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ON CERTAIN TOPOLOGICAL INDICES OF NANOSTRUCTURES USING $Q(G)$ AND $R(G)$ OPERATORS

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Abstract. The invention of new nanostructures gives a key measurement to industry, electronics, pharmaceutical and biological therapeutics. By considering the importance of this key point, in here we compute the 2*D-lattice*, *nanotube* and *nanotorus* of $TUC_4C_8[p,q]$ over the graphs $Q(G)$ and $R(G)$ in terms of certain topological indices, namely first, second and third Zagreb indices, hyper Zagreb index and forgotten topological index. These indices are numerical propensity that often characterizes the quantitative structural activity/property/toxicity relationships, and also correlates physico-chemical properties such as boiling point, melting point and stability of respective nanostructures.

1. Introduction and Preliminaries

In the fields of chemical graph theory, molecular topology and mathematical chemistry, a *topological index* is actually a molecular graph invariant which making matches the physio-chemical properties of a molecular graph with a number. Furthermore, in some cases, a topological index known as a *connectivity index* which is a type of a molecular descriptor and is calculated based on the molecular graph of a chemical compound. A large amount of chemical experiments require a determination of the chemical properties of new compounds.

If we enumerate all octagons of $TUC_4C_8[p,q]$ (any cycle C_8) and all quadrangles (any cycle C_4), where p and q denotes number of octagons in a fixed row and column, respectively, of a 2-dimensional lattice (see Figure 1-(a)), then

- the *nanotube* is obtained from the lattice by wrapping it up so that each dangling edge from the left-hand side connects to the right most vertex of the same row (see Figure 1-(b)), or

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- the *nanotorus* is obtained from again the lattice by wrapping it up so that each dangling edge from the left-hand side connects to the right most vertex of the same row and each dangling edge from up side connects to the down most vertex of the same row (see Figure 1-(c)).

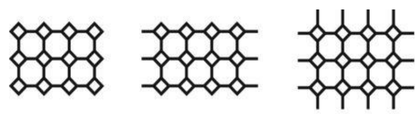

FIGURE 1. (a) $2D$-lattice of $TUC_4C_8[p,q]$; (b) nanotubes of $TUC_4C_8[p,q]$; (c) nanotores of $TUC_4C_8[p,q]$.

Recently, in [10], Hosamani has been computed the topological properties of the line graphs of subdivision graphs of certain nanostructures-II, and also obtained upper bounds for Wiener index of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. In [14], V. Lokesha et al. established on model graph structure of Alveoli in human lungs in terms of graph operators such as subdivision, double graph, $Q(G)$ and $R(G)$ of certain topological indices. In the same reference, by using $Q(G)$ and $R(G)$, the authors also exhibited the relation between indices. At this point let us remind the graph operators $Q(G)$ and $R(G)$ which are directly related to the main aim of this paper.

- The $Q(G)$ graph is obtained from G by inserting a new vertex into each edge of G and by joining edges those pairs of new vertices which lie on adjacent edges of G.
- The $R(G)$ graph is obtained from G by adding a new vertex corresponding to every edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.

We note that the first and third authors of this paper utilized these above graph operators previously (cf. [14, 19]). On the other hand, Diudea et al. considered the problem of computing topological indices of some chemical graphs related to nanostructurer in joint works (cf. [3, 4, 12]). In addition to these above studies, Ashrafi et al. computed some topological indices of nanotubes in [1, 2], and Nadeem et al. ([16]) obtained the expressions for certain topological indices for the line graph of subdivision graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. Moreover, Lokesha et al. in [15] studied on nanostructurer in terms of SDD, ABC_4 and GA_5 indices.

