different forms of edge partitions based on the degrees of the end vertices of each edge which are indicated in Table [5].

Edge partition (d_a, d_b)	Number of edges
(r, q)	2
(r, s)	2
(q, q)	n-3
(q, t)	2(n-3)
(q,s)	2
(t, t)	$\sum_{k=5}^{n-1} (n-k)$
(t, s)	2(n-4)
(s, s)	1

Table 5. Edge partition of P_n^{+-+} .

Using definition (5) together with Table [5], we get $M_1^e(P_n^{+-+})$

$$= M_1(P_n^{+-+}) + \frac{F(P_n^{+-+})}{q} + 2M_2(P_n^{+-+}) + EM_1(P_n^{+-+}) - 2(n-3)q^2$$

-2 $\sum_{k=5}^{n-1} (n-k)t^2 - 2s^2 - 4(n-4)st - (n-2)q^2 - 4rq - 4rs - 4qt(n-3)$
-4qs - 2 $\frac{r^3}{q} - \frac{(n-3)}{q}t^3 - \frac{2s^3}{q}$ where $M_1(P_n^{+-+}) = 2r^2 + (n-3)t^2 + 2s^2$
+ (n-2)q^2, $M_2(P_n^{+-+}) = 2rq + 2rs + (n-3)q^2 + 2(n-3)qt + 2qs$
+ $\sum_{k=5}^{n-1} (n-k)t^2 + 2(n-4)st + s^2$, $F(P_n^{+-+}) = 2r^3 + (n-3)t^3 + 2s^3 + (n-2)q^3$
and $EM_1(P_n^{+-+}) = 4r^2 - 16r + q^2[6n - 14] + q[32 - 16n] + 2ns^2$
+ $t^2 \left[4n - 14 + 4\sum_{k=5}^{n-1} (n-k) \right] + t \left[56 - 16n - 8\sum_{k=5}^{n-1} (n-k) \right]$
+ $s[8 - 8n] + 4rq + 4rs + 4(n-3)qt + 4qs + 4st(n-4).$

Theorem 2.6. The FEZI of P_n^{-+-} is given by $M_1^e(P_n^{-+-}) = M_1(P_n^{-+-})$ + $\frac{F(P_n^{\mp -})}{r} + 2M_2(P_n^{-+-}) + EM_1(P_n^{-+-}) - 4pq - 4(n-3)qr - 4ps - 2(n-3)$ [(n-4)qr + 2qs + 2rs].

Proof. Let P_n^{-+-} be a graph with degree sequence (p, q, r, s) where p = n - 1, q = n, r = 2n - 6 and s = 2n - 4. Here $|V(P_n^{-+-})| = (2n - 1)$ and $|E(P_n^{-+-})| = \frac{1}{2}[3n^2 - 7n + 2]$. In P_n^{-+-} , there are nine different forms of edge partitions based on the degrees of the end vertices of each edge which are indicated in Table [6].

Edge partition (d_a, d_b)	Number of edges
(p,q)	2
(p, r)	2(n-3)
(p, s)	2

Table 6. Edge partition of P_n^{-+-} .

(q, q)	n-4
(q, r)	(n-4)(n-3)
(q, s)	2(n-3)
(r, r)	$\sum_{k=4}^{n-1} (n-k)$
(r, s)	2(n-3)
(s, s)	1

Using Definition (5) together with Table [6], we get the desired result, where

$$M_{1}(P_{n}^{-+-}) = 2p^{2} + (n-2)r^{2} + 2s^{2} + (n-3)q^{2},$$

$$F(P_{n}^{-+-}) = 2pq + 2(n-3)pr + 2ps + (n-4)q^{2} + (n-4)(n-3)qr$$

$$+ 2(n-3)qs + \sum_{k=4}^{n-1} (n-k)r^{2} + 2(n-3)rs + s^{2}$$

$$EM_{1}(P_{n}^{-+-}) = 2p^{2}[n-1] + q^{2}[n^{2} - n - 8] + r^{2} \left[4\sum_{k=4}^{n-1} (n-k) - 3n \right]$$

$$+2s^{2}[2n-3]+16s[2-n]-8p[n+5]-4qn[n-3]+4r\left[3n-n^{2}-2\sum_{k=4}^{n-1}(n-k)\right]$$

$$+4[pq+pr(n-3)+ps+qs(n-3)+rs(n-3)]+2qr(n^{2}-7n+12)$$

$$+4\left[n^{2}+2n-5+\sum_{k=4}^{n-1}(n-k)\right].$$

Theorem 2.7. The FEZI of P_n^{-++} is given by $M_1^e(P_n^{-++}) = M_1(P_n^{-++})$ + $\frac{F(P_n^{-++})}{r} + 2M_2(P_n^{-++}) + EM_1(P_n^{-++}) - 4pq - 8pr - 4(n-3)qr - nr^2 - \frac{2p^3}{r}$ $- \frac{(n-3)q^3}{r} - 2(n-4)q^2 - 2\sum_{k=1}^{n-2} kr^2.$

Proof. Let P_n^{-++} be a graph with degree sequence (p, q, r) where p = 3, q = 4, r = n - 1. Here $|V(P_n^{-++})| = 2n - 1$ and $|E(P_n^{-++})| = \frac{1}{2}[n^2 + 3n - 6]$. Edge partitions are classified into six types based on the degrees of the end vertices of each edge in P_n^{-++} which are indicated in Table [7].

Edge Partition (d_a, d_b)	Number of edges
(p, p)	2
(p,q)	4
(p, r)	n-4
(r, r)	$\sum_{k=1}^{n-2}k$
(q, r)	2n - 6

Table 7. Edge partition of P_n^{-++} .

