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Minus F and Square F-Indices and Their Polynomials of Certain Dendrimers

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Abstract

We introduce the minus F-index and square F-index of a graph. In this study, we determine the minus F-index, square F-index and their polynomials of porphyrin dendrimer, propyl ether imine dendrimer, zinc porphyrin dendrimer and poly ethylene amide amine dendrimer.

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of edges incident to v. The edge connecting vertices u and v will be denoted by uv. For other definitions and notations, readers are referred to [1].

Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A molecular graph or chemical graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In Chemistry, topological indices have been found to be useful in discrimination, chemical documentation, structure property relationships, structure activity relationships and pharmaceutical drug design. There has been considerable interest in the general problem of determining topological indices, see [2, 3].

The first F-index [4] and second F-index [5] of a graph G are defined respectively as

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$$F_1(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2], \qquad F_2(G) = \sum_{uv \in E(G)} d_G(u)^2 d_G(v)^2.$$

Recently some novel variants of F indices were introduced and studied such as F-indices [5], connectivity F-indices [6], multiplicative F-indices [7].

The irregularity index (called as minus index [8]) was introduced by Albertson in [9] and defined as

$$M_i(G) = \sum_{uv \in E(G)} | d_G(u) - d_G(v) |.$$

Recently, the square *ve*-degree index was introduced by Kulli in [10] and defined as

$$Q_{ve}(G) = \sum_{uv \in E(G)} [d_{ve}(u) - d_{ve}(v)]^2.$$

Very recently, some square indices were introduced and studied such as square reverse index [11], square Revan index [12] square leap index [13], square KV index [14].

We now introduce the minus F-index and square F-index of a graph G as follows:

The *minus F-index* of a graph G is defined as

$$MF(G) = \sum_{uv \in E(G)} | d_G(u)^2 - d_G(v)^2 |. \tag{1}$$

The *square F-index* of a graph G is defined as

$$QF(G) = \sum_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2. \tag{2}$$

Considering the minus F and square F indices, we define the minus F and square F polynomials of a graph G as

$$MF(G, x) = \sum_{uv \in E(G)} x^{| d_G(u)^2 - d_G(v)^2 |}, \tag{3}$$

$$QF(G, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}. \tag{4}$$

In this paper, we consider the porphyrin, propyl ether imine, zinc porphyrin and poly ethylene amide amine dendrimers. Some degree based topological indices, eccentricity based topological indices of these dendrimers were studied in [15, 16, 17, 18, 19, 20]. In Chemical Graph Theory, graph polynomials related to molecular graph were studied in [21, 22, 23, 24, 25, 26, 27, 28, 29]. Graph polynomials and topological based numbers have significant importance to collect information about properties of chemical compounds [30]. In this paper, the minus F and square F indices and their polynomials of porphyrin, propyl ether imine, zine porphyrin and poly ethylene amide amine dendrimers are determined.

2. Results for Porphyrin Dendrimer D_nP_n

We consider the porphyrin dendrimer which is denoted by D_nP_n. The porphyrin dendrimer is shown in Figure 1.

