Open Journal of
Discrete Applied Mathematics

Article

The forgotten index of complement graph operations and its applications of molecular graph

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Received: 6 August 2020; Accepted: 23 September 2020; Published: 24 October 2020.

Abstract: A topological index of graph G is a numerical parameter related to graph which characterizes its molecular topology and is usually graph invariant. Topological indices are widely used to determine the correlation between the specific properties of molecules and the biological activity with their configuration in the study of quantitative structure-activity relationships (QSARs). In this paper some basic mathematical operations for the forgotten index of complement graph operations such as join $\overline{G_1 + G_2}$, tensor product $\overline{G_1 \otimes G_2}$, Cartesian product $\overline{G_1 \times G_2}$, composition $\overline{G_1 \circ G_2}$, strong product $\overline{G_1 * G_2}$, disjunction $\overline{G_1 \vee G_2}$ and symmetric difference $\overline{G_1 \oplus G_2}$ will be explained. The results are applied to molecular graph of nanotorus and titania nanotubes.

Keywords: Forgotten index, Zagreb indices, complement graph, graph operation.

MSC: 05C92.

1. Introduction

Theory of chemical graphs is the branch of mathematical chemistry that applies theory of graphs to mathematical modeling of chemical phenomena. In chemical graph theory a molecular graph is a simple graph in which the vertices and edges represent atoms and chemical bonds between them. In this paper, G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of elements in $V(G)$ and $E(G)$ is represented as $|V(G)|$ and $|E(G)|$, respectively. For a vertex $u \in V(G)$, the number of vertices adjacent to the vertex u is called the degree of u, denoted by $\delta_G(u)$. The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv, if and only if they are not adjacent in G. Hence, $uv \in E(\overline{G})$, if and only if $uv \notin E(G)$. Obviously $E(G) \cup E(\overline{G}) = E(K_n)$, and $\overline{m} = |E(\overline{G})| = \binom{n}{2} - m$, the degree of a vertex u in $\overline{G}$, is the number of edges incident to u, denoted by $\delta_{\overline{G}}(u) = n - 1 - \delta_G(u)$ [1]. The well-known Zagreb indices introduced in [2] are among the most important topological indices. The first and second Zagreb indices M_1 and M_2, respectively, are defined for a molecular graph G as:

$$M_1(G) = \sum_{v \in V(G)} \delta_G{}^2(v) = \sum_{uv \in E(G)} [\delta_G(u) + \delta_G(v)], \qquad M_2(G) = \sum_{uv \in E(G)} \delta_G(u)\, \delta_G(v).$$

The first and second Zagreb coindices have been introduced by Ashrafi *et al.,* in 2010 [3], they are respectively defined as:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} [\delta_G(u) + \delta_G(v)], \qquad \overline{M}_2(G) = \sum_{uv \notin E(G)} \delta_G(u)\, \delta_G(v).$$

Furtula and Gutman in 2015 introduced forgotten index (F-index) [4] which is defined as:

$$F(G) = \sum_{v \in V(G)} \delta_G{}^3(v) = \sum_{uv \in E(G)} \left(\delta_G{}^2(u) + \delta_G{}^2(v)\right).$$

De *et al.*, in 2016 defined forgotten coindex (F-coindex)[5] which is defined as:

$$\overline{F}(G) = \sum_{uv \notin E(G)} \left({\delta_G}^2(u) + {\delta_G}^2(v) \right).$$

Then, De *et al.*, in 2016 [6] computed the forgotten index of join $G_1 + G_2$, tensor product $G_1 \otimes G_2$, Cartesian product $G_1 \times G_2$, composition $G_1 \circ G_2$, strong product $G_1 * G_2$, disjunction $G_1 \vee G_2$ and symmetric difference $G_1 \oplus G_2$ of two graphs. Here we continue this line of research by exploring the behavior of the forgotten index under the same operations of complement graphs. The results are applied to molecular graph of nanotorus and titania nanotubes. In recent years, there has been considerable interest in general problems of determining topological indices and their operations [1,7–9].

2. Preliminaries

In this section we give some basic and preliminary concepts which we shall use later.

