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Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

COMPUTING THE MODIFIED ECCENTRIC CONNECTIVITY POLYNOMIAL OF NAPHTHYLENIC LATTICES

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ABSTRACT. Let $G = (V, E)$ be a graph, where G is a non-empty set of vertices $V(G)$ and $E(G)$ is a set of edges. In such chemical graphs the vertices of the graph corresponds to the atoms of the molecule, and the edges represent the chemical bonds. The aim of this paper is to compute the modified eccentric connectivity polynomial for the naphthylenic molecular graph.

Keywords: *modified eccentric connectivity polynomial, molecular graph, naphthylenic lattice*

INTRODUCTION

Molecular descriptors, especially topological indices, play an important role in the research of chemical compounds. A topological index is a numeric quantity derived from the structure of a graph which is invariant under automorphisms of the graph under consideration.

There are known many topological indices that have found some usage in QSPR/QSAR investigation. All graphs in this paper are finite and simple. A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of a graph correspond to the atoms of a molecule, and the edges represent chemical bonds. A distance-

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based topological index for a graph G is a topological index related to the distance function $d(-,-): V(G) \times V(G) \to \mathbb{R}$ in which $d(u,v)$ is defined as the length of a minimal path connecting u and v. The eccentricity of a vertex u in $V(G)$, denoted $ecc(u)$, is defined as $ecc(u) = Max\{d(u,v)|\ v \in\ V(G)\}$ $[1-5]$.

The eccentric connectivity index of the molecular graph, $ecc(G)$, was proposed by Sharma, Goswami and Madan [6]. It is defined as $\xi^c(G) = \sum_{u \in V(G)} \deg(u)\, ecc(u)$, where $deg(u)$ denotes the degree of vertex u in G.

The modified eccentric connectivity polynomial was proposed by Ashrafi [7] and it is defined as $\Lambda(G,x) = \sum_{u \in V(G)} \mathrm{n}_G(u)\, x^{ecc(u)}$, where $\mathrm{n}_G(u)$ is the sum of the degrees of neighborhoods of a vertex u. As a result, MEC index is the first derivative of this polynomial in $x = 1$.

The aim of this paper is to compute modified eccentric connectivity (MEC) polynomial for an infinite family of naphthylenic graphs. We encourage the reader to consult the papers [7-12] for more details about some properties of this topological index of some nanostructures.

RESULTS AND DISCUSSION

Following Diudea [13,14], we propose now the naphthylenic net, with the sequence: $C_6, C_{6,}, C_4, C_6,\ C_6 \ldots C_6, C_{6,}, C_4, C_6, C_6$, and repeat unit $C_6, C_{6,}, C_4$. The naphthylenic patterns, $NP[n,n]$ was designed as in Figure 1.

