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Some computational aspects of carbon nanocone using $Q(G)$ operator, hexagonal network and probabilistic neural network

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ABSTRACT. In this article, we first find closed forms of M-polynomials of carbon nanocones using $Q(G)$ operator, hexagonal networks and probabilistic neural network. We also reckon closed forms of various degree-based topological indices of these structures. These indices are numerical tendencies that generally interprit quantitative structural activity/property/toxicity relationships and correlate certain physico-chemical properties, such as boiling point, stability, and strain energy, of respective nanomaterial.

1. INTRODUCTION

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 those of the laboratory made nanocones. 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 [9].

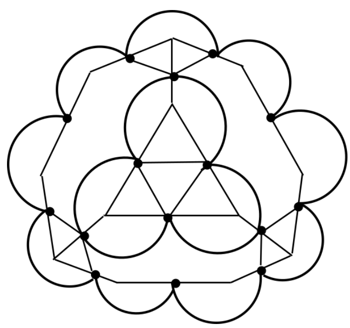

FIGURE 1. Graph of $Q[CNC_3[1]]$.

In hexagonal network there exist three regular plane tilings with composition of same kind of regular polygons such as triangular, hexagonal and square. In the construction of hexagonal networks, triangular tiling is used as shown in FIGURE 2. A hexagonal network of dimension n is usually denoted as HX_n, where n is the number of vertices on each side of hexagon.

A neural network is a computer system modelled on the nerve tissue and nervous system. Recently, these networks are applied in chemical and environmental sciences [16].

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Mainly, the probabilistic neural networks are used in biochemical field for the toxicological and metabolic responses [10]. For more details about the construction of probabilistic neural network we refer the reader to [11].

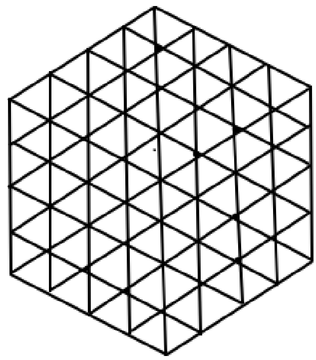

FIGURE 2. Graph of HX_5

In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges, respectively. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there is a connection between any pair of vertices in G. The degree d_u of a vertex u is the number of edges that are incident to it. 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.

The aim of this paper is to compute the zagreb indices, generalized randic index, inverse randic index and SDD index, M-polynomials of carbon nanocones using $Q(G)$ operator, hexagonal networks and probabilistic neural network.

Definition 1.1. M-polynomial of graph G is defined as

$$M(G, x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j$$

where $m_{ij}(G)$, $(i, j \geq 1)$ be the number of edges $e = uv$ of G such that $(d_u, d_v) = (i, j)$.

The Wiener index is originally the first and most studied topological index. The Randić index, [15] denoted by $R_{\frac{1}{2}}(G)$ and introduced by Milan Randić in 1975, is also one of the oldest topological indices. The general Randić index is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}.$$

Gutman and Trinajstić [3, 4] introduced first Zagreb index and second Zagreb index, which are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v$$

respectively. Both the first Zagreb index and the second Zagreb index give greater weights to the inner vertices and edges, and smaller weights to the outer vertices and edges, which opposes intuitive reasoning. For a simple connected graph G, the second modified Zagreb index [18] is defined as

$$^{m}M_2(G) = \sum_{uv\in E(G)} \{\frac{1}{d_u d_v}\}.$$

Symmetric division deg index is one of the discrete Adriatic indices, [5,6,12,17]. It is a good predictor of total surface area for polychlorobiphenyls and is defined as

$$SDD(G) = \sum_{uv\in E(G)} \left\{\frac{d_u^2 + d_v^2}{d_u d_v}\right\}.$$

The figuration of the probabilistic neural network have three layers of nodes.

