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SK INDICES, FORGOTTEN TOPOLOGICAL INDICES AND HYPER ZAGREB INDEX OF Q OPERATOR OF CARBON NANOCONE

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Abstract. Carbon nanocones are conical structures made from carbon and they have one dimension of order one micrometer. The physical features of these structures can be easily understood by exploiting topological indices. In this article we established SK, F, S and Hyper Zagreb index of carbon nanocones using $Q(G)$ operator.

Keywords: Carbon nanocones, Topological indices, $Q(G)$ operator, SK indices, Forgotten topological index, Hyper zagreb index, Sum connectivity index.

AMS Subject Classification: 05C90; 05C35; 05C12

1. Introduction

Molecular graphs are a peculiar type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a molecule is represented in a two-dimensional basis, it is called structural graph [[1], [14]]. All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Topological indices are the mathematical measures which correspond to the structure of any simple finite graph. They are invariant under the graph isomorphism. The significance of topological indices is usually associated with QSPR and QSAR [[8], [10]].

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Here $d_G(u)$ represents the degree of the vertex u. The operator $Q(G)$ is the graph obtained from G by inserting a new vertex into each edge of G and by joining edges to new vertices which lie on adjacent edges of G.

Carbon nanocones have been observed since 1968 or even earlier, on the surface of naturally occurring Graphite. Their bases are attached to the graphite and their height varies between 1 and 40 micrometers. Their walls are often curved and are less regular than

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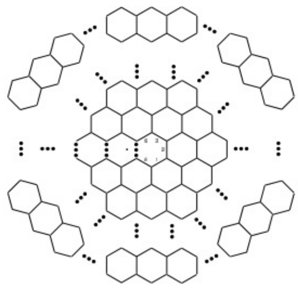

Figure 1: $CNC_k[n]$

those of the laboratory made nanocones. Carbon nanostructures have attached considerable attention due to their potential use in many applications including energy storage, gas sensors, biosensors, nano electronic device and chemical probes. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices. More recently, carbon nanocones have gained increased scientific interest due to their unique properties and promising uses in many novel applications such as energy and gas storage [6].

In [7] Yuhong Huo et. al proposed topological indices ABC_4 and GA_5 based on the degree of vertices of line graph of $CNC_k[n]$ nanocones.

In [9] M. Faisal Nadeem et. al proposed R_α, M_α, χ_α, ABC, GA, ABC_4 and GA_5 indices of $L(S(CNC_k(n)))$.

This paper is motivated from Yuhong Huo, M. F. Nadeem and their co-workers. Here we deal with the SK indices, Forgotten topological indices, Hyper zagreb index and Sum connectivity index of carbon nanocones by using operator $Q(G)$.
The graphical structure of $CNC_k[n]$ nanocones have a cycle of k-length at its central part and n-levels of hexagons positioned at the conical exterior around its central part. The graph of $CNC_k[n]$ has $\frac{k(n+1)(3n+2)}{2}$ edges and $k(n+1)^2$ vertices and is shown in $Figure 1$.

Table 1

The edge partition of Carbon Nanocone $Q[CNC_k[n]]$ based on degree of end vertices $k \geq 3$, $n = 1, 2, 3, ...,$

(d_u, d_v) where $uv \in E(G)$	(2,4)	(2,5)	(3,5)	(3,6)	(4,5)	(5,5)	(5,6)	(6,6)
Number of edges	$2k$	$2kn$	$2kn$	$kn(3n+1)$	$2k$	$k(2n-1)$	$2kn$	$3kn^2$

In [11] V. S. Shegehalli and R. Kanabur introduced new degree based topological indices (SK indices) as follows;

$$SK(G) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_G(u) d_G(v)}{2}.$$

$$SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2.$$

In [2] Furtula and Gutman introduced Forgotten topological index and established its some basic properties. This index is defined as

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

In [16] B. Zhou and N. Trinajstic et. al developed Sum Connectivity index. The Sum Connectivity index is defined as

$$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}.$$

In [13] G. H. Shirdel and H. Rezapour et. al introduced Hyper-zagreb index. The Hyper zagreb index is defined as follows

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

The paper is organized as follows: Starts with an preliminaries which are essential for development of the main results. In coming section established the Q-operator on nanocones general form of SK indices, Forgotten topological index, Sum connectivity index and Hyper Zagreb index. Finally conclusions and appropriated references are appended.

2. Main Results

In this section, we established Q-operator on $CNC_k[n]$ with different topological indices.