Lemma 1. *[10,11] Let G_1 and G_2 be two connected graphs with $|V(G_1)| = n_1$, $|V(G_2)| = n_2$, $|E(G_1)| = m_1$, and $|E(G_2)| = m_2$. Then*

1. $|V(G_1 \times G_2)| = |V(G_1 \vee G_2)| = |V(G_1 \circ G_2)| = |V(G_1 \otimes G_2)| = |V(G_1 * G_2)| = |V(G_1 \oplus G_2)| = n_1 n_2$, $|V(G_1 + G_2)| = n_1 + n_2$,
2. $|E(G_1 \times G_2)| = m_1 n_2 + n_1 m_2$,
   $|E(G_1 * G_2)| = m_1 n_2 + n_1 m_2 + 2m_1 m_2$,
   $|E(G_1 + G_2)| = m_1 + m_2 + n_1 n_2$,
   $|E(G_1 \circ G_2)| = m_1 {n_2}^2 + m_2 n_1$,
   $|E(G_1 \vee G_2)| = m_1 {n_2}^2 + m_2 {n_1}^2 - 2m_1 m_2$,
   $|E(G_1 \otimes G_2)| = 2m_1 m_2$,
   $|E(G_1 \oplus G_2)| = m_1 {n_2}^2 + m_2 {n_1}^2 - 4m_1 m_2$.

Proposition 1. *[12] Let G be a simple graph on n vertices and m edges. Then.*

$$F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G).$$

3. Discussion and main results

In this section, we study the forgotten index of various complement graph binary operations such as join, tensor product, Cartesian product, composition, strong product, disjunction and symmetric difference of two simple connected graphs. We use the notation $V(G_i)$ for the vertex set, $E(G_i)$, $E(\overline{G}_i)$ for the edge sets, n_i for the number of vertices and m_i, $\overline{m}_i$ for the number of edges of the graph G_i, $\overline{G}_i$ respectively. All graphs here offer are simple graphs.

Definition 1 (Join)**.** The join $G_1 + G_2$ of two graphs G_1 and G_2 is a graph with vertex set $V(G_1 + G_2) = V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_1) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$.

Theorem 1. *The $F-$index of the complement of $G_1 + G_2$ is given by*

$$\begin{aligned} F(\overline{G_1 + G_2}) \;\; = \;\; & (n_1 + n_2)(n_1 + n_2 - 1)^3 - 6(m_1 + m_2 + n_1 n_2)(n_1 + n_2 - 1)^2 \\ & + 3(n_1 + n_2 - 1)[M_1(G_1) + M_1(G_2) + n_1 n_2^2 + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1] \\ & - [F(G_1) + F(G_2) + 3n_2 M_1(G_1) + 3n_1 M_1(G_2) + 6n_2^2 m_1 + 6n_1^2 m_2 + n_1 n_2^3 + n_2 n_1^3]. \end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(G_1 + G_2) = M_1(G_1) + M_1(G_2) + n_1 n_2^2 + n_2 n_1^2 + 4m_1 n_2 + 4m_2 n_1$, given in [10], $F(G_1 + G_2) = F(G_1) +$

$F(G_2) + 3n_2M_1(G_1) + 3n_1M_1(G_2) + 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3$, given in [6]. and $|E(G_1 + G_2)| = m_1 + m_2 + n_1n_2$, $|V(G_1 + G_2)| = n_1 + n_2$ given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 + G_2}) &= |V(G_1 + G_2)|(|V(G_1 + G_2)| - 1)^3 - 6|E(G_1 + G_2)|(|V(G_1 + G_2)| - 1)^2 \\ &\quad +3(|V(G_1 + G_2)| - 1)M_1(G_1 + G_2) - F(G_1 + G_2) \\ &= (n_1 + n_2)(n_1 + n_2 - 1)^3 - 6(m_1 + m_2 + n_1n_2)(n_1 + n_2 - 1)^2 \\ &\quad +3(n_1 + n_2 - 1)[M_1(G_1) + M_1(G_2) + n_1n_2^2 + n_2n_1^2 + 4m_1n_2 + 4m_2n_1] \\ &\quad -[F(G_1) + F(G_2) + 3n_2M_1(G_1) + 3n_1M_1(G_2) + 6n_2^2m_1 + 6n_1^2m_2 + n_1n_2^3 + n_2n_1^3]. \end{aligned}$$

□

Definition 2 (Tensor product)**.** The tensor product $G_1 \otimes G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and any two vertices (u_1, v_1) and (u_2, v_2) are adjacent if and only if $u_1u_2 \in E(G_1)$ and $v_1v_2 \in E(G_2)$.

