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Computation of Minus *F*-indices and their Polynomials of Titania Nanotubes

V.R.Kulli

Department of Mathematics
Gulbarga University, Gulbarga 585 106, India
E-mail: vrkulli@gmail.com

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Abstract. In Chemical Graph Theory, a forgotten topological index or *F*-index has significant importance to collect information about properties of chemical compounds. In this study, we introduce the modified minus *F*-index, minus connectivity *F*-index, reciprocal minus connectivity *F*-index, general minus *F*-index and their polynomials of a molecular graph. Furthermore, we present exact expressions for these minus *F*-indices and their polynomials of titania nanotubes.

Keywords: modified minus *F*-index, reciprocal minus connectivity *F*-index, general minus *F*-index, titania nanotube.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*40, 05*C*92

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. For definitions and notations, we refer the book [1].

Chemical Graph Theory is a branch of Mathematical Chemistry, which has an important effect on the development of Chemical Sciences. 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, 4].

The first *F*-index [5] and second *F*-index [6] of a graph *G* are defined respectively as

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

Recently some novel variants of *F*-indices were introduced and studied such as multiplicative *F*-indices [7], connectivity *F*-indices [8], multiplicative first *F*-index [9, 10].

The irregularity index (called as minus index [11]) was introduced by Albertson in [12], defined as

$$M_i(G)=\sum\left|d_G(u)-d_G(v)\right|.$$

The minus *F*-index or nano Zagreb index was introduced and studied independently by Kulli in [13] and Jahanbani et al. in [14] and defined it as

$$MF(G)=\sum\left|d_G(u)^2-d_G(v)^2\right|.$$

Recently, the multiplicative minus indices were studied in [15].

In [16], Gutman et al. introduced the sigma index of a graph *G* and defined it as

$$\sigma(G)=\sum\left[d_G(u)-d_G(v)\right]^2.$$

Similarly, in [13], Kulli introduced the square *F*-index (or sigma *F*-index) of a graph *G*, defined as

$$QF(G) \text{ or } \sigma F(G)=\sum_{uv\in E(G)}\left[d_G(u)^2-d_G(v)^2\right]^2.$$

We now introduce the following minus *F*-indices:

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

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

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

$$RMF_C(G)=\sum_{uv\in E(G)}\sqrt{\left|d_G(u)^2-d_G(v)^2\right|}.$$

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

$$MF^a(G)=\sum_{uv\in E(G)}\left[\left|d_G(u)^2-d_G(v)^2\right|\right]^a, \tag{1}$$

where *a* is real number.

The minus *F*-polynomial and sigma *F*-polynomial (or square *F*-polynomial) of a graph were introduced by Kulli in [11], and they are defined as

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

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

We now introduce the minus *F*-polynomials of a graph *G* as follows:

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

$${}^{m}MF(G,x)=\sum_{uv\in E(G)}x^{\frac{1}{\left|d_G(u)^2-d_G(v)^2\right|}}.$$

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

$$MF_C(G,x)=\sum_{uv\in E(G)}x^{\frac{1}{\sqrt{\left|d_G(u)^2-d_G(v)^2\right|}}}.$$

The reciprocal minus connectivity *F*-polynomial of a graph *G* is defined as

$$RMF_C(G,x)=\sum_{uv\in E(G)}x^{\sqrt{\left|d_G(u)^2-d_G(v)^2\right|}}.$$

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

$$MF^a(G,x) = \sum_{uv \in E(G)} x^{\left[\left|d_G(u)^2 - d_G(v)^2\right|\right]^a}, \tag{2}$$

where *a* is real number.

Recently some graph polynomials were studied in [17, 18, 19, 20, 21,22, 23].

In this paper, some minus *F*-indices and their corresponding polynomial versions of titania nanotubes are determined.

