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Degree Based Topological Indices of Graphene Using M_{hr}- Polynomial

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Abstract

Graphene is a two-dimensional material consisting of a single layer of carbon atom arranged in a honeycomb structure. Graphine exhibits important intrinsic properties such as high strength, excellent conductor of heat and electricity. In this research, M_{hr}-polynomial, when of HDR indices for the line graph of Graphene is established, the degree-based topological indices, such as first, second HDR indices are obtained. Accordingly, by using the derivative of M_{hr}-polynomial of Graphene the first, second HDR hyper-Zagreb indices, and HDR forgotten topological index of Graphene, are found.

Keywords: Topological index; ψ_k-Polynomial; M_{hr}- Polynomial.
2020 Mathematics Subject Classification: 05C10, 05C07, 05C05, 05C90.

1. Introduction

Graph theory provides simple rules by which chemists may obtain qualitative predictions about the structure and reactivity of various compounds. It may be used as a foundation for the representation, classification, and categorization of a very large number of chemical systems. Chemical graph theory is a branch of mathematical chemistry that is concerned with all aspects of the application of graph theory to chemistry. A molecular graph is a connected graph whose vertices correspond to the atoms of the compound and edges correspond to the chemical bonds. A topological index is a number related to a graph G which is invariant under graph isomorphism, that is. it does not depend on the labelling or the pictorial representation of a graph [21]. The molecular graphs considered in this paper are simple connected undirected graphs, where the atoms of the molecule are represented as vertices and the bonds between them as edges. A graph $G = (V, E)$ consists of a vertex set $V(G)$ and an edge set $E(G)$. The number of vertices of G which are at a degree distance k from v is said to be k^{th} degree distance of the vertex and denoted by $d_k(v)$, $\delta_k(G)$ and $\Delta_k(G)$ are the k^{th} minimum degree distance and k^{th} maximum degree distance respectively. Graphene is an atomic-scale honeycomb lattice made of the

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carbon atoms. It is the first $2D$ material that was isolated from graphite in 2004 by Professor Andre Geim and Professor Kostya Novoselov. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and the world's most conductive material. Duo to these unique properties Graphene has captured the attention of scientists, researchers, and industries worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for potential applications ranging from electronics to optics, sensors, and bio-devices. Also, it is the most effective material for electromagnetic interference (EMI) shielding. Sridhara et al. has calculated some topological indices of Graphene in [17]. There are some recent papers devoted to the computation of degree-based topological indices using some polynomials ([12, 15, 16, 18, 22]). For more discussion, see [3–6, 8–10, 19, 20]. The line graph $L(G)$ of a graph G is the graph each of whose vertex represents an edge of G and two of its vertices are adjacent if their corresponding edges are adjacent in G. In this paper, we compute the closed-form of some degree-based topological indices of Graphene and its line graph by using the ψ_2-polynomial [1].

2. Basic Definitions and Literature Review

Definition 2.1. *The M_k-polynomial of a graph G is defined as*

$$M_k(G,x,y) = \sum_{\delta_k \leq i \leq j \leq \Delta_k} M_{hr}(i,j)x^i y^j,$$

where $M_{hr}(i,j)$ be the number of edges uv in G such that $\{d_k(v), d_k(u)\} = \{i,j\}$ and $d_k(v)$, $d_k(u)$ are the k^{th} degree distance of v and u respectively.

In this paper, we use M_k-polynomial. The degree based topological indices for a graph G can be expressed $I(G) = \sum_{uv \in E(G)} f(d_k(u), d_k(v))$, where $f = f(x,y)$ is a function appropriately selected for possible chemical application . The above result can also be written as