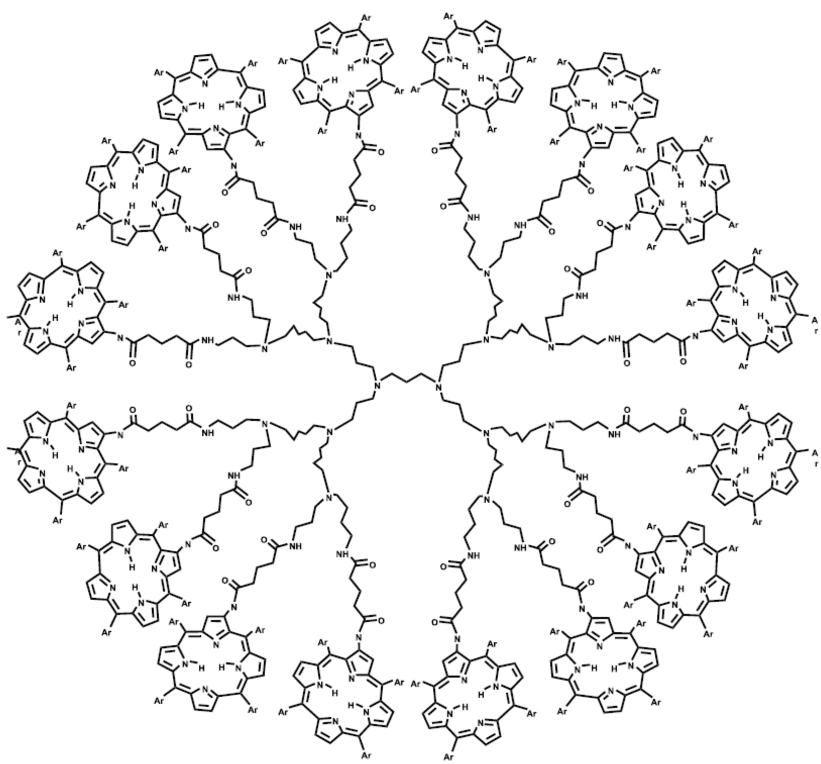

Figure 1. Porphyrin dendrimer D_nP_n.

Let $G = D_n P_n$ be a porphyrin dendrimer. By calculation, G has $96n - 10$ vertices and $105n - 11$ edges. In G, there are six types of edges based on degrees of end vertices of each edge. By calculation, the edge partition of G is given in Table 1.

Table 1. Edge partition of $D_n P_n$.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$2n$	$24n$	$10n - 5$	$48n - 6$	$13n$	$8n$

Theorem 1. *The minus F-index of* $D_n P_n$ *is*

$$MF(D_n P_n) = 672n - 30.$$

Proof. Let $G = D_n P_n$. By using equation (1) and Table 1, we obtain

$$MF(D_n P_n) = \sum_{uv \in E(G)} | d_G(u)^2 - d_G(v)^2 |$$

$$= | 1^2 - 3^2 | 2n + | 1^2 - 4^2 | 24n + | 2^2 - 2^2 | (10n - 5)$$

$$+ | 2^2 - 3^2 | (48n - 6) + | 3^2 - 3^2 | 13n + | 3^2 - 4^2 | 8n$$

$$= 672n - 30.$$

Theorem 2. *The minus F polynomial of* $D_n P_n$ *is*

$$MF(D_n P_n, x) = 24nx^{15} + 2nx^8 + 8nx^7 + (48n - 6)x^5 + (23n - 5)x^0.$$

Proof. Let $G = D_n P_n$. By using equation (3) and Table 1, we have

$$MF(D_n P_n, x) = \sum_{uv \in E(G)} x^{| d_G(u)^2 - d_G(v)^2 |}$$

$$= 2nx^{| 1^2 - 3^2 |} + 24nx^{| 1^2 - 4^2 |} + (10n - 5)x^{| 2^2 - 2^2 |}$$

$$+ (48n - 6)x^{| 2^2 - 3^2 |} + 13nx^{| 3^2 - 3^2 |} + 8nx^{| 3^2 - 4^2 |}$$

$$= 24nx^{15} + 2nx^8 + 8nx^7 + (48n - 6)x^5 + (23n - 5)x^0.$$

Theorem 3. *The square F-index of* D_nP_n *is*

$$QF(D_nP_n) = 7120n - 150.$$

Proof. Let $G = D_nP_n$. From equation (2) and using Table 1, we deduce

$$QF(D_nP_n) = \sum_{uv\in E(G)} [d_G(u)^2 - d_G(v)^2]^2$$

$$= (1^2 - 3^2)^2 2n + (1^2 - 4^2)^2 24n + (2^2 - 2^2)^2 (10n - 5)$$

$$+ (2^2 - 3^2)^2 (48n - 6) + (3^2 - 3^2)^2 13n + (3^2 - 4^2)^2 8n$$

$$= 7120n - 150.$$

Theorem 4. *The square F-polynomial of* D_nP_n *is*

$$QF(D_nP_n,\ x) = 24nx^{225} + 2nx^{64} + 8nx^{49} + (48n - 6)x^{25} + (23n - 5)x^0.$$

Proof. Let $G = D_nP_n$. From equation (4) and by using Table 1, we derive

$$QF(D_nP_n,\ x) = \sum_{uv\in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}$$

$$= 2nx^{(1^2-3^2)^2} + 24nx^{(1^2-4^2)^2} + (10n-5)x^{(2^2-2^2)^2}$$

$$+ (48n-6)x^{(2^2-3^2)^2} + 13nx^{(3^2-3^2)^2} + 8nx^{(3^2-4^2)^2}$$

$$= 24nx^{225} + 2nx^{64} + 8nx^{49} + (48n - 6)x^{25} + (23n - 5)x^0.$$

3. Results for Propyl Ether Imine Dendrimer *PETIM*

We consider the propyl ether imine dendrimer which is denoted by *PETIM*. This dendrimer is presented in Figure 2.