Theorem 2. *The $F-$index of the complement of $G_1 \otimes G_2$ is given by*

$$F(\overline{G_1 \otimes G_2}) = n_1n_2(n_1n_2 - 1)^3 - 12m_1m_2(n_1n_2 - 1)^2 + 3(n_1n_2 - 1)M_1(G_1)M_1(G_2) - F(G_1)F(G_2).$$

Proof. From Proposition 1 we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(G_1 \otimes G_2) = M_1(G_1)M_1(G_2)$ given in [13], $F(G_1 \otimes G_2) = F(G_1)F(G_2)$ given in [6] and $|E(G_1 \otimes G_2)| = 2m_1m_2$, $|V(G_1 \otimes G_2)| = n_1n_2$ given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 \otimes G_2}) &= |V(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^3 - 6|E(G_1 \otimes G_2)|(|V(G_1 \otimes G_2)| - 1)^2 \\ &\quad +3(|V(G_1 \otimes G_2)| - 1)M_1(G_1 \otimes G_2) - F(G_1 \otimes G_2) \\ &= n_1n_2(n_1n_2 - 1)^3 - 12m_1m_2(n_1n_2 - 1)^2 + 3(n_1n_2 - 1)M_1(G_1)M_1(G_2) - F(G_1)F(G_2). \end{aligned}$$

□

Definition 3 (Cartesian product)**.** The Cartesian product $G_1 \times G_2$, of two simple and connected graphs G_1 and G_2 has the vertex set$V(G_1 \times G_2) = V(G_1) \times V(G_2)$ and $(a, x)(b, y)$ is an edge of $G_1 \times G_2$ if $a = b$ and $xy \in E(G_2)$, or $ab \in E(G_1)$ and $x = y$.

Theorem 3. *The $F-$index of the complement of $G_1 \times G_2$ is given by*

$$\begin{aligned} F(\overline{G_1 \times G_2}) &= n_1n_2(n_1n_2 - 1)^3 - 6(m_1n_2 + n_1m_2)(n_1n_2 - 1)^2 + 3(n_1n_2 - 1)[n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2] \\ &\quad -[n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)]. \end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(G_1 \times G_2) = n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2$, given in [14], $F(G_1 \times G_2) = n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)$, given in [6]. and $|E(G_1 \times G_2)| = m_1n_2 + n_1m_2$, $|V(G_1 \times G_2)| = n_1n_2$ given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 \times G_2}) &= |V(G_1 * G_2)|(|V(G_1 * G_2)| - 1)^3 - 6|E(G_1 * G_2)|(|V(G_1 * G_2)| - 1)^2 \\ &\quad +3(|V(G_1 * G_2)| - 1)M_1(G_1 * G_2) - F(G_1 * G_2) \\ &= n_1n_2(n_1n_2 - 1)^3 - 6(m_1n_2 + n_1m_2)(n_1n_2 - 1)^2 \\ &\quad +3(n_1n_2 - 1)[n_2M_1(G_1) + n_1M_1(G_2) + 8m_1m_2] \\ &\quad -[n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)]. \end{aligned}$$

□

Definition 4 (Composition)**.** The composition $G_1 \circ G_2$, of two simple and connected graphs G_1 and G_2 with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph with vertex set $V(G_1) \times V(G_2)$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or $\{u_1 = u_2$ and v_1 is adjacent with $v_2\}$.