Motivated from the above references, in here we aimed to compute the first, second and third Zagreb indices, the hyper Zagreb index and the forgotten topological index of $Q(G)$ and $R(G)$ graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. To reach the aim, let us recall the following topological indices that will be needed in our results:

The *first* and *second Zagreb indices* were introduced more than thirty years ago by I. Gutman and Trinajstic [8] which are defined as

$$\left.\begin{aligned} M_1(G) &= \sum_{e=uv\in E(G)} [d_G(u)+d_G(v)] \\ \text{and} \qquad & \\ M_2(G) &= \sum_{e=uv\in E(G)} d_G(u).d_G(v) \end{aligned}\right\}, \tag{1.1}$$

where $d_G(u)$ denotes the degree of a vertex u in G. We may refer [9, 11, 13, 17, 18, 20] for more detailed works on Zagreb indices. On the other hand, the *third Zagreb index*

$$M_3(G) = \sum_{e=uv\in E(G)} |d_G(u) - d_G(v)| \tag{1.2}$$

was introduced by Fath-Tabar in [5]. Although this modified version of Zagreb indices has been taken interest since 2011, another modified version, namely the *hyper-Zagreb index* (cf. [21]) had to be created depending on the importance of these indices. The hyper-Zagreb index is defined as

$$HM(G) = \sum_{e=uv\in E(G)} [d_G(u)+d_G(v)]^2 . \tag{1.3}$$

Unfortunately another the degree based graph invariant has not attracted any attention in the literature of mathematical chemistry for more than forty years. In view of this fact, B. Furtula et al. ([6, 7]) named it as *forgotten (topological) index* in 2015 and defined it as

$$F(G) = \sum_{e=uv\in E(G)} [d_G(u)^2 + d_G(v)^2] . \tag{1.4}$$

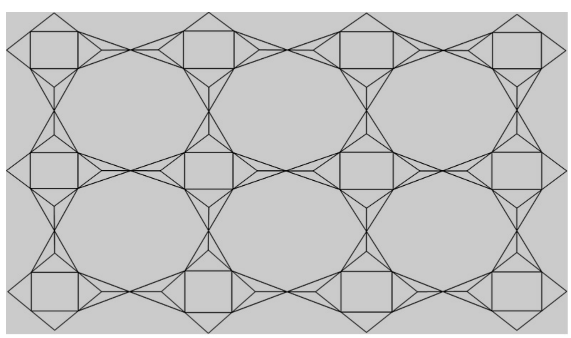

FIGURE 2. $Q(G)$ of 2D-lattice of $TUC_4C_8[p,q]$.

Forthcoming two sections, we shall give the results on the topological indices (indicated in (1.1), (1.2), (1.3) and (1.4)) of the graphs $Q(G)$ and $R(G)$ for $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, respectively.

2. The case on $Q(G)$

In this section, by considering Equations (1.1)-(1.4) and the operator $Q(G)$, we discuss the results on $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

Theorem 1. *Let H be the $Q(G)$ of 2D-lattice of $TUC_4C_8[p,q]$ (see Figure 2). Then*

$$\begin{aligned} M_1(H) &= 4(p+q)\,[11(q-1)+15]+9q^2(q-6)+18p(6q-5)+9(q+2)+ \\ & 18q(5-q)+10pq(q-5)+20(4p+q)+44(p-q)+ \\ & (q-2)[8(q-3)-11(2p+q-1)(q-1)]-188\,, \\ M_2(H) &= 18q^2(q-6)+36p(6q-5)+18(q+2)+40q(5-q)+25pq(q-5)+ \\ & 50(4p+q)+120(p-q)+100(p+q)+16(q-2)(q-3)+ \\ & (q-1)[12(p+q)-30(2p+q-1)(q-2)+36q(5p-6)- \\ & 36(q-2)((p-1)(p-2)+5)]-416 \end{aligned}$$

and

$$\begin{aligned} M_3(H) &= 4(p+q)[(q-1)+5]+3q^2(q-6)+6p(6q-5)+3(q+2)+ \\ & 2q(5-q)+4(p-q)-(2p+q-1)(q-1)(q-2)-28\,, \\ HM(H) &= 4(p+q)[121(q-1)+113]+81q^2(q-6)+162p(6q-5)+ \\ & 81(q+2)+64(q-2)(q-3)+162q(5-q)+100pq(q-5)+ \\ & 200(4p+q)+484(p-q)+144q(q-1)(5p-6)- \\ & (q-1)(q-2)[121(2p+q-1)+(p-1)(p-2)+5]-1740\,, \\ F(H) &= 90p(6q-5)+45(q+2)+32(q-2)(q-3)+82q(5-q)+ \\ & 50pq(q-5)+45q^2(q-6)+100(4p+q)+244(p-q)+ \\ & 252(p+q)+(q-1)[244(p+q)-61(2p+q-1)(q-2)+ \\ & 72q(5p-6)-72(q-2)((p-1)(p-2)+5)]-908. \end{aligned}$$