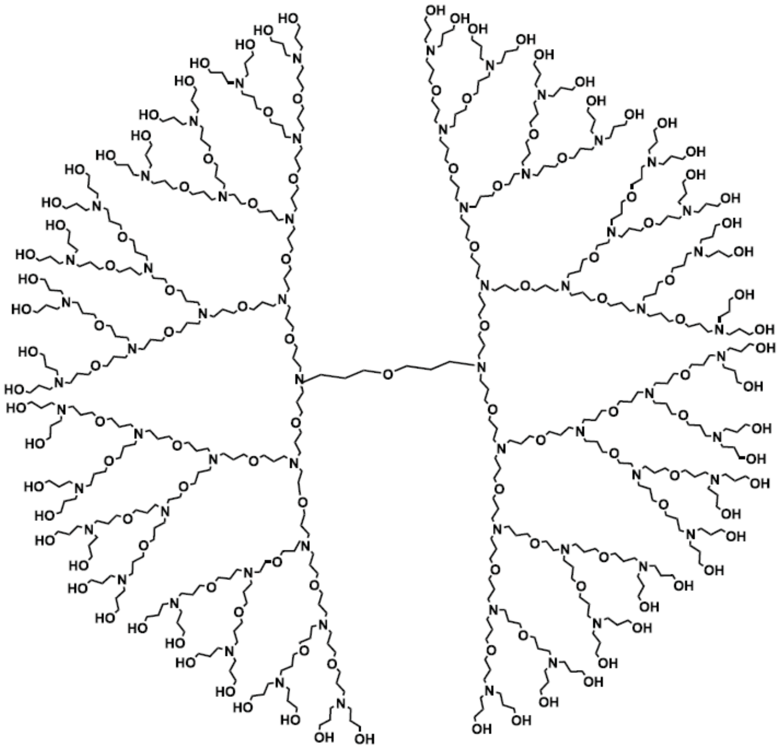

Figure 2. Propyl ether imine dendrimer *PETIM*.

Let G be a propyl ether imine dendrimer *PETIM*. By calculation, G has $24 \times 2^n - 23$ vertices and $24 \times 2^n - 24$ edges.

In G, there are exactly three types of edges based on degrees of end vertices of each edge. Also by calculation, the edge partition of G is given in Table 2.

Table 2. Edge partition of *PETIM*.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(2, 2)	(2, 3)
Number of edges	2^{n+1}	$2^{n+4} - 18$	$6 \times 2^n - 6$

Theorem 5. *The minus F-index of PETIM is*

$$MF(PETIM) = 3 \times 2^{n+1} + 30 \times 2^n - 30.$$

Proof. Let $G = PETIM$. By using equation (1) and Table 2, we deduce

$$MF(PETIM) = \sum_{uv \in E(G)} | d_G(u)^2 - d_G(v)^2 |$$

$$= | 1^2 - 2^2 | 2^{n+1} + | 2^2 - 2^2 | (2^{n+4} - 18) + | 2^2 - 3^2 | (6 \times 2^n - 6)$$

$$= 3 \times 2^{n+1} + 30 \times 2^n - 30.$$

Theorem 6. *The minus F polynomial of PETIM is*

$$MF(PETIM, x) = (6 \times 2^n - 6) x^5 + 2^{n+1} x^3 + (2^{n+4} - 18) x^0.$$

Proof. Let $G = PETIM$ from equation (3) and by using Table 2, we derive

$$QF(PETIM, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}$$

$$= 2^{n+1} x^{| 1^2 - 2^2 |} + (2^{n+4} - 18) x^{| 2^2 - 2^2 |} + (6 \times 2^n - 6) x^{| 2^2 - 3^2 |}$$