Theorem 4. *The $F-$ index of the complement of $G_1 \circ G_2$ is given by*

$$\begin{aligned} F(\overline{G_1 \circ G_2}) &= n_1n_2(n_1n_2-1)^3 - 6(m_1{n_2}^2 + m_2n_1)(n_1n_2-1)^2 \\ &\quad +3(n_1n_2-1)[n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] \\ &\quad -[n_2^4F(G_1) + n_1F(G_2) + 6n_2^2m_2M_1(G_1) + 6n_2m_1M_1(G_2)]. \end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(G_1 \circ G_2) = n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1$, given in [14]. $F(G_1 \circ G_2) = n_2^4F(G_1) + n_1F(G_2) + 6n_2^2m_2M_1(G_1) + 6n_2m_1M_1(G_2)$, given in [6]. and $|E(G_1 \circ G_2)| = m_1{n_2}^2 + m_2n_1$, $|V(G_1 \circ G_2)| = n_1n_2$ given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 \circ G_2}) &= |V(G_1 \circ G_2)|(|V(G_1 \circ G_2)|-1)^3 - 6|E(G_1 \circ G_2)|(|V(G_1 \circ G_2)|-1)^2 \\ &\quad +3(|V(G_1 \circ G_2)|-1)M_1(G_1 \circ G_2) - F(G_1 \circ G_2) \\ &= n_1n_2(n_1n_2-1)^3 - 6(m_1{n_2}^2 + m_2n_1)(n_1n_2-1)^2 \\ &\quad +3(n_1n_2-1)[n_2^3M_1(G_1) + n_1M_1(G_2) + 8n_2m_2m_1] \\ &\quad -[n_2^4F(G_1) + n_1F(G_2) + 6n_2^2m_2M_1(G_1) + 6n_2m_1M_1(G_2)]. \end{aligned}$$

□

Definition 5 (Strong product)**.** The strong product $G_1 * G_2$, of two simple and connected graphs G_1 and G_2 is a graph with vertex set $V(G_1 * G_2) = V(G_1) \times V(G_2)$ and any two vertices (u_1, v_1) and (u_2, v_2) are adjacent if and only if $\{u_1 = u_2 \in V(G_1)$ and $v_1v_2 \in E(G_2)\}$ or $\{v_1 = v_2 \in V(G_2)$ and $u_1u_2 \in E(G_1)\}$.

Proposition 2. *[15] Let G_1, G_2 be two graphs with n_1, n_2 vertices and m_1, m_2 edges, respectively. Then*

$$M_1(G_1 * G_2) = (n_2 + 6m_2)M_1(G_1) + 8m_2m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2).$$

Theorem 5. *The $F-$ index of the complement of $G_1 * G_2$ is given by*

$$\begin{aligned} F(\overline{G_1 * G_2}) &= n_1n_2(n_1n_2-1)^3 - 6(m_1n_2 + n_1m_2 + 2m_1m_2)(n_1n_2-1)^2 \\ &\quad +3(n_1n_2-1)[(n_2+6m_2)M_1(G_1) + 8m_2m_1 + (6m_1+n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)] \\ &\quad -[n_2F(G_1) + n_1F(G_2) + F(G_1)F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2) \\ &\quad +6m_2F(G_1) + 6m_1F(G_2) + 3F(G_2)M_1(G_1) + 3F(G_1)M_1(G_2) + 6M_1(G_1)M_1(G_2)]. \end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(G_1 * G_2) = (n_2 + 6m_2)M_1(G_1) + 8m_2m_1 + (6m_1 + n_1)M_1(G_2) + 2M_1(G_1)M_1(G_2)$, given in Proposition 2, and by [6] we have

$$\begin{aligned} F(G_1 * G_2) &= n_2F(G_1) + n_1F(G_2) + F(G_1)F(G_2) + 6m_2M_1(G_1) + 6M_1(G_1)M_1(G_2) \\ &\quad +6m_1M_1(G_2) + 6m_2F(G_1) + 6m_1F(G_2) + 3F(G_2)M_1(G_1) + 3F(G_1)M_1(G_2). \end{aligned}$$