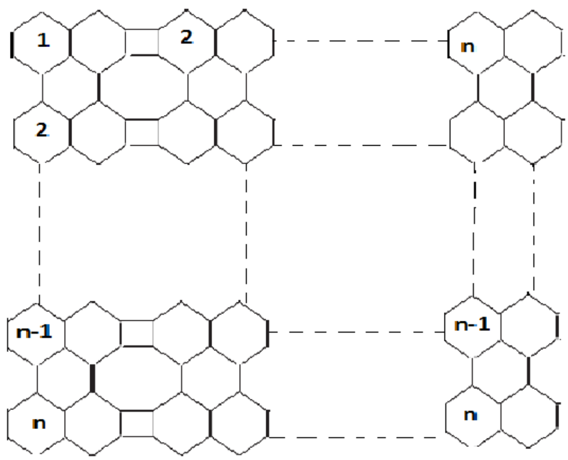

Figure 1. The 2D lattice of $NP[n,n]$

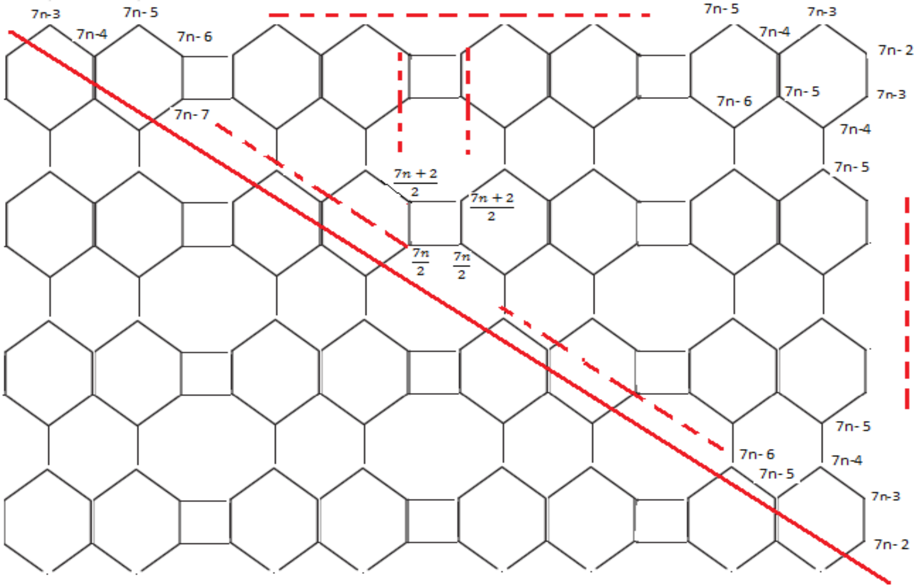

Figure 2. The maximum and minimum eccentricity of $NP[2k, 2k]$

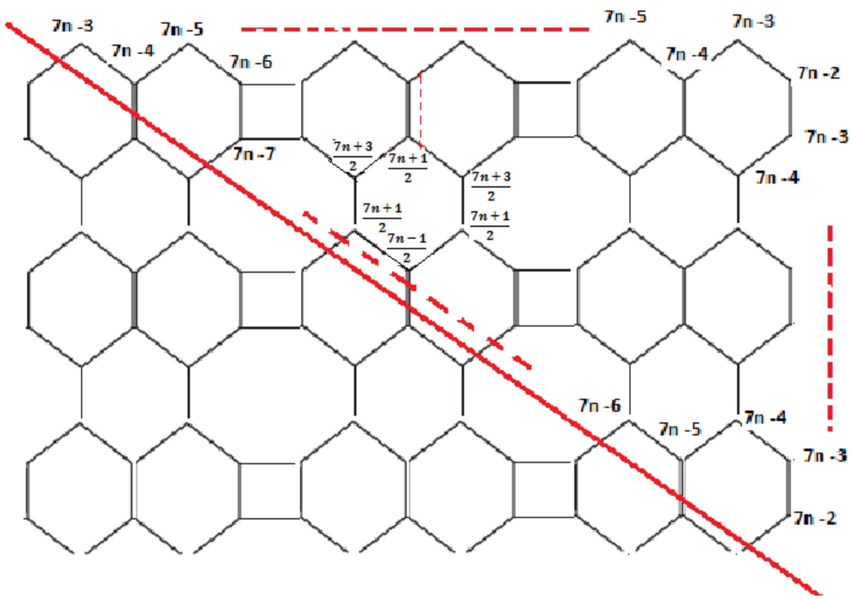

Figure 3. The maximum and minimum eccentricity of $NP[2k+1, 2k+1]$

In the following lemma, the maximum and minimum eccentric connectivity of $NP[n,n]$ is computed.

Lemma 1. *For any vertex* u *in* $V(NP[n,n])$, *we have:*

$$Max\ (ecc(u)) = 7n-2,$$

$$Min\ (ecc(u)) = \begin{cases} \frac{7n}{2} & if\ 2|n, \\ \frac{7n-1}{2} & if\ 2 \nmid n. \end{cases}$$

Proof. Suppose u is a vertex of $NP[n,n]$, then from Figures 2 and 3, one can see that for each vertex *v*, the longest path with maximum length is $7n-2$, and the shortest paths with maximum length, when n is even or odd, are $\frac{7n}{2}$ and $\frac{7n-1}{2}$, respectively. Thus the proof is completed.

In the following theorem we compute the modified eccentric connectivity polynomial for $NP(n,n)$.

Theorem 2. The modified eccentric connectivity polynomial of $NP(n,n)$ is computed as:

$$\Lambda(NP(n,n),x) = 8x^{7n-2} + 20x^{7n-3} + 40x^{7n-4} + 56x^{7n-5} + 78x^{7n-6}$$
$$+192x^{7n-7} + \begin{cases} \mathrm{A} & 2|n \quad n \geq 6 \\ \mathrm{B} & 2 \nmid n, \quad n \geq 7 \end{cases}$$

A and B are as follows, respectively.