- The first layer has a certain number of nodes also known as input layer, the hidden layer or second layer subsist certain number of classes such that each class contains a particular number of nodes, and the third layer called by output layer has a number of nodes equal to the number of classes of the second layer.
- The formation of a PNN, each node of the first/input layer is joined to all the nodes of each class of the second/hidden layer and all the nodes of each class of the hidden layer are joined to a particular node of the third/output layer.
- Consider p, k, q nodes are the input, hidden and output layers respectively. Thus, a probabilistic neural network symbolized by $PNN(p, k, q)$ such that

  $$|V(PNN(p, k, q))| = p + k(q + 1)$$

  and

  $$|E(PNN(p, k, q))| = kq(p + 1).$$

The following figure shows the probabilistic neural network $PNN(4, 2, 3)$.

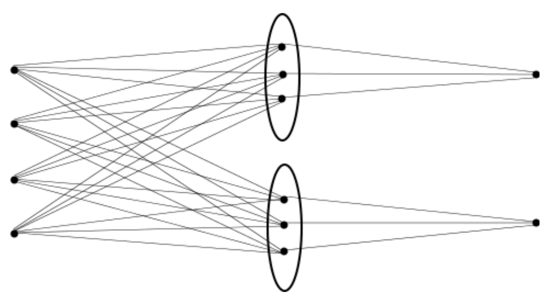

FIGURE 3. Graph of $PNN(4, 2, 3)$.

The following Table 1 relates some well-known degree-based topological indices with M-polynomials.

where $D_x = \frac{\partial(f(x,y))}{\partial x}$, $D_y = \frac{\partial(f(x,y))}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t} dt$ and $S_y = \int_0^y \frac{f(x,t)}{t} dt$.

This paper is organised as follows. Section 1 consists of a brief introduction which is essential for the development of main results. Section 2 will consist of the first zagreb, second zagreb, modified second zagreb indices, generalized randic, inverse randic indices and SDD index of M-polynomials of carbon nanocones using $Q(G)$ operator, hexagonal networks and probabilistic neural network. Finally, conclusions and appropriate references are appended.

TABLE 1. Derivation of some degree-based topological indices from M-polynomials.

Topological index	$f(x,y)$	Derivation from $M(G;x,y)$
First Zagreb	$x+y$	$(D_x+D_y)(M(G;x,y))\mid_{x=y=1}$
Second Zagreb	xy	$(D_xD_y)(M(G;x,y))\mid_{x=y=1}$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_xS_y)(M(G;x,y))\mid_{x=y=1}$
Randić	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\mid_{x=y=1}$
Generalized Randić	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\mid_{x=y=1}$
Symmetric Division Deg	$\frac{x^2+y^2}{xy}$	$(D_xS_y+S_xD_y)(M(G;x,y))\mid_{x=y=1}$

2. M-POLYNOMIALS OF CARBON NANOCONE USING $Q(G)$ OPERATOR, HEXAGONAL NETWORK AND PROBABILISTIC NEURAL NETWORK

In this section closed forms of M-polynomials of carbon nanocones using $Q(G)$ operator, hexagonal networks and probabilistic neural networks is calculated and closed forms of various degree-based topological indices of these structures is also computed.

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

$$\begin{aligned} M(G,x,y) &= 2kx^2y^4 + 2knx^2y^5 + 2knx^3y^5 + kn(3n+1)x^3y^6 + 2kx^4y^5 \\ &+ k(2n-1)x^5y^5 + 2knx^5y^6 + 3kn^2x^6y^6. \end{aligned}$$