And since $|E(G_1 * G_2)| = m_1n_2 + n_1m_2 + 2m_1m_2$, $|V(G_1 * G_2)| = n_1n_2$, given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 * G_2}) &= |V(G_1 * G_2)|(|V(G_1 * G_2)|-1)^3 - 6|E(G_1 * G_2)|(|V(G_1 * G_2)|-1)^2 \\ &\quad +3(|V(G_1 * G_2)|-1)M_1(G_1 * G_2) - F(G_1 * G_2) \end{aligned}$$

$$\begin{aligned}
&= n_1n_2(n_1n_2-1)^3 - 6(m_1n_2+n_1m_2+2m_1m_2)(n_1n_2-1)^2 \\
&\quad +3(n_1n_2-1)[(n_2+6m_2)M_1(G_1)+8m_2m_1+(6m_1+n_1)M_1(G_2)+2M_1(G_1)M_1(G_2)] \\
&\quad -[n_2F(G_1)+n_1F(G_2)+F(G_1)F(G_2)+6m_2M_1(G_1)+6m_1M_1(G_2) \\
&\quad +6m_2F(G_1)+6m_1F(G_2)+3F(G_2)M_1(G_1)+3F(G_1)M_1(G_2)+6M_1(G_1)M_1(G_2)].
\end{aligned}$$

□

Definition 6 (Disjunction)**.** The disjunction $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and (u_1, v_1) is adjacent with (u_2, v_2), whenever $(u_1, u_2) \in E(G_1)$ or $(v_1, v_2) \in E(G_2)$.

Theorem 6. *The first Zagreb index of $G_1 \vee G_2$ is given by*

$$M_1(G_1 \vee G_2) = [n_2^3 - 4n_2m_2]M_1(G_1) + [n_1^3 - 4n_1m_1]M_1(G_2) + 8n_1n_2m_1m_2 + M_1(G_1)M_1(G_2).$$

Theorem 7. *The $F-$index of the complement of $G_1 \vee G_2$ is given by*

$$\begin{aligned}
F(\overline{G_1 \vee G_2}) &= n_1n_2(n_1n_2-1)^3 - 6[m_1{n_2}^2+m_2{n_1}^2-2m_1m_2](n_1n_2-1)^2 \\
&\quad +3(n_1n_2-1)\big[[n_2^3-4n_2m_2]M_1(G_1)+[n_1^3-4n_1m_1]M_1(G_2) \\
&\quad +8n_1n_2m_1m_2+M_1(G_1)M_1(G_2)\big] - [n_2^4F(G_1)+n_1^4F(G_2)-F(G_1)F(G_2) \\
&\quad +6n_1n_2^2m_2M_1(G_1)+6n_2n_1^2m_1M_1(G_2)+3n_2F(G_1)M_1(G_2)+3n_1F(G_2)M_1(G_1) \\
&\quad -6n_2^2m_2F(G_1)-6n_1^2m_1F(G_2)-6n_1n_2M_1(G_1)M_1(G_2)].
\end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and by Theorem 6 and [6], respectively, we have

$$M_1(G_1 \vee G_2) = [n_2^3 - 4n_2m_2]M_1(G_1) + [n_1^3 - 4n_1m_1]M_1(G_2) + 8n_1n_2m_1m_2 + M_1(G_1)M_1(G_2).$$

$$\begin{aligned}
F(G_1 \vee G_2) &= n_2^4F(G_1)+n_1^4F(G_2)-F(G_1)F(G_2)+6n_1n_2^2m_2M_1(G_1) \\
&\quad +6n_2n_1^2m_1M_1(G_2)+3n_2F(G_1)M_1(G_2)+3n_1F(G_2)M_1(G_1) \\
&\quad -6n_2^2m_2F(G_1)-6n_1^2m_1F(G_2)-6n_1n_2M_1(G_1)M_1(G_2).
\end{aligned}$$

And since $|E(G_1 \vee G_2)| = m_1{n_2}^2 + m_2{n_1}^2 - 2m_1m_2, \quad |V(G_1 \vee G_2)| = n_1n_2$ given in Lemma 1. Then