$$I(G) = \sum_{i \leq j} M_{hr}(i,j) f(i,j).$$

The first HDR Zagreb index [1] is defined as

$$HDRM_1^*(G) = \sum_{uv \in E(G)} [d_{hr}(u) + d_{hr}(v)].$$

The second HDR Zagreb index [1] is defined as

$$HDRM_2(G) = \sum_{uv \in E(G)} d_{hr}(u) d_{hr}(v).$$

The third HDR Zagreb index [1] is defined as

$$HDRM_3(G) = \sum_{uv \in E(G)} [d_{hr}(u) + d_{hr}(v)].$$

The first HDR hyper-Zagreb index [1] is defined as

$$HDRHM_1(G) = \sum_{uv \in E(G)} [d_{hr}(u) + d_{hr}(v)]^2.$$

The second HDR hyper-Zagreb index [1] is defined as

$$HLM_2(G) = \sum_{uv \in E(G)} [d_{hr}(u) d_{hr}(v)]^2.$$

In [11] The leap forgotten topological index was defined as

$$HDRF(G) = \sum_{uv \in E(G)} [d^2_{hr}(u) + d^2_{hr}(v)].$$

The relation of some degree-based topological indices with the M_{hr}-Polynomial is shown in Table 1.

Topological Index	$f(x,y)$	*Derivation From* $M_{hr}(G)$
$HDRM_1^*$	$x+y$	$(D_x + D_y)(M_2(G))\|_{x=y=1}$
$HDRM_2$	xy	$(D_x D_y)(M_2(G))\|_{x=y=1}$
$HDRM_3$	$x+y$	$(D_x + D_y)(M_2(G))\|_{x=y=1}$
$HDRHM_1$	$(x+y)^2$	$(D_x + D_y)^2(M_{hr}(G))\|_{x=y=1}$
$HDRHM_2$	$(xy)^2$	$(D_x D_y)^2(M_{hr}(G))\|_{x=y=1}$
$HDRF$	x^2+y^2	$(D_x^2 + D_y^2)(M_{hr}(G))\|_{x=y=1}$

Table 1: Derivation of some degree based topological indices

$$D_x(f(x,y)) = x\frac{\partial(f(x,y))}{\partial x}, \quad D_y(f(x,y)) = y\frac{\partial(f(x,y))}{\partial y}.$$

3. Main Results

In this section, we presented our main results in two subsection.

3.1 Computing the ψ_2-polynomial and degree based topological indices of line graph of graphene

Consider the line graph $L(G)$ of graphene with t rows and s benzene rings in each row. We have $M_{hr}(i,j)$ is the number of edges uv in G such that $\{d_k(v), d_k(u)\} = \{i,j\}$ and $d_k(v)$, $d_k(u)$ are the k^{th} degree distance of v and u respectively. We compute M_{hr}-polynomial of $L(G)$ of graphene. We start by considering the first, second and third leap Zagreb indices, also we compute the first and second leap hyper-Zagreb indices, and leap forgotten topological index of graphene by the derivative.

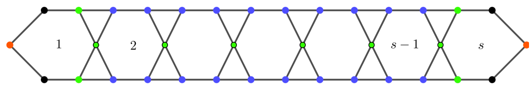


Figure 1: Line graph of Graphene, with $t = 1$ and $s > 2$.

$M_{hr}(2,3)$	$M_{hr}(3,4)$	$M_{hr}(4,4)$	$M_{hr}(4,5)$	$M_{hr}(5,5)$
2	5	5	$5(s-1)$	$(5s-10)$

Table 2: The number of edges in the different types of edges of line graph of Graphene, with $t = 1$ and $s > 2$.

Theorem 3.1. *Let $L(G)$ be the line graph of Graphene, with $t = 1$ and $s > 2$. Then*

$$\psi_2(L(G), x, y) = 2x^2y^3 + 5x^3y^4 + 5x^4y^4 + 3(s-1)x^4y^5 + (6s-10)x^5y^5.$$

Proof. We have $L(G)$ be the line graph of Graphene with $t = 1$ and $s > 2$ as in Figure 1. Then from the Table 2, we get

$$\begin{aligned} M_{hr}(L(G), x, y) &= \sum_{\delta_2 \le i \le j \le \Delta_2} \psi_2(i,j)x^iy^j \\ &= 2x^2y^3 + 5x^3y^4 + 5x^4y^4 + 3(s-1)x^4y^5 + (6s-10)x^5y^5. \end{aligned}$$

□

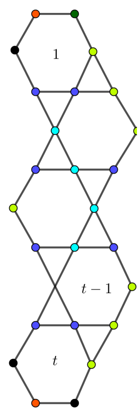


Figure 2: line graph of Graphene, with $s = 1$ and $t > 2$.