2. Results for titania nanotubes

Titania nanotube is studied in material science. The titania nanotubes denoted by $TiO_2[m, n]$ for any $m, n \in N$, in which *m* is the number of octagons C_8 in a row and *n* is the number of octagons C_8 in a column. The molecular graph of $TiO_2[m, n]$ is presented in Figure 1.

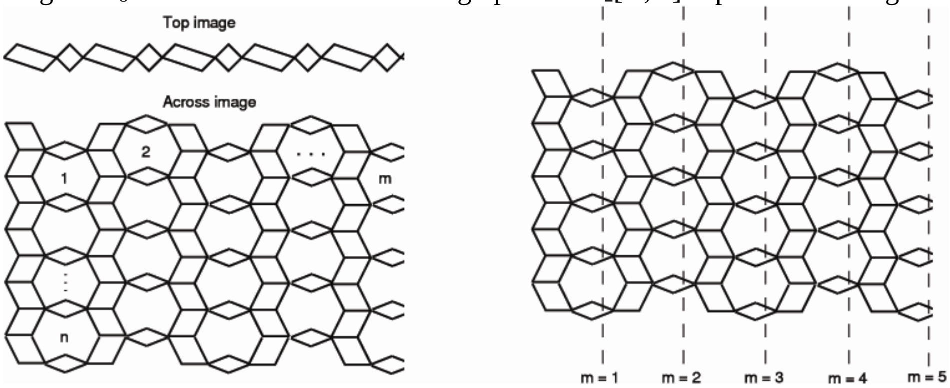

Figure 1: Molecular graph of $TiO_2[m, n]$

Let *G* be the graph of titania nanotube $TiO_2[m, n]$. The graph *G* has $6n(m+1)$ vertices and $10mn+8n$ edges. By calculation, we obtain that *G* has four types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2,4)	(2, 5)	(3, 4)	(3, 5)
Number of edges	$6n$	$4mn+2n$	$2n$	$6mn - 2n$

Table 1: Edge partition of $TiO_2[m, n]$

In the following theorem, we compute the general minus *F*-index of $TiO_2[m, n]$.

Theorem 1. The general minus *F*-index of $TiO_2[m, n]$ titania nanotubes is

$$MF^a(TiO_2) = \left(4\times 21^a + 6\times 16^a\right)mn + \left(6\times 12^a + 2\times 21^a + 2\times 7^a - 2\times 16^a\right)n. \tag{3}$$

Proof: Let *G* be the graph of $TiO_2[m, n]$ titania nanotube. By using equation (1) and Table 1, we deduce

$$\begin{aligned} MF^a(TiO_2) &= \sum_{uv\in E(G)} \left[\left|d_G(u)^2 - d_G(v)^2\right|\right]^a \\ &= \left(\left|2^2-4^2\right|\right)^a 6n + \left(\left|2^2-5^2\right|\right)^a (4mn+2n) \\ &\quad + \left(\left|3^2-4^2\right|\right)^a 2n + \left(\left|3^2-5^2\right|\right)^a (6mn-2n). \end{aligned}$$

$$=\left(4\times 21^{a}+6\times 16^{a}\right)mn+\left(6\times 12^{a}+2\times 21^{a}+2\times 7^{a}-2\times 16^{a}\right)n.$$

We establish the following results by using Theorem 1.

Corollary 1.1. The minus F-index of $TiO_2[m, n]$ is

$$MF(TiO_2) = 180mn + 96n.$$

Corollary 1.2. The square F-index of $TiO_2[m, n]$ is

$$QF(TiO_2) = 3300mn + 1332n.$$

Corollary 1.3. The modified minus F-index of $TiO_2[m, n]$ is

$${}^{m}MF\left(TiO_2\right)=\frac{95}{168}mn+\frac{889}{1176}n.$$

Corollary 1.4. The minus connectivity F-index of $TiO_2[m, n]$ is

$$MF_C\left(TiO_2\right)=\left(\frac{4}{\sqrt{21}}+\frac{3}{2}\right)mn+\left(\frac{3}{\sqrt{3}}+\frac{2}{\sqrt{21}}+\frac{2}{\sqrt{7}}-\frac{1}{2}\right)n.$$

Corollary 1.5. The reciprocal minus connectivity F-index of $TiO_2[m, n]$ is

$$RMF_C\left(TiO_2\right)=\left(4\sqrt{21}+24\right)mn+\left(12\sqrt{3}+2\sqrt{21}+2\sqrt{7}-8\right)n.$$

Proof: Put a = 1, 2, – 1, –½, ½ in equation (3), we get the desired results.