$$\begin{aligned}
F(\overline{G_1 \vee G_2}) &= |V(G_1 \vee G_2)|(|V(G_1 \vee G_2)|-1)^3 - 6|E(G_1 \vee G_2)|(|V(G_1 \vee G_2)|-1)^2 \\
&\quad +3(|V(G_1 \vee G_2)|-1)M_1(G_1 \vee G_2) - F(G_1 \vee G_2) \\
&= n_1n_2(n_1n_2-1)^3 - 6[m_1{n_2}^2+m_2{n_1}^2-2m_1m_2](n_1n_2-1)^2 \\
&\quad +3(n_1n_2-1)\big[[n_2^3-4n_2m_2]M_1(G_1)+[n_1^3-4n_1m_1]M_1(G_2) \\
&\quad +8n_1n_2m_1m_2+M_1(G_1)M_1(G_2)\big] - [n_2^4F(G_1)+n_1^4F(G_2)-F(G_1)F(G_2) \\
&\quad +6n_1n_2^2m_2M_1(G_1)+6n_2n_1^2m_1M_1(G_2)+3n_2F(G_1)M_1(G_2)+3n_1F(G_2)M_1(G_1) \\
&\quad -6n_2^2m_2F(G_1)-6n_1^2m_1F(G_2)-6n_1n_2M_1(G_1)M_1(G_2)].
\end{aligned}$$

□

Definition 7 (Symmetric difference)**.** The symmetric difference $G_1 \oplus G_2$, of two simple and connected graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ and $E(G_1 \oplus G_2) = (u_1, u_2)(v_1, v_2)|u_1v_1 \in E(G_1)$ or $u_2v_2 \in E(G_2)$ but not both.

Theorem 8. *The first Zagreb index of $G_1 \oplus G_2$ is given by*

$$M_1(G_1 \oplus G_2) = [n_2^3 - 8n_2m_2]M_1(G_1) + [n_1^3 - 8n_1m_1]M_1(G_2) + 8n_1n_2m_1m_2 + 4M_1(G_1)M_1(G_2).$$

Theorem 9. *The $F-$ index of the complement of $G_1 \oplus G_2$ is given by*

$$\begin{aligned} F(\overline{G_1 \oplus G_2}) &= n_1n_2(n_1n_2-1)^3 - 6[m_1{n_2}^2 + m_2{n_1}^2 - 4m_1m_2](n_1n_2-1)^2 \\ &+3(n_1n_2-1)\big[[n_2^3 - 8n_2m_2]M_1(G_1) + [n_1^3 - 8n_1m_1]M_1(G_2) \\ &+8n_1n_2m_1m_2 + 4M_1(G_1)M_1(G_2)\big] - \big[n_2^4F(G_1) + n_1^4F(G_2) \\ &-8F(G_1)F(G_2) + 6n_1n_2^2m_2M_1(G_1) + 6n_2n_1^2m_1M_1(G_2) \\ &+12n_2F(G_1)M_1(G_2) + 12n_1F(G_2)M_1(G_1) - 12n_2^2m_2F(G_1) \\ &-12n_1^2m_1F(G_2) - 12n_1n_2M_1(G_1)M_1(G_2)\big]. \end{aligned}$$

Proof. From Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and by Theorem 8 and [6], respectively, we have

$$M_1(G_1 \oplus G_2) = [n_2^3 - 8n_2m_2]M_1(G_1) + [n_1^3 - 8n_1m_1]M_1(G_2) + 8n_1n_2m_1m_2 + 4M_1(G_1)M_1(G_2).$$

$$\begin{aligned} F(G_1 \oplus G_2) &= n_2^4F(G_1) + n_1^4F(G_2) - 8F(G_1)F(G_2) + 6n_1n_2^2m_2M_1(G_1) \\ &+6n_2n_1^2m_1M_1(G_2) + 12n_2F(G_1)M_1(G_2) + 12n_1F(G_2)M_1(G_1) \\ &-12n_2^2m_2F(G_1) - 12n_1^2m_1F(G_2) - 12n_1n_2M_1(G_1)M_1(G_2). \end{aligned}$$