$$A = 2(5n+70)x^{7n-8} + 2(12n+32)x^{7n-9} + 2(17n+16)x^{7n-10}$$
$$+ 18\sum_{k=0}^{n-2}(2k+2)x^{\frac{7n}{2}+k} + 36\sum_{k=n-1}^{\frac{7n-22}{2}}(n-1)\,x^{\frac{7n}{2}+k}$$
$$+ 32\sum_{k=0}^{\frac{n-4}{2}} x^{\frac{9n-2}{2}+5k} + 24\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n}{2}+5k} + 28\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+2}{2}+5k}$$
$$+ 24\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+4}{2}+5k} + 32\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+6}{2}+5k},$$

$$B = 220x^{7n-8} + 2(5n+85)x^{7n-9} + 2(13n+29)x^{7n-10} + 2(17n+5)x^{7n-11} + 18\sum_{k=0}^{n-2}(2k+1)x^{\frac{7n-1}{2}+k} + 36\sum_{k=n-1}^{3n-7}(n-1)\,x^{\frac{7n-1}{2}+k} + 28\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n-3}{2}+5k} + 24\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n-1}{2}+5k} + 32\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n+1}{2}+5k} + 32\sum_{k=0}^{\frac{n-7}{2}} x^{\frac{9n+3}{2}+5k} + 24\sum_{k=0}^{\frac{n-7}{2}} x^{\frac{9n+5}{2}+5k} - 14x^{\frac{9n-3}{2}}.$$

Proof. Considering Figures 2 and 3, it can be seen that there are several types of vertices. By computing the eccentricity of these vertices we have the results in Tables 1 and 2.

Table 1. Types of vertices of $NP(2k,2k)$

Number	ECC	$N_G(u)$
2	$7n-2$	4
4	$7n-3$	5
2	$7n-4$	8
2	$7n-4$	7
2	$7n-4$	5
2	$7n-5$	9
2	$7n-5$	8
2	$7n-5$	6
2	$7n-5$	5
4	$7n-6$	9
4	$7n-6$	8
2	$7n-6$	5
6	$7n-7$	9
4	$7n-7$	8
2	$7n-7$	5
8	$7n-8$	9
2	$7n-8$	8
2	$7n-8$	6
$n-6$	$7n-8$	5
10	$7n-9$	9

Number	**ECC**	$N_G(u)$
$n-6$	$7n-9$	8
2	$7n-9$	7
$n-6$	$7n-9$	5
$n+4$	$7n-10$	9
$n-4$	$7n-10$	8
2	$7n-10$	6
$2\ (n-1)$	$7n-11$	9
2	$7n-11$	8
000	…	...
$2\ (n-1)$	$(7n+2(n-2))/2$	9
$2\ (n-2)$	$(7n+2(n-3))/2$	9
000	…	...
6	$(7n+4)/2$	9
4	$(7n+2)/2$	9
2	$7n/2$	9

Table 2. Types of vertices of $NP(2k+1, 2k+1)$

Number	**ECC**	$N_G(u)$
2	$7n-2$	4
4	$7n-3$	5
2	$7n-4$	8
2	$7n-4$	7
2	$7n-4$	5
2	$7n-5$	9
2	$7n-5$	8
2	$7n-5$	6
2	$7n-5$	5
4	$7n-6$	9
4	$7n-6$	8
2	$7n-6$	5
6	$7n-7$	9
4	$7n-7$	8
2	$7n-7$	5
8	$7n-8$	9
2	$7n-8$	8
2	$7n-8$	6

Number	ECC	$N_G(u)$
2	$7n-8$	5
10	$7n-9$	9
2	$7n-9$	8
2	$7n-9$	7
$n-7$	$7n-9$	5
12	$7n-10$	9
$n-7$	$7n-10$	8
2	$7n-10$	6
$n-7$	$7n-10$	5
$n+5$	$7n-11$	9
$n-7$	$7n-11$	8
$2(n-1)$	$7n-12$	9
2	$7n-12$	8
000	…	…
$2n-3$	$(7n-1+2(n-2))/2$	9
$2n-5$	$(7n-1+2(n-3))/2$	9
000	…	...
5	$7n+3/2$	9
3	$7n+1/2$	9
1	$7n-1/2$	9

This implies that:

$$\begin{aligned}\Lambda\,(NP(2k,2k),x) &= 2(2\times 4x^{7n-2}+4\times 5x^{7n-3}+(2\times 8+2\times 7+2\times 5)x^{7n-4}\\ &+(2\times 9+2\times 8+2\times 6+2\times 5)x^{7n-5}\\ &+(4\times 9+4\times 8+2\times 5)x^{7n-6}+(6\times 9+4\times 8+2\times 5)x^{7n-7}\\ &+\left(8\times 9+2\times 8+2\times 6+5(n-6)\right)x^{7n-8}\\ &+(10\times 9+8(n-6)+2\times 7+5(n-6))x^{7n-9}\\ &+(9(n+4)+8(n-4)+6\times 2)x^{7n-10}\\ &+(18(n-1)+2\times 8)x^{7n-11}+\cdots)\\ &+\left(2\times 9x^{\frac{7n}{2}}+4\times 9x^{\frac{7n+2}{2}}+\cdots+2(n-1)\times 9x^{\frac{7n}{2}+(n-2)}\right),\end{aligned}$$