Proof. For the graph H, there are $p^2(3q-q^2-2)+q^2(7p-12)+3q(p+10)+8p-24$ number of edges. Among these number of edges;

8 edges are of the type $(2,4)$,
$4[(p+q)-2]$ edges are of type $(2,5)$,
$4[(p+q)-2]$ edges are of the type $(3,5)$,
$[q(q^2-6q+12p+1)-10p+2]$ edges are of type $(3,6)$,
(q^2-5q+6) edges are of the type $(4,4)$,
$[2q(5-q)-4]$ edges are of the type $(4,5)$,
$[pq^2-5pq+2(4p+q-4)]$ edges are of the type $(5,5)$,
$(q(8q-q^2-13)+2p(5q-q^2-2)+2)$ edges are of the type $(5,6)$, and
$[pq(8q-14-pq+3p)+q(27-13q)+2p(3-p)-14]$ edges are of the type $(6,6)$.

Now, by taking into account of edge partition and then applying Equations (1.1)-(1.4) to H, we obtain the required results. □

Theorem 2. *Let S be the $Q(G)$ of nanotubes of $TUC_4C_8[p,q]$ (see Figure 3). Then*

$$\begin{aligned} M_1(S) &= 68p+12q+16pq(5-q)-32(2p-1)+44(p-1)+ \\ &\quad (q-1)[9(16p-pq+q-2)+10p(q-4)-22p(q-4)+ \\ &\quad 12(8p+5q+q(p-q)-10)]. \\ M_2(S) &= 140p+18q+30pq(5-q)-60(2p-1)+120(p-1)+ \\ &\quad (q-1)[18(16p-pq+q-2)+25p(q-4)-60p(q-4)+ \\ &\quad 36(8p+5q+q(p-q)-10)]. \end{aligned}$$

and

$$\begin{aligned} M_3(S) &= 12p+4pq(5-q)-8(2q-1)+4(p-1)+ \\ &\quad (q-1)[3(16p-pq+q-2)-2p(q-4)]. \\ HM(S) &= 596p+72q+128pq(5-q)-256(2p-1)+484(p-1)+ \\ &\quad (q-1)[81(16p-pq+q-2)-142p(q-4)+ \\ &\quad 144(8p+5q+q(p-q)-10)]. \\ F(S) &= 316p+36q+68pq(5-q)-136(2p-1)+244(p-1)+ \\ &\quad (q-1)[45(16p-pq+q-2)-72p(q-4)+ \\ &\quad 72(8p+5q+q(p-q)-10)]. \end{aligned}$$

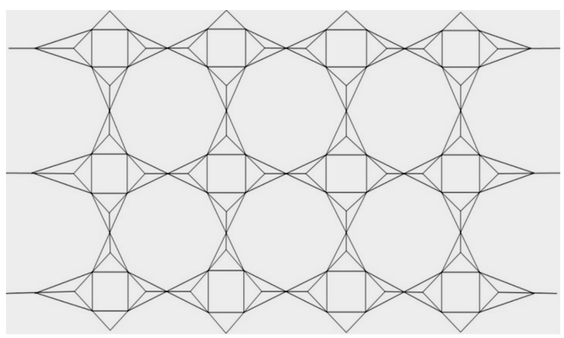

FIGURE 3. $Q(G)$ of nanotube of $TUC_4C_8[p,q]$.