$$= (6 \times 2^n - 6) x^5 + 2^{n+1} x^3 + (2^{n+4} - 18) x^0.$$

Theorem 7. *The square F index of PETIM is*

$$QF(PETIM) = 9 \times 2^{n+1} + 150 \times 2^n - 150.$$

Proof. Let $G = PETIM$. By using equation (2) and Table 2, we obtain

$$QF(PETIM) = \sum_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2$$

$$= (1^2 - 2^2)^2 2^{n+1} + (2^2 - 2^2)^2 (2^{n+4} - 18) + (2^2 - 3^2)^2 (6 \times 2^n - 6)$$

$$= 9 \times 2^{n+1} + 150 \times 2^n - 150.$$

Theorem 8. *The square F-polynomial of PETIM is*

$$QF(PETIM, x) = (6 \times 2^n - 6) x^{25} + 2^{n+1} x^9 + (2^{n+4} - 18) x^0.$$

Proof. Let $G = PETIM$. From equation (4) and by using Table 2, we have

$$QF(PETIM, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}$$

$$= 2^{n+1} x^{(1^2-2^2)^2} + (2^{n+4} - 18) x^{(2^2-2^2)^2} + (6 \times 2^n - 6) x^{(2^2-3^2)^2}$$

$$= (6 \times 2^n - 6) x^{25} + 2^{n+1} x^9 + (2^{n+4} - 18) x^0.$$

4. Results for Zinc Porphyrin Dendrimer DPZ_n

We consider the zinc porphyrin dendrimer and it is symbolized by DPZ_n. The zinc porphyrin dendrimer is depicted in Figure 3.

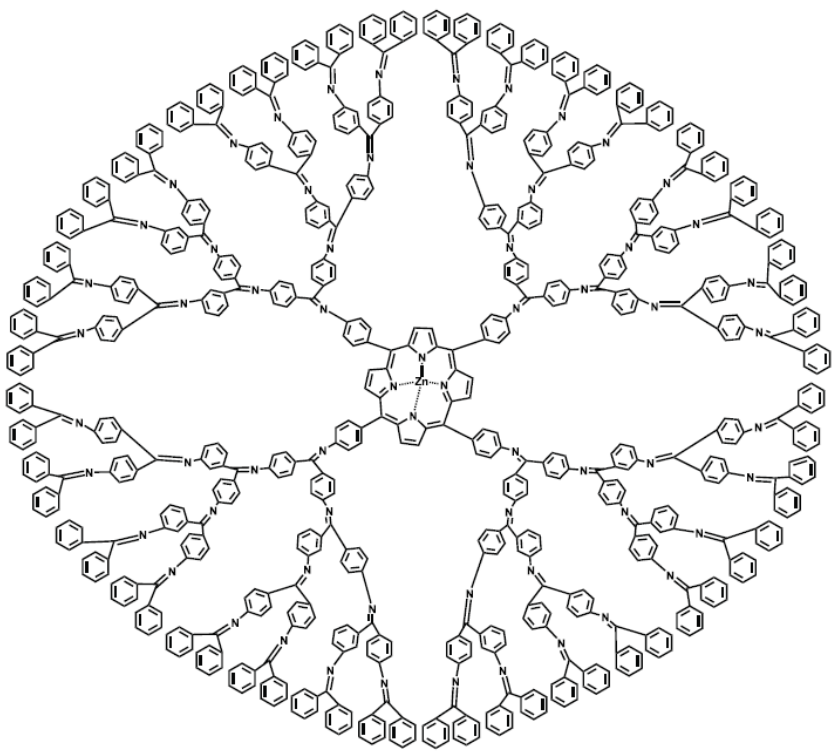

Figure 3. Zinc porphyrin dendrimer DPZ_n.

Let $G = DPZ_n$ be a zinc porphyrin dendrimer. By calculation, G has $64 \times 2^n - 4$ edges. In G, there are four different types of edges based on degrees of end vertices of each edge. Also by calculation, the edge partition of G is given in Table 3.