Proof. Let G be the $Q[CNC_k[n]]$ where k is the length of cycle at its central part and n is the level of hexagons positioned at the conical exterior around its central part as shown in FIGURE 1. The graph G consists of $\frac{k(n+1)(5n+4)}{2}$ and $3k[1+n(3+2n)]$ edges. Graph G have 8 types of edges as folllows

$$\begin{aligned} E_{(2,4)} &= \{e = uv \in E(G) \mid d_u = 2, d_v = 4\} \rightarrow |E_{(2,4)}| = 2k \\ E_{(2,5)} &= \{e = uv \in E(G) \mid d_u = 2, d_v = 5\} \rightarrow |E_{(2,5)}| = 2kn \\ E_{(3,5)} &= \{e = uv \in E(G) \mid d_u = 3, d_v = 5\} \rightarrow |E_{(3,5)}| = 2kn \\ E_{(3,6)} &= \{e = uv \in E(G) \mid d_u = 3, d_v = 6\} \rightarrow |E_{(3,6)}| = kn(3n+1) \\ E_{(4,5)} &= \{e = uv \in E(G) \mid d_u = 4, d_v = 5\} \rightarrow |E_{(4,5)}| = 2k \\ E_{(5,5)} &= \{e = uv \in E(G) \mid d_u = 5, d_v = 5\} \rightarrow |E_{(5,5)}| = k(2n-1) \\ E_{(5,6)} &= \{e = uv \in E(G) \mid d_u = 5, d_v = 6\} \rightarrow |E_{(5,6)}| = 2kn \\ E_{(6,6)} &= \{e = uv \in E(G) \mid d_u = 6, d_v = 6\} \rightarrow |E_{(6,6)}| = 3kn^2 \end{aligned}$$

Thus, the M-polynomial of $Q[CNC_k(n)]$ is

$$\begin{aligned} M(G,x,y) &= \sum_{i\leq j} m_{ij}(G)x^iy^j \\ &= \sum_{2\leq 4} m_{24}(G)x^2y^4 + \sum_{2\leq 5} m_{25}(G)x^2y^5 + \sum_{3\leq 5} m_{35}(G)x^3y^5 \\ &+ \sum_{3\leq 6} m_{36}(G)x^3y^6 + \sum_{4\leq 5} m_{45}(G)x^4y^5 + \sum_{i=j=5} m_{55}(G)x^5y^5 \\ &+ \sum_{5\leq 6} m_{56}(G)x^5y^6 + \sum_{i=j=6} m_{66}(G)x^6y^6 \\ &= \mid E_{(2,4)} \mid x^2y^4 + \mid E_{(2,5)} \mid x^2y^5 + \mid E_{(3,5)} \mid x^3y^5 \\ &+ \mid E_{(3,6)} \mid x^3y^6 + \mid E_{(4,5)} \mid x^4y^5 + \mid E_{(5,5)} \mid x^5y^5 \end{aligned}$$

$$\begin{aligned} &+ \quad | E_{(5,6)} | x^5y^6 + | E_{(6,6)} | x^6y^6 \\ \therefore M(G,x,y) &= 2kx^2y^4 + 2knx^2y^5 + 2knx^3y^5 + kn(3n+1)x^3y^6 + 2kx^4y^5 \\ &+ k(2n-1)x^5y^5 + 2knx^5y^6 + 3kn^2x^6y^6. \end{aligned}$$

□

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

$$\begin{aligned} 1.\ M_1(G) &= 20k + 81kn + 63kn^2. \\ 2.\ M_2(G) &= k^2[91 + 3n[324n^3 + 828n^2 + 729n + 255]]. \\ 3.\ {}^mM_2(G) &= k^2\left[\frac{3}{2}n^4 + \frac{107}{20}n^3 + \frac{711}{100}n^2 + \frac{417}{100}n + \frac{91}{100}\right]. \\ 4.\ R_\alpha(G) &= [k^2[91 + 3n[324n^3 + 828n^2 + 729n + 255]]]^\alpha. \\ 5.\ R'_\alpha(G) &= \left[k^2\left[\frac{3}{2}n^4 + \frac{107}{20}n^3 + \frac{711}{100}n^2 + \frac{417}{100}n + \frac{91}{100}\right]\right]^\alpha. \\ 6.\ SDD(G) &= k^2\left[81n^4 + \frac{2517}{10}n^3 + \frac{2827}{10}n^2 + \frac{669}{5}n + \frac{109}{5}\right]. \end{aligned}$$