$M_{hr}(2,3)$	$M_{hr}(3,4)$	$M_{hr}(3,5)$	$M_{hr}(4,4)$	$M_{hr}(4,5)$	$M_{hr}(5,5)$	$M_{hr}(5,6)$	$M_{hr}(6,6)$
3	3	4	2	$3(t-2)$	1	$(2t-8)$	$(2t-6)$

Table 3: The number of edges of the different types of edges of line graph of Graphene, with $s = 1$ and $t > 2$.

Theorem 3.2. *Let $L(G)$ be the line graph of Graphene, with $s = 1$ and $t > 2$. Then*

$$M_{hr}(L(G),x,y) = 3x^2y^3 + 3x^3y^4 + 4x^3y^5 + 2x^4y^4 + 3(t-2)x^4y^5 + x^5y^5 + (2t-8)x^5y^6 + (2t-6)x^6y^6.$$

Proof. We have $L(G)$ be the line graph of Graphene with $s = 1$ and $t > 2$ as in Figure 2. Then from the Table 3, we get

$$\begin{aligned} M_{hr}(L(G),x,y) &= \sum_{\delta_2 \le i \le j \le \Delta_2} \psi_2(i,j)x^iy^j \\ &= 3x^2y^3 + 3x^3y^4 + 4x^3y^5 + 2x^4y^4 + 3(t-2)x^4y^5 + x^5y^5 + (2t-8)x^5y^6 + (2t-6)x^6y^6. \end{aligned}$$

□

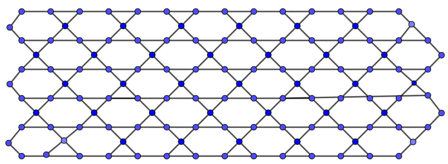


Figure 3: line graph of Graphene, with $s > 1$ and $t > 1$.

Row	$M_{hr}(3,3)$	$M_{hr}(3,4)$	$M_{hr}(3,5)$	$M_{hr}(4,4)$	$M_{hr}(4,5)$	$M_{hr}(4,6)$	$M_{hr}(5,5)$
1	1	1	1	3	2	3	$2s-5$
2	0	0	0	1	1	0	0
3	0	0	0	0	2	0	0
4	0	0	0	0	2	0	0
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
$t-1$	0	0	0	1	1	1	0
t	1	1	1	3	2	3	$2s-5$
total	2	2	2	8	$(2t-2)$	7	$(4s-10)$

Table 4: The number of edges of the different types of edges of line graph of Graphene, with $s > 1$ and $t > 1$.

Row	$M_{hr}(5,6)$	$M_{hr}(5,7)$	$M_{hr}(6,7)$	$M_{hr}(6,8)$	$M_{hr}(7,8)$	$M_{hr}(8,8)$
1	$2s-4$	1	1	$2s-2$	1	$2s-4$
2	2	2	2	0	4	$6s-8$
3	2	2	2	0	4	$6s-8$
4	2	2	2	0	4	$6s-8$
.	.	.	.	.	.	.
.	.	.	.	.	.	.
$t-1$	2	2	2	2	4	$6s-8$
t	$2s-4$	1	1	$2s-3$	2	0
total	$(4s+2t-12)$	$(2t-4)$	$(2t-2)$	$(4s-3)$	$(2t-4)$	$(6st-8t-10s+12)$

Table 5: The number of edges of the different types of edges of the line graph of Graphene, with$s > 1$ and $t > 1$.