Table 3. Edge partition of DPZ_n.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16 \times 2^n - 4$	$40 \times 2^n - 16$	$8 \times 2^n + 12$	4

Theorem 9. *The minus F-index of DPZ_n is*

$$MF(DPZ_n) = 200 \times 2^n - 52.$$

Proof. Let $G = DPZ_n$. By using equation (1) and Table 3, we have

$$MF(DPZ_n) = \sum_{uv \in E(G)} | d_G(u)^2 - d_G(v)^2 |$$

$$= | 2^2 - 2^2 |(16 \times 2^n - 4) + | 2^2 - 3^2 |(40 \times 2^n - 16)$$

$$+ | 3^2 - 3^2 |(8 \times 2^n - 12) + | 3^2 - 4^2 | 4$$

$$= 200 \times 2^n - 52.$$

Theorem 10. *The minus F-polynomial of DPZ_n* is

$$QF(PETIM, x) = 4x^7 + (40 \times 2^n - 16) x^5 + (24 \times 2^n + 8) x^0.$$

Proof. Let $G = DPZ_n$. From equation (3) and by using Table 3, we obtain

$$MF(DPZ_n, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]}$$

$$= (16 \times 2^n - 4) x^{| 2^2 - 2^2 |} + (40 \times 2^n - 16) x^{| 2^2 - 3^2 |}$$

$$+ (8 \times 2^n - 12) x^{| 3^2 - 3^2 |} + 4x^{| 3^2 - 4^2 |}$$

$$= 4x^7 + (40 \times 2^n - 16) x^5 + (24 \times 2^n + 8) x^0.$$

Theorem 11. *The square F-index of DPZ_n is*

$$QF(DPZ_n) = 1000 \times 2^n - 204.$$

Proof. Let $G = DPZ_n$. By using equation (2) and Table 3, we deduce

$$QF(DPZ_n) = \sum_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2$$

$$= (2^2 - 2^2)^2 (16 \times 2^n - 4) + (2^2 - 3^2)^2 (40 \times 2^n - 16)$$

$$+ (3^2 - 3^2)^2 (8 \times 2^n + 12) + (3^2 - 4^2)^2 4$$

$$= 1000 \times 2^n - 204.$$

Theorem 12. *The square F-polynomial of* DPZ_n *is*

$$QF(DPZ_n, x) = 4x^{49} + (40 \times 2^n - 16) x^{25} + (24 \times 2^n + 8) x^0.$$

Proof. Let $G = DPZ_n$. From equation (4) and by using Table 3. We derive

$$QF(DPZ_n, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}$$

$$= (16 \times 2^n - 4) x^{(1^2 - 2^2)^2} + (40 \times 2^n - 16) x^{(2^2 - 3^2)^2}$$

$$+ (8 \times 2^n + 12) x^{(3^2 - 3^2)^2} + 4x^{(3^2 - 4^2)^2}$$

$$= 4x^{49} + (40 \times 2^n - 16) x^{25} + (24 \times 2^n + 8) x^0.$$

5. Results for Poly Ethylene Amide Amine Dendrimer *PETAA*

We consider the poly ethylene amide amine dendrimer which is denoted by *PETAA*. This dendrimer is shown in Figure 4.

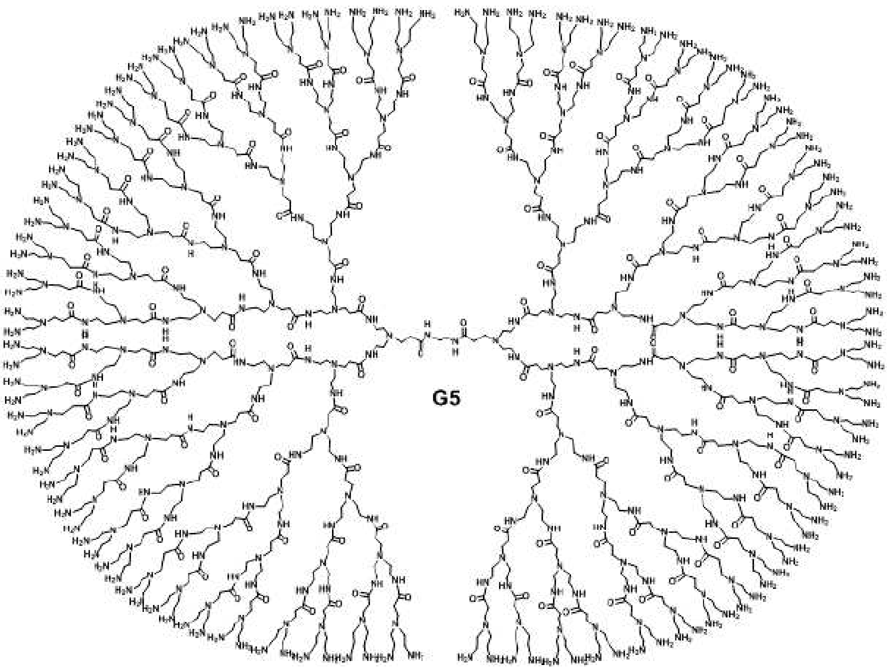

Figure 4. Poly ethylene amide amine dendrimer *PETAA*.