And since $|E(G_1 \oplus G_2)| = m_1{n_2}^2 + m_2{n_1}^2 - 4m_1m_2, \quad |V(G_1 \oplus G_2)| = n_1n_2$ given in Lemma 1. Then

$$\begin{aligned} F(\overline{G_1 \oplus G_2}) &= |V(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^3 - 6|E(G_1 \oplus G_2)|(|V(G_1 \oplus G_2)| - 1)^2 \\ &+3(|V(G_1 \oplus G_2)| - 1)M_1(G_1 \oplus G_2) - F(G_1 \oplus G_2) \\ &= n_1n_2(n_1n_2-1)^3 - 6[m_1{n_2}^2 + m_2{n_1}^2 - 4m_1m_2](n_1n_2-1)^2 \\ &+3(n_1n_2-1)\big[[n_2^3 - 8n_2m_2]M_1(G_1) + [n_1^3 - 8n_1m_1]M_1(G_2) \\ &+8n_1n_2m_1m_2 + 4M_1(G_1)M_1(G_2)\big] - \big[n_2^4F(G_1) + n_1^4F(G_2) \\ &-8F(G_1)F(G_2) + 6n_1n_2^2m_2M_1(G_1) + 6n_2n_1^2m_1M_1(G_2) \\ &+12n_2F(G_1)M_1(G_2) + 12n_1F(G_2)M_1(G_1) - 12n_2^2m_2F(G_1) \\ &-12n_1^2m_1F(G_2) - 12n_1n_2M_1(G_1)M_1(G_2)\big]. \end{aligned}$$

□

4. Application

In this section, the forgotten index have been investigated for complement titania TiO_2 nanotubes and molecular graph of nanotorus.

Corollary 1. *The forgotten index of complement $TiO_2[n,m]$ nanotube Figure 1 is given by*

$$\begin{aligned} F(\overline{TiO_2[n,m]}) &= (6mn+6n)(6mn+6n-1)^3 - 4(10mn+8n)(6mn+6n-1)^2 \\ &+3(6mn+6n-1)(76mn+48n) - 320mn - 160n. \end{aligned}$$

Proof. By Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 4m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $F(TiO_2[n,m]) = 320mn + 160n$, and $M_1(TiO_2[n,m]) = 76mn + 48n$ given in [16]. In [17] the partitions of the vertex set and edge set $\sum |V(TiO_2[n,m])| = 6mn + 6n, \sum |E(TiO_2[n,m])| = 10mn + 8n$ of titania nanotubes. Then

$$\begin{aligned} F(\overline{TiO_2[n,m]}) &= \sum |V(TiO_2[n,m])|(\sum |V(TiO_2[n,m])| - 1)^3 - 4\sum |E(TiO_2[n,m])|(\sum |V(TiO_2[n,m])| - 1)^2 \\ &+3(\sum |V(TiO_2[n,m])| - 1)M_1(TiO_2[n,m]) - F(TiO_2[n,m]) \\ &= (6mn+6n)(6mn+6n-1)^3 - 4(10mn+8n)(6mn+6n-1)^2 \\ &+3(6mn+6n-1)(76mn+48n) - 320mn - 160n. \end{aligned}$$

□

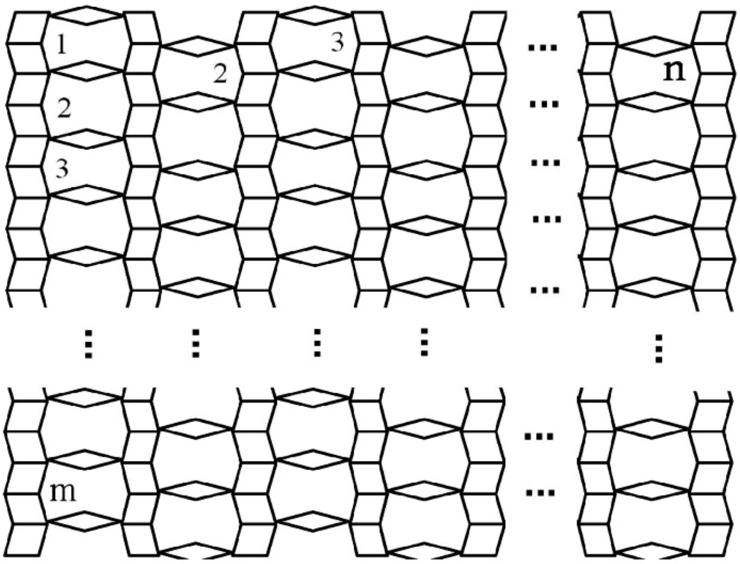

Figure 1. 2-Dimensional Lattice of molecular graph of $TiO_2[n,m]$ nanotube ($n, m \in \mathbb{N}$).