Proof. For polynomial equation applying the Table 1 values, we obtained the required results. □

Theorem 2.3. *Let H be the graph of hexagonal network HX_n. Then the M-polynomial is*

$$\begin{aligned} M(H,x,y) &= 12x^3y^4 + 6x^3y^6 + (6n-18)x^4y^4 + (12n-24)x^4y^6 \\ &+ (9n^2 - 33n + 30)x^6y^6. \end{aligned}$$

Proof. Let H be the graph of hexagonal network HX_n where n is the number of vertices on each side of hexagon. The graph H consists of $3n^2 - 3n + 1$ vertices and $9n^2 - 15n + 6$ edges. Graph H have 5 types of edges as folllows

$$E_{(3,4)} = \{e = uv \in E(H) \mid d_u = 3, d_v = 4\} \rightarrow |E_{(3,4)}| = 12$$
$$E_{(3,6)} = \{e = uv \in E(H) \mid d_u = 3, d_v = 6\} \rightarrow |E_{(3,6)}| = 6$$
$$E_{(4,4)} = \{e = uv \in E(H) \mid d_u = 4, d_v = 4\} \rightarrow |E_{(4,4)}| = 6n - 18$$
$$E_{(4,6)} = \{e = uv \in E(H) \mid d_u = 4, d_v = 6\} \rightarrow |E_{(4,6)}| = 12n - 24$$
$$E_{(6,6)} = \{e = uv \in E(H) \mid d_u = 6, d_v = 6\} \rightarrow |E_{(6,6)}| = 9n^2 - 33n + 30$$

Thus, the M-polynomial of HX_n is

$$\begin{aligned} M(H,x,y) &= \sum_{i \leq j} m_{ij}(H)x^iy^j \\ &= \sum_{3 \leq 4} m_{34}(H)x^3y^4 + \sum_{3 \leq 6} m_{36}(H)x^3y^6 + \sum_{i=j=4} m_{44}(H)x^4y^4 \\ &+ \sum_{4 \leq 6} m_{46}(H)x^4y^6 + \sum_{i=j=6} m_{66}(H)x^6y^6 \\ &= | E_{(3,4)} | x^3y^4 + | E_{(3,6)} | x^3y^6 + | E_{(4,4)} | x^4y^4 \\ &+ | E_{(4,6)} | x^4y^6 + | E_{(6,6)} | x^6y^6 \\ \therefore M(H,x,y) &= 12kx^3y^4 + 6x^3y^6 + (6n-18)x^4y^4 + (12n-24)x^4y^6 \\ &+ (9n^2 - 33n + 30)x^6y^6. \end{aligned}$$

□

Theorem 2.4. *Let H be a graph of Hexagonal network HX_n . Then*

$$\begin{aligned}
1.M_1(H) &= 108n^2 - 372n + 114.\\
2.M_2(H) &= 2916n^4 - 20088n^3 + 37152n^2 - 10188.\\
3.{}^mM_2(H) &= \frac{9}{4}n^4 - \frac{9}{2}n^3 + \frac{7}{2}n^2 - \frac{3}{2}n + \frac{1}{4}.\\
4.R_\alpha(H) &= [108n^2 - 372n + 114]^\alpha.\\
5.R'_\alpha(H) &= \left[\frac{9}{4}n^4 - \frac{9}{2}n^3 + \frac{7}{2}n^2 - \frac{3}{2}n + \frac{1}{4}\right]^\alpha.\\
6.SDD(H) &= 3[54n^4 - 240n^3 + 241n^2 - 8n + 19].
\end{aligned}$$

Proof. For polynomial equation applying the Table 1 values, we obtained the required results. □