In the following Theorem, we compute the general minus F-polynomial of $TiO_2[m, n]$.

Theorem 2. The general minus F-polynomial of $TiO_2[m, n]$ titania nanotubes is

$$MF^{a}\left(TiO_2,x\right)=6nx^{12^{a}}+\left(4mn+2n\right)x^{21^{a}}+2nx^{7^{a}}+\left(6mn-2n\right)x^{16^{a}}. \qquad (4)$$

Proof: Let G be the graph of $TiO_2[m, n]$. By using equation (2) and Table 1, we derive

$$MF^{a}(TiO_2,x)=\sum_{uv\in E(G)} x^{\left[\left|d_G(u)^2-d_G(v)^2\right|\right]^{a}}$$

$$=6nx^{\left(\left|2^2-4^2\right|\right)^{a}}+\left(4mn+6n\right)x^{\left(\left|2^2-5^2\right|\right)^{a}}$$

$$+2nx^{\left(\left|3^2-4^2\right|\right)^{a}}+\left(6mn-2n\right)x^{\left(\left|3^2-5^2\right|\right)^{a}}$$

$$=6nx^{12^{a}}+\left(4mn+2n\right)x^{21^{a}}+2nx^{7^{a}}+\left(6mn-2n\right)x^{16^{a}}.$$

The following results are obtained by using Theorem 2.

Corollary 2.1. The minus F-polynomial of $TiO_2[m, n]$ is

$$MF(TiO_2, x) = (4mn + 2n)x^{21} + (6mn – 2n)x^{16} + 6nx^{12} + 2nx^{7}.$$

Corollary 2.2. The square F-polynomial of $TiO_2[m, n]$ is

$$QF(TiO_2, x) = (4mn + 2n)x^{441} + (6mn – 2n)x^{256} + 6nx^{144} + 2nx^{49}.$$

Corollary 2.3. The modified minus F-polynomial of $TiO_2[m, n]$ is

$$ {}^{m}MF\left(TiO_2,x\right)=\left(4mn+2n\right)x^{\frac{1}{21}}+\left(6mn-2n\right)x^{\frac{1}{16}}+6nx^{\frac{1}{12}}+2nx^{\frac{1}{7}}. $$

Corollary 2.4. The minus connectivity *F*-polynomial of $TiO_2[m, n]$ is

$$ MF_C\left(TiO_2,x\right)=\left(4mn+2n\right)x^{\frac{1}{\sqrt{21}}}+\left(6mn-2n\right)x^{\frac{1}{4}}+6nx^{\frac{1}{\sqrt{12}}}+2nx^{\frac{1}{\sqrt{7}}}. $$

Corollary 2.5. The reciprocal minus connectivity *F*-index of $TiO_2[m, n]$ is

$$ RMF_C\left(TiO_2,x\right)=\left(4mn+2n\right)x^{\sqrt{21}}+\left(6mn-2n\right)x^{4}+6nx^{\sqrt{12}}+2nx^{\sqrt{7}}. $$

Proof: Put a = 1, 2, – 1, –½, ½ in equation (4), we obtain the desired results.

3. Conclusion

In this study, we have proposed the modified minus *F*-index, minus connectivity *F*-index, reciprocal minus connectivity *F*-index, general minus *F*-index and their corresponding polynomials of a molecular graph. We have computed these minus *F*-indices and their corresponding polynomial versions of titania nanotubes.

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