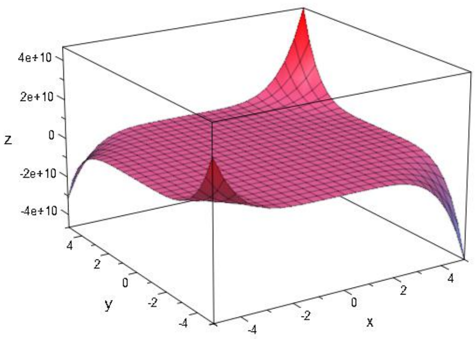
Theorem 3.3. *Let $L(G)$ be the line graph of Graphene, with $s > 1$ and $t > 1$. Then*

$$\begin{aligned} M_{hr}(L(G), x, y) = {} & 2x^3y^3 + 2x^3y^4 + 2x^3y^5 + 8x^4y^4 + (2t-2)x^4y^5 \\ & + 7x^4y^6 + (4s-10)x^5y^5 + (4s+2t-12)x^5y^6 \\ & + (2t-4)x^5y^7 + (2t-2)x^6y^7 + (4s-3)x^6y^8 \\ & + (2t-4)x^7y^8 + (6st-8t-10s+12)x^8y^8. \end{aligned}$$

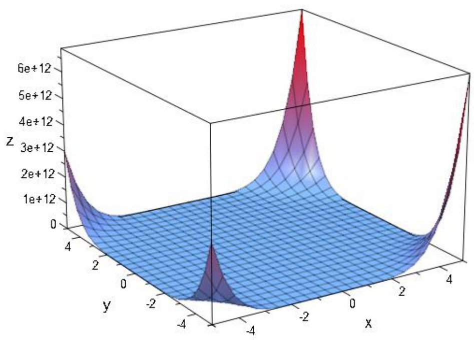
Proof. Let $L(G)$ be the line graph of Graphene with $s > 1$ and $t > 1$ as in the Figure 3. Then from the Table 4 and 5. We get

$$\begin{aligned} M_2(L(G), x, y) = {} & \sum_{\delta_2 \le i \le j \le \Delta_2} M_{hr}(i,j)x^iy^j \\ = {} & 2x^3y^3 + 2x^3y^4 + 2x^3y^5 + 8x^4y^4 + (2t-2)x^4y^5 \\ & + 7x^4y^6 + (4s-10)x^5y^5 + (4s+2t-12)x^5y^6 \\ & + (2t-4)x^5y^7 + (2t-2)x^6y^7 + (4s-3)x^6y^8 \\ & + (2t-4)x^7y^8 + (6st-8t-10s+12)x^8y^8. \end{aligned}$$

□



(a) M_{hr}-polynomial of the line graph of Graphene with $t = 1$, and $s = 1000$



(b) M_{hr}-polynomial of line graph of Graphene, with $s = t = 1000$

Figure 4

Now, by using the M_{hr}-polynomial, we have calculated some degree based topological indices of the line graph of Graphene in the following theorems.

Theorem 3.4. *Let $L(G)$ be the line graph of Graphene, with $s > 2$, $t = 1$ and $M_2(L(G), x, y) = 4x^2y^3 + 4x^3y^4 + 4x^4y^4 + 4(s-1)x^4y^5 + (4s-10)x^5y^5$. Then*

(1). $HDRM_1^*(L(G)) = 76s - 56.$

(2). $HDRM_2(L(G)) = 180s - 194.$

(3). $HDRHM_1(L(G)) = 724s - 772.$

(4). $HDRHM_2(L(G)) = 4100s - 5506.$

(5). $HDRF(L(G)) = 364s - 384.$

Proof. Let $M_{hr}(L(G), x, y) = f(x, y) = 4x^2y^3 + 4x^3y^4 + 4x^4y^4 + 4(s-1)x^4y^5 + (4s-10)x^5y^5$. Then, we have