Corollary 2. *Let $T = T[p,q]$ be the molecular graph of a nanotorus such that $|V(T)| = pq$, $|E(T)| = \frac{3}{2}pq$, Figure 2. Then*

a. $F(\overline{T[p,q]}) = pq[(pq-1)^2(pq-7) + 27(pq-1) - 27]$.
b. $F(P_n \times T) = pq[125n - 122]$.
c. $F(\overline{P_n \times T}) = pq[(npq-1)^2(n^2pq - 11n + 4) + 3(npq-1)(25n-18) - 125n + 122]$.

Proof. a. By Proposition 1, we have $F(\overline{G}) = n(n-1)^3 - 4m(n-1)^2 + 3(n-1)M_1(G) - F(G)$, and since $M_1(T) = 9pq$ given in [14]. and $F(T) = 27pq$ given in [18]. Then

$$\begin{aligned}
F(\overline{T[p,q]}) &= |V(T)|(|V(T)|-1)^3 - 4|E(T)|(|V(T)|-1)^2 + 3(|V(T)|-1)M_1(T) - F(T) \\
&= pq(pq-1)^3 - 6pq(pq-1)^2 + 27pq(pq-1) - 27pq \\
&= pq[(pq-1)^2(pq-7) + 27(pq-1) - 27].
\end{aligned}$$

b. By $F(G_1 \times G_2) = n_2F(G_1) + n_1F(G_2) + 6m_2M_1(G_1) + 6m_1M_1(G_2)$, given in [6]. and since $M_1(P_n) = 4n-6$, $M_1(T) = 9pq$ given in [14]. and $F(P_n) = 8n-14$, $F(T) = 27pq$ given in [18]. Then

$$\begin{aligned}
F(P_n \times T) &= |V(T)|F(P_n) + |V(P_n)|F(T) + 6|E(T)|M_1(P_n) + 6|E(P_n)|M_1(T) \\
&= 2pq(4n-7) + 27npq + 18pq(2n-3) + 54pq(n-1) \\
&= pq[125n - 122].
\end{aligned}$$

c. By [19], $M_1(P_n \times T) = pq(25n-18)$, and by using Lemma 1, $|E(P_n \times T)| = pq(\frac{5}{2}n - 1)$, $|V(P_n \times T)| = npq$, and applying Proposition 1 and item (b) we get

$$\begin{aligned}
F(\overline{P_n \times T}) &= |V(P_n \times T)|(|V(P_n \times T)|-1)^3 - 4|E(P_n \times T)|(|V(P_n \times T)|-1)^2 \\
&\quad +3(|V(P_n \times T)|-1)M_1(P_n \times T) - F(P_n \times T) \\
&= npq(npq-1)^3 - 4pq(\frac{5}{2}n-1)(npq-1)^2 \\
&\quad +3pq(npq-1)(25n-18) - pq[125n-122] \\
&= pq[(npq-1)^2(n^2pq - 11n + 4) + 3(npq-1)(25n-18) - 125n + 122].
\end{aligned}$$

□

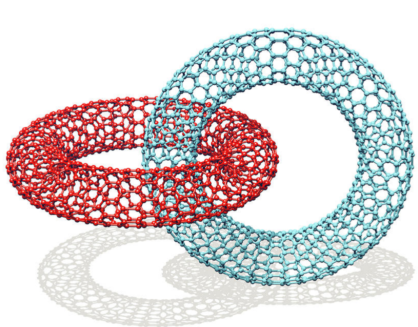

Figure 2. Molecular graph of a nanotorus

5. Conclusion

The forgotten index one of the most important topological indices which preserve the symmetry of molecular structures and provide a mathematical formulation to predict their physical and chemical properties. In this article, we computed the forgotten index of some basic mathematical operations and obtained explicit formula for their values under complement graph operations, and we computed the forgotten index of molecular complement graph of nanotorus and titania nanotubes $TiO_2[n,m]$.

Author Contributions: All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

Conflicts of Interest: "The authors declare no conflict of interest."

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