Proof. For the graph S, we have total $[3pq(13-q)+q(7q-q^2-16)-24p+12]$ number of edges. From Figure 3, it can be observed that there are seven partition of those edges such that

$(2,5)$ having $4p$ edges,
$(3,3)$ are of $2q$ edges,
$(3,5)$ are of $[2pq(5-q)-4(2p-1)]$ edges,
$(3,6)$ are of $[17pq-(16p+3q)+q^2(1-p)+2]$ edges,
$(5,5)$ are of $[8p-5pq+pq^2]$ edges,
$(5,6)$ are of $[2(5pq-pq^2-2p-2)]$ edges, and

$(6,6)$ are of $[q(6q-15-q^2)+p(7q+q^2-8)+10]$ edges.
Similarly as in the proof of Theorem 1, by considering the edge partition and also applying Equations (1.1)-(1.4) to S, we get the results. □

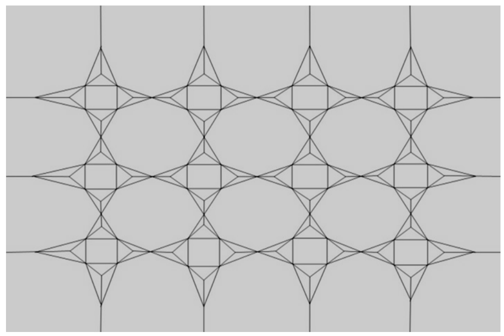

FIGURE 4. $Q(G)$ of nanotorus of $TUC_4C_8[p,q]$.

Theorem 3. *Let K be the $Q(G)$ of nanotorus of $TUC_4C_8[p,q]$ (see Figure 4). Then*

$$M_1(K)=252pq-18(p+q)\,,\qquad M_2(K)=648pq-90(p+q)\,,$$
$$M_3(K)=6(p+q+6pq)\,,\qquad HM(K)=2700pq-342(p+q)\,,$$
$$F(K)=1404pq-162(p+q)\,.$$

Proof. The graph K has $24pq$ number of edges from Figure 4. The partitions of edges are of $(3,3)$, $(3,6)$ and $(6,6)$ having $2(p+q)$, $2(p+q+6pq)$ and $4(3pq-p-q)$ edges, respectively. Similarly as in the final parts of the proofs of Theorems 1 and 2, we obtain the results. □

3. THE CASE ON $R(G)$

With a quite parallel approximation as in Section 2, by considering Equations (1.1)-(1.4) and the operator $R(G)$, we shall present the results on $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

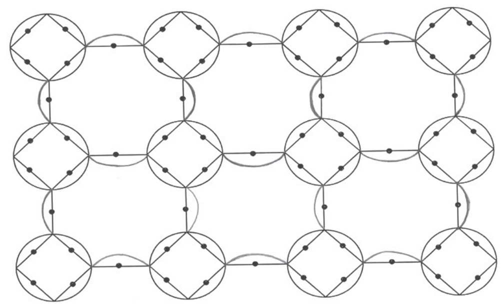

FIGURE 5. $R(G)$ of 2D-lattice of $TUC_4C_8[p,q]$.

Theorem 4. *Let H_1 be the $R(G)$ of 2D-lattice of $TUC_4C_8[p,q]$ (see Figure 5). Then we have the following equations:*

$$\begin{aligned}
M_1(H_1) &= 48(p-q) - 36(p+q) + 40(p+q-2) + \\
&\quad 8pq[9 - 2(q-1)(q-5)] + 80\,, \\
M_2(H_1) &= 72(p-q) - 148(p+q) + 96(p+q-2) + \\
&\quad 24pq[9 - (q-1)(q-5)] + 208\,, \\
M_3(H_1) &= 8(p+q) + 24(p-q) - 8pq(q-1)(q-5) + 8(p+q-2)\,, \\
HM(H_1) &= 384(p-q) + 400(p+q-2) - 576(p+q) + \\
&\quad 16pq[54 - 8(q-1)(q-5)] + 832\,, \\
F(H_1) &= 208(p+q-2) + 16pq[27 - 5(q-1)(q-5)] - 208(p+q) + \\
&\quad 240(p-q) + 416\,.
\end{aligned}$$

Proof. The total number of edges for the graph H_1 is $3(3p-q)+2pq[3-(q-1)(q-5)]$. Among these number of edges, there are

$4(p+q)$ edges are of type $(2,4)$,
$6(p-q) - 2pq(q-1)(q-5)$ edges are of the type $(2,6)$,
4 edges are of type $(4,4)$,
$4(p+q-2)$ edges are of the type $(4,6)$, and
$6pq - 5(p+q) + 4$ edges are of the type $(6,6)$.