Theorem 2.1. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, ...$ Then*

$$SK[G] = \frac{k}{2}\left[9(7n^2 + 9) + 5\right].$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1 + n(3 + 2n)]$ edges. Graph G, have 8-types of edges, which are shown in Table 1. Utilizing table values to $SK(G)$ we obtain □

Theorem 2.2. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, ...$ Then*

$$SK_1[G] = \frac{1}{2}\left[2k[n[89 + 81n]] + 31\right].$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1 + n(3 + 2n)]$ edges. Graph G, have 8-types of edges, which are shown in Table 1. Utilizing table values to $SK_1[G]$ we obtain

$$SK_1[G] = 2k\left[\frac{2.4}{2}\right] + 2kn\left[\frac{2.5}{2}\right] + 2kn\left[\frac{3.5}{2}\right] + kn(3n+1)\left[\frac{3.6}{2}\right] + 2k\left[\frac{4.5}{2}\right] + k(2n-1)k\left[\frac{5.5}{2}\right]$$
$$+ 2kn\left[\frac{5.6}{2}\right] + 3kn^2\left[\frac{6.6}{2}\right].$$

$$= \frac{1}{2}\left[2k[n[89+81n]]+31\right].$$

□

Theorem 2.3. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$SK_2[G] = \frac{k}{2}\left[n(847+675n)+134\right].$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1+n(3+2n)]$ edges. Graph G, have 8-types of edges, which are shown in Table 1. Utilizing table values to $SK_2[G]$ we obtain

$$SK_2[G] = 2k\left[\frac{2+4}{2}\right]^2 + 2kn\left[\frac{2+5}{2}\right]^2 + 2kn\left[\frac{3+5}{2}\right]^2 + kn(3n+1)\left[\frac{3+6}{2}\right]^2$$
$$+2k\left[\frac{4+5}{2}\right]^2 + k(2n-1)k\left[\frac{5+5}{2}\right]^2 + 2kn\left[\frac{5+6}{2}\right] + 3kn^2\left[\frac{6+6}{2}\right]^2.$$

$$= \frac{k}{2}\left[n(847+675n)+134\right].$$

□

Theorem 2.4. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$F[G] = k(kn(351n+393)+72).$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1+n(3+2n)]$ edges. Graph G, have 8-types of edges, which are shown in Table 1. Utilizing table values to $F(G)$ we obtain

$$F(G) = 2k(2^2+4^2)+2kn(2^2+5^2)+2kn(3^2+5^2)+kn(3n+1)(3^2+6^2)+2k(4^2+5^2)+k(2n-1)(5^2+5^2)$$
$$+2kn(5^2+6^2)+3kn^2(6^2+6^2).$$
$$= k(kn(351n+393)+72).$$

□

Theorem 2.5. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$S[G] = k\left[n\left[n\left(\frac{2\sqrt{3}+3}{2\sqrt{3}}\right) + \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{2}} + \frac{1}{3} + \frac{2}{\sqrt{10}} + \frac{2}{\sqrt{11}}\right]\right.$$
$$\left. + \frac{2}{\sqrt{6}} - \frac{1}{\sqrt{10}} + \frac{2}{3}\right].$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1+n(3+2n)]$edges. Graph G, have 8-types of edges, which are shown in Table 1. Utilizing table values to $S[G]$ we obtain

$$S[G] = 2k\frac{1}{\sqrt{2+4}}+2kn\frac{1}{\sqrt{2+5}}+2kn\frac{1}{\sqrt{3+5}}+kn(3n+1)\frac{1}{\sqrt{3+6}}+2k\frac{1}{\sqrt{4+5}}+k(2n-1)\frac{1}{\sqrt{5+5}}$$
$$+2kn\frac{1}{\sqrt{5+6}}+3kn^2\frac{1}{\sqrt{6+6}}.$$
$$= k\left[n\left[n\left(\frac{2\sqrt{3}+3}{2\sqrt{3}}\right)+\frac{2}{\sqrt{5}}+\frac{1}{\sqrt{2}}+\frac{1}{3}+\frac{2}{\sqrt{10}}+\frac{2}{\sqrt{11}}\right]+\frac{2}{\sqrt{6}}-\frac{1}{\sqrt{10}}+\frac{2}{3}\right].$$

□

Theorem 2.6. *Let G be a graph of $Q[CNC_k[n]]$ nanocones for $k \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$HM[G] = k[675n^2 + 749n + 134].$$

Proof. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ vertices and $3k[1+n(3+2n)]$ edges. Graph G, have 8-types of edges, which are shown in Table 1. Now Utilizing table values to $HM[G]$ we obtain

$$HM[G] = 2k(2+4)^2+2kn(2+5)^2+2kn(3+5)^2+kn(3n+1)(3+6)^2+2k(4+5)^2+k(2n-1)(5+5)^2$$
$$+2kn(5+6)^2+3kn^2(6+6)^2.$$
$$= k[675n^2 + 749n + 134].$$

□

3. CONCLUSIONS

Chemical graph theory is an important tool for studying molecular structure and has an important effect on the development of chemical sciences. The study of topological indices is one of the most active research fields in chemical graph theory. We have presented here some theoretical results on the SK indices, Forgotten topological index, Sum connectivity index and Hyper zagreb index of Carbon Nanocones by using Q operator for carbon nanocones. These formulae make it possible to correlate the chemical structure of nanostructures with a large amount of information about their physical features.

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