Theorem 2.5. *Let P be a graph of $PNN(n,k,m)$. Then the M-polynomial is*

$$M(P,x,y) = nkmx^{n+1}y^{km} + kmx^my^{n+1}.$$

Proof. Let P be the $PNN(n,k,m)$ where n is the number of vertices in first layer, k is the number of class in hidden layer and m is the number of vertices in each class. The graph P consists of $n + k(m + 1)$ vertices and $km(n + 1)$ edges as shown in FIGURE 3. Graph P have 2 types of edges as folllows

$$\begin{aligned}
E_{(n+1,km)} &= \{e = uv \in E(G) \mid d_u = n+1, d_v = km\} \to |E_{(n+1,km)}| = nkm\\
E_{(m,n+1)} &= \{e = uv \in E(G) \mid d_u = m, d_v = n+1\} \to |E_{(m,n+1)}| = km
\end{aligned}$$

Thus, the M-polynomial of $PNN(n,k,m)$ is

$$\begin{aligned}
M(P,x,y) &= \sum_{i\le j} m_{ij}(P)x^iy^j\\
&= \sum_{n+1\le km} m_{(n+1)(km)}(P)x^{n+1}y^{km} + \sum_{m\le n+1} m_{(m)(n+1)}(P)x^my^{n+1}\\
&= \mid E_{(n+1,km)} \mid x^{n+1}y^{km} + \mid E_{(m,n+1)} \mid x^my^{n+1}\\
\therefore M(P,x,y) &= nkmx^{n+1}y^{km} + kmx^my^{n+1}.
\end{aligned}$$

□

Theorem 2.6. *Let P be a graph of $PNN(n,k,m)$ neural network. Then*

$$\begin{aligned}
1.\quad M_1(P) &= km[n[km + n + 2] + m + 1].\\
2.\quad M_2(P) &= k^2m^2[n[km(n^2 + n + 1) + (n + 1)^2 + m] + m].\\
3.\quad {}^mM_2(P) &= \frac{kn(m+1)}{(n+1)^2}\left(km + (n+1)^2\right).\\
4.\quad R_\alpha(P) &= [k^2m^2[n[km(n^2 + n + 1) + (n + 1)^2 + m] + m]]^\alpha.\\
5.\quad R'_\alpha(P) &= \left[\frac{kn(m+1)}{(n+1)^2}\left(km + (n+1)^2\right)\right]^\alpha.\\
6.\ SDD(P) &= km\Bigg[kmn + \frac{1}{n+1}(2 + kmn(km + kn + n + 2)\\
&+ n(kn + 2)) + n(n^2 + n + m)\Bigg].
\end{aligned}$$

Proof. For polynomial equation applying the Table 1 values, we obtained the required results. □

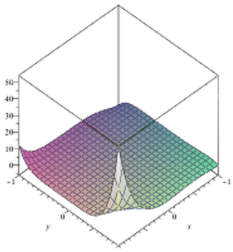

FIGURE 4(a)
M-Polynomial of Q[CNC3[1]]

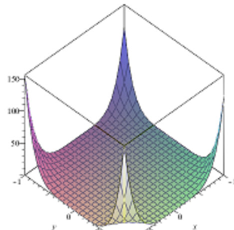

FIGURE 4(b)
M-Polynomial of HX5

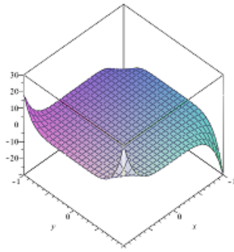

FIGURE 4(c)
M-Polynomial of PNN(4,2,3)

3. Conclusions

In this article, we computed the closed form of M-polynomial for carbon nanocones using Q operator, hexagonal networks HX_n and probabilistic neural network $PNN(n,k,m)$. Then, we derived certain degree-based topological indices for these structures. Also we plot surfaces associated with these structures that show the dependence of each topological index on the parameters of the structure.

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