Let $G = PETAA$ be a poly ethylene amide amine dendrimer. By calculation, *G* has $44 \times 2^n - 18$ vertices and $44 \times 2^n - 19$ edges. In *G*, there are four different types of edges based on degrees of end vertices of each edge. Also by calculation, the edge partition of *G* is given in Table 4.

Table 4. Edge partition of *PETAA*.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	4×2^n	$4 \times 2^n - 2$	$16 \times 2^n - 8$	$20 \times 2^n - 9$

Theorem 13. *The minus F-index of PETAA is*

$$MF(PETAA) = 144 \times 2^n - 61.$$

Proof. Let $G = PETAA.$ From equation (1) and by using Table 4, we obtain

$$MF(PETAA) = \sum_{uv \in E(G)} | d_G(u)^2 - d_G(v)^2 |$$

$$= |1^2 - 2^2| 4 \times 2^n + |1^2 - 3^2| (4 \times 2^n - 2)$$

$$+ |2^2 - 2^2| (16 \times 2^n - 8) + |2^2 - 3^2| (20 \times 2^n - 9)$$

$$= 144 \times 2^n - 61.$$

Theorem 14. *The minus F-polynomial of PETAA is*

$$MF(PETAA, x) = (4 \times 2^n - 2) x^8 + (20 \times 2^n - 9) x^5 + 4 \times 2^n x^3$$

$$+ (16 \times 2^n - 8) x^0.$$

Proof. Let $G = PETAA$. By using equation (3) and Table 4, we deduce

$$MF(PETAA, x) = \sum_{uv \in E(G)} x^{[d_G(u)^2 - d_G(v)^2]}$$

$$= 4 \times 2^n x^{|1^2 - 2^2|} + (4 \times 2^n - 2) x^{|1^2 - 3^2|}$$

$$+ (16 \times 2^n - 8) x^{|2^2 - 2^2|} + (20 \times 2^n - 9) x^{|2^2 - 3^2|}$$

$$= (4 \times 2^n - 2) x^8 + (20 \times 2^n - 9) x^5 + 4 \times 2^n x^3$$

$$+ (16 \times 2^n - 8) x^0.$$

Theorem 15. *The square F-index of PETAA is*

$$QF(PETAA) = 792 \times 2^n - 353.$$

Proof. Let $G = PETAA$. By using equation (2) and Table 5, we derive

$$QF(PETAA) = \sum_{uv \in E(G)} [d_G(u)^2 - d_G(v)^2]^2$$

$$= (1^2 - 2^2)^2 4 \times 2^n + (1^2 - 3^2)^2 (4 \times 2^n - 2)$$

$$+ (2^2 - 2^2)^2 (16 \times 2^n - 8) + (2^2 - 3^2)^2 (20 \times 2^n - 9)$$

$$= 792 \times 2^n - 353.$$

Theorem 16. *The square F-polynomial of PETAA is*

$$QF(PETAA,\ x) = (4\times 2^n - 2)\,x^{64} + (20\times 2^n - 9)\,x^{25} + 4\times 2^n x^9 + (16\times 2^n - 8)\,x^0.$$

Proof. Let $G = PETAA$. From equation (4) and by using Table 4, we get

$$QF(PETAA,\ x) = \sum_{uv\in E(G)} x^{[d_G(u)^2 - d_G(v)^2]^2}$$

$$= 4\times 2^n x^{(1^2-2^2)^2} + (4\times 2^n - 2)\,x^{(1^2-3^2)^2} + (16\times 2^n - 8)\,x^{(2^2-2^2)^2} + (20\times 2^n - 9)\,x^{(2^2-3^2)^2}$$

$$= (4\times 2^n - 2)\,x^{64} + (20\times 2^n - 9)\,x^{25} + 4\times 2^n x^9 + (16\times 2^n - 8)\,x^0.$$

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