Using definition (5) together with Table [7], we get the desired result where

$$\begin{split} M_1(P_n^{-++}) &= 2p^2 + (n-3)q^2 + nr^2, \\ M_2(P_n^{-++}) &= 2pq + 4pr + (n-4)q^2 + 2(n-3)qr + \sum_{k=1}^{n-2}k(r^2) \text{ and} \\ & EM_1(P_n^{-++}) = (6p^2 - 24p) + [(6n-20)q^2 + 48q] + (12n-16) \\ &+ 4\sum_{k=1}^{n-2}k + p(4q+8r) + q[4(n-3)r - 16n] + 8r[1 - n - \sum_{k=1}^{n-2}k] \\ &+ r^2[2n-2 + 4\sum_{k=1}^{n-2}k]. \end{split}$$
Theorem 2.8. The FEZI of P_n^{+--} is given by $M_1^e(P_n^{+--}) = M_1(P_n^{+--}) \\ &- 2r^2 + \frac{F(P_n^{+--})}{r} + 4M_2(P_n^{+--}) + EM_1(P_n^{+--}) - 4(n-1)p^2 - 4\sum_{k=1}^{n-5}kr - 4r^2 \end{split}$

$$-\frac{np^3}{r} - \frac{(n-3)q^3}{r} - 4(n-2)(n-3)pq - 8(n-2)pr - 8(n-4)qr.$$

Proof. Let P_n^{+--} be a graph with degree sequence (p, q, r) where p = n - 1, q = 2n - 6, r = 2n - 5. Here $|V(P_n^{+--})| = 2n - 1$ and $|E(P_n^{+--})| = \frac{1}{2}[3n^2 - 9n + 8]$. There are six different forms of edge partitions in P_n^{+--} based on the degrees of the end vertices of each edge which are indicated in Table [8].

Edge Partition (d_a, d_b)	Number of edges
(p, p)	n-1
(p,q)	$n^2 - 5n + 6$
(p, r)	2n - 4
(r, r)	$\sum_{k=1}^{n-5}k$
(q, r)	2n - 8
(<i>r</i> , <i>r</i>)	1

Table 8. Edge partition of P_n^{+--} .

Using definition (5) together with Table [8], we get the desired result where

$$\begin{split} M_1(P_n^{+--}) &= np^2 + (n-3)q^2 + 2r^2, \\ M_2(P_n^{+--}) &= (n-1)p^2 + (n-2)(n-3)pq + 2(n-2)pr + \sum_{k=1}^{n-5}k(r^2) \\ &+ 2(n-4)qr + r^2, \\ EM_1(P_n^{+--}) &= p^2(n^2 + n - 2) + q^2(n^2 - 3n - 2) + r^2 \bigg(4n + 4\sum_{k=1}^{n-5}k - 8 \bigg) \\ &+ p(4n - 4n^2 + 2qn^2 + 12q) + q(-4n^2 + 12n + 8 - 10pn) \\ &+ r \bigg(4pn - 8p - 16n + 40 - 8\sum_{k=1}^{n-5}k + 4nq + 16q \bigg) + \bigg(4n^2 - 24 + 4\sum_{k=1}^{n-5}k \bigg). \end{split}$$

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Conclusion

In this article, we determine the exact expression for the first entire Zagreb index of the eight distinct transformations of path graph in terms of M_1 , M_2 , Forgotten index, and EM_1 .

References

- A. Alwardi, A. Alqesmah, R. Rangarajan and I. Naci Cangul, Entire Zagreb indices of graphs, Discrete Mathematics, Algorithms and Applications 10(16) (2018), Article ID 1850037.
- [2] K. C. Das and I. Gutman, Some properties of the second Zagreb index, MATCH Communications in Mathematical and in Computer Chemistry 52 (2004), 103-112.
- [3] K. C. Das and I. Gutman, The first Zagreb index 30 years after, MATCH Communications in Mathematical and in Computer Chemistry 50 (2004), 83-92.
- [4] B. Furtula and I. Gutman, A forgotten topological index, J. Math. Chem. 53 (2015), 1184-1190.
- [5] A. Ghalavand and A. R. Ashrafi, Bounds on the entire Zagreb indices of graphs, MATCH Communications in Mathematical and in Computer Chemistry 81 (2019), 371-381.
- [6] I. Gutman, B. Ruscic, N. Trinajstic and C. F. Wilcox, Graph theory and molecular orbitals, XII, Acyclic polyenes, The Journal of Chemical Physics 62 (1975), 3399-3405.
- [7] I. Gutman and N. Trinajstic, Graph theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons, Chemical Physics Letters 17 (1972), 535-538.
- [8] Y. Ma, S. Cao, Y. Shi, I. Gutman, M. Dehmer and B. Furtula, From the connectivity index to various Randić-type descriptors, MATCH Communications in Mathematical and in Computer Chemistry 80 (2018), 85-106.
- [9] A. Millicevic, S. Nikolic and N. Trinajstic, On reformulated Zagreb indices, Mol Divers, 8 (2004), 393-399.
- [10] D. B. West, Introduction to Graph Theory, Prentice-Hall, Upper Saddle River, NJ, USA, 2nd edition, 2001.
- [11] B. Wu and J. Meng, Basic properties of total transformation graphs, J. Math. Study 34(2) (2001), 109-116.
- [12] D. Zhao, Z. Iqbal, R. Irfan et al., Comparison of irregularity indices of several dendrimers structures, Processes 7(10) (2019), 1-14.
- [13] F. Zhan, Y. Qiao and J. Cai, Relations between the first Zagreb index and spectral moment of graphs, MATCH Communications in Mathematical and in Computer Chemistry 81 (2019), 383-392.