Therefore,

$$
\begin{aligned}
&\wedge (NP(2k,2k),x)\\
&= 16x^{7n-2} + 40x^{7n-3} + 80x^{7n-4} + 112x^{7n-5} + 156x^{7n-6}\\
&+ 192x^{7n-7} + 2(5n+70)x^{7n-8} + 2(12n+32)x^{7n-9}\\
&+ 2(17n+16)x^{7n-10}\\
&+ 18\sum_{k=0}^{n-2}(2k+2)x^{\frac{7n}{2}+k} + 36\sum_{k=n-1}^{\frac{7n-22}{2}}(n-1)\,x^{\frac{7n}{2}+k} + 32\sum_{k=0}^{\frac{n-4}{2}} x^{\frac{9n-2}{2}+5k}\\
&+ 24\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n}{2}+5k} + 28\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+2}{2}+5k}\\
&+ 24\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+4}{2}+5k} + 32\sum_{k=0}^{\frac{n-6}{2}} x^{\frac{9n+6}{2}+5k}.
\end{aligned}
$$

and for $n = 2k+1$ we have:

$$
\begin{aligned}
&\wedge (NP(2k+1,2k+1),x)\\
&= 2(2\times 4x^{7n-2} + 2\times 5x^{7n-3} + (2\times 8 + 2\times 7 + 2\times 5)x^{7n-4}\\
&+ (2\times 9 + 2\times 8 + 2\times 6 + 2\times 5)x^{7n-5}\\
&+ (4\times 9 + 4\times 8 + 4\times 5)x^{7n-6} + (6\times 9 + 4\times 8 + 2\times 5)x^{7n-7}\\
&+ (8\times 9 + 2\times 8 + 2\times 6 + 2\times 5)x^{7n-8}\\
&+ \left(10\times 9 + 2\times 8 + 2\times 7 + 5(n-7)\right)x^{7n-9}\\
&+ (12\times 9 + 8(n-7) + 2\times 6 + 5(n-7)x^{7n-10}\\
&+ \left(9(n+5) + 8(n-5)\right)x^{7n-11} + (18(n-1) + 2\times 8)x^{7n-12} + \cdots)\\
&+ \left(1\times 9x^{\frac{7n-1}{2}} + 3\times 9x^{\frac{7n+1}{2}} + \cdots + (2n-3)\times 9x^{\frac{7n-1}{2}+(n-2)}\right).
\end{aligned}
$$

Therefore,

$$\Lambda\,(NP(2k+1,2k+1),x) = 16x^{7n-2} + 40x^{7n-3} + 80x^{7n-4} + 112x^{7n-5} + 156x^{7n-6} + 192x^{7n-7} + 220x^{7n-8} + 2(5n+85)x^{7n-9} + 2(13n+29)x^{7n-10} + 2(17n+5)x^{7n-11} + 18\sum_{k=0}^{n-2}(2k+1)x^{\frac{7n-1}{2}+k} + 36\sum_{k=n-1}^{3n-7}(n-1)\,x^{\frac{7n-1}{2}+k} + 28\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n-3}{2}+5k} + 24\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n-1}{2}+5k} + 32\sum_{k=0}^{\frac{n-5}{2}} x^{\frac{9n+1}{2}+5k} + 32\sum_{k=0}^{\frac{n-7}{2}} x^{\frac{9n+3}{2}+5k} + 24\sum_{k=0}^{\frac{n-7}{2}} x^{\frac{9n+5}{2}+5k} - 14x^{\frac{9n-3}{2}}.$$

Some exceptional cases are given in Table 3.

Table 3. Some exceptional cases of $NP(n,n)$

Naphtylenic graph	MEC polynomial, 2$\leq n \leq 5$
$NP(2,2)$	$16x^{12} + 40x^{11} + 80x^{10} + 60x^9 + 68x^8 + 36x^7$
$NP(3,3)$	$16x^{26} + 40x^{25} + 80x^{24} + 112x^{23} + 104x^{22} + 104x^{21} + 132x^{20} + 136x^{19} + 132x^{18} + 140x^{17} + 108x^{16} + 72x^{15} + 36x^{14}$.
$NP(4,4)$	$16x^{26} + 40x^{25} + 80x^{24} + 112x^{23} + 104x^{22} + 104x^{21} + 132x^{20} + 136x^{19} + 132x^{18} + 140x^{17} + 108x^{16} + 72x^{15} + 36x^{14}$
$NP(5,5)$	$16x^{33} + 40x^{32} + 80x^{31} + 112x^{30} + 156x^{29} + 172x^{28} + 176x^{27} + 172x^{26} + 168x^{25} + 176x^{24} + 176x^{23} + 168x^{22} + 158x^{21} + 126x^{20} + 90x^{19} + 54x^{18} + 18x^{17}$

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