As in the proof of Theorem 1, by taking into account of edge partition and then applying Equations (1.1)-(1.4) to H_1, we reached the results as required. □

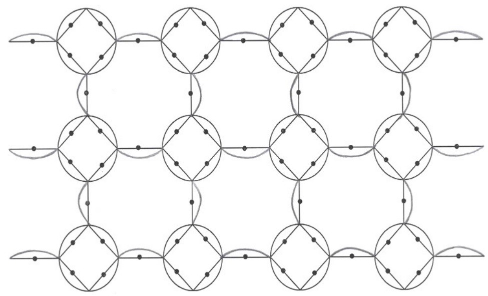

FIGURE 6. $R(G)$ of nanotube of $TUC_4C_8[p,q]$.

Theorem 5. *Let S_1 be the $R(G)$ of nanotubes of $TUC_4C_8[p,q]$ (see Figure 6). Therefore the following bounds are eligible.*

$$\begin{aligned} M_1(S_1) &= 64p + 8[6p(2q-1)+2q] + 12(6pq - 5p + q)\,, \\ M_2(S_1) &= 36(6pq-5p+q) + 128p + 12[6p(2q-1)+2q]\,, \\ M_3(S_1) &= 4[6p(2q-1)+2q] + 16p\,, \\ HM(S_1) &= 544p + 384p(2q-1) + 144(6pq-5p) + 272q\,, \\ F(S_1) &= 40[6p(2q-1)+2q] + 72(6pq+q) - 72p\,. \end{aligned}$$

Proof. By Figure 6, it is easy to observe that the total number of edges for the graph S_1 is $3[q(6p+1)-p]$. It can be also observed that there are four partition of edges such that

$(2,4)$ having $4p$ edges,

$(2,6)$ are of $6p(2q-1)+2q$ edges,

$(4,6)$ are of $4p$ edges and $(6,6)$ are of $6pq-5p+q$ edges.

With a completely same idea as in the final parts of the proofs of previous theorems, the result follows. □

Theorem 6. *Let K_1 be the $R(G)$ of nanotorus of $TUC_4C_8[p,q]$ (see Figure 7). Then*

$$M_1(K_1) = 28(p+q) + 168pq\,, \quad M_2(K_1) = 60(p+q) + 360pq\,,$$

$$M_3(K_1) = 8(p+q) + 48pq\,, \qquad HM(K_1) = 272(p+q) + 1632pq\,,$$

$$F(K_1) = 152(p+q) + 912pq\,.$$

Proof. By Figure 7, the graph K_1 has $3p+3q+18pq$ number of edges. In here, the partitions of edges are of $(2,6)$ and $(6,6)$ having $2(p+q+6pq)$ and $p+q+6pq$ edges, respectively. Now, by considering the edge partition and then applying Equations (1.1)-(1.4) to K_1, the correctness of the theorem is shown. □

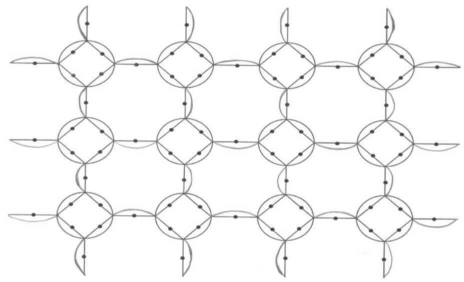

FIGURE 7. $R(G)$ of nanotorus of $TUC_4C_8[p,q]$.

Conclusion 1. *In this paper, we computed the nanostructures through degree-based topological indices over* $TUC_4C_8[p,q]$. *The topological indices calculated in here can help us to understand the physical features, chemical reactivity, and biological activities of these structures. From this view point, topological indices in graph theory can be regarded as a score function that maps each molecular structure to a real number, and are used as descriptors of the molecular under testing.*

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