$$\begin{aligned}
(D_x + D_y)(f(x,y)) &= 20x^2y^3 + 28x^3y^4 + 32x^4y^4 + 36(s-1)x^4y^5 + 10(4s-10)x^5y^5. \\
D_xD_y(f(x,y)) &= 24x^2y^3 + 48x^3y^4 + 64x^4y^4 + 80(s-1)x^4y^5 + 25(4s-10)x^5y^5. \\
(D_x + D_y)^2(f(x,y)) &= 100x^2y^3 + 196x^3y^4 + 256x^4y^4 + 324(s-1)x^4y^5 + 100(4s-10)x^5y^5. \\
(D_xD_y)^2(f(x,y)) &= 144x^2y^3 + 576x^3y^4 + 1024x^4y^4 + 1600(s-1)x^4y^5 + 625(4s-10)x^5y^5. \\
(D_x^2 + D_y^2)(f(x,y)) &= 52x^2y^3 + 100x^3y^4 + 128x^4y^4 + 164(s-1)x^4y^5 + 50(4s-10)x^5y^5.
\end{aligned}$$

The required result can obtain by using Table 1. □

Theorem 3.5. *Let $L(G)$ be the line graph of Graphene, with $s = 1$, $t > 2$ and*

$$M_{hr}(L(G), x, y) = 4x^2y^3 + 2x^3y^4 + 2x^3y^5 + 4x^4y^4 + 2(t-2)x^4y^5 + 2x^5y^5 + (4t-8)x^5y^6 + (2t-6)x^6y^6.$$

Then

(1). $HDRM_1^*(L(G)) = 86t - 94.$

(2). $HDRM_2(L(G)) = 323t - 344.$

(3). $HDRHM_1(L(G)) = 464t - 366.$

(4). $HDRHM_2(L(G)) = 69922t - 13420.$

(5). $HDRF(L(G)) = 670ts - 686.$

Proof. Let

$$\begin{aligned}
M_2(L(G), x, y) &= f(x, y) \\
&= 4x^2y^3 + 2x^3y^4 + 2x^3y^5 + 4x^4y^4 + 2(t-2)x^4y^5 + 2x^5y^5 + (4t-8)x^5y^6 + (2t-6)x^6y^6.
\end{aligned}$$

Then we have

$$\begin{aligned}
(D_x+D_y)(f(x,y)) &= 20x^2y^3+14x^3y^4+16x^3y^5+32x^4y^4+18(t-2)x^4y^5+20x^5y^5\\
&\quad +11(4t-8)x^5y^6+12(2t-6)x^6y^6.\\
D_xD_y(f(x,y)) &= 24x^2y^3+24x^3y^4+30x^3y^5+64x^4y^4\\
&\quad +40(t-2)x^4y^5+50x^5y^5+30(4t-8)x^5y^6+36(2t-6)x^6y^6.\\
(D_x+D_y)^2(f(x,y)) &= 100x^2y^3+98x^3y^4+128x^3y^5+256x^4y^4\\
&\quad +162(t-2)x^4y^5+200x^5y^5+121(4t-8)x^5y^6+144(2t-6)x^6y^6.\\
(D_xD_y)^2(f(x,y)) &= 144x^2y^3+288x^3y^4+450x^3y^5+1024x^4y^4\\
&\quad +800(t-2)x^4y^5+1250x^5y^5+900(4t-8)x^5y^6+1296(2t-6)x^6y^6.\\
(D_x^2+D_y^2)(f(x,y)) &= 52x^2y^3+50x^3y^4+68x^3y^5+128x^4y^4\\
&\quad +82(t-2)x^4y^5+100x^5y^5+61(4t-8)x^5y^6+72(2t-6)x^6y^6.
\end{aligned}$$

The required result can obtain by using Table 1. □

Theorem 3.6. *Let $L(G)$ be the line graph of Graphene, with $s>1$, $t>1$ and*

$$\begin{aligned}
M_{hr}(L(G),x,y) &= 2x^3y^3+2x^3y^4+2x^3y^5+8x^4y^4+(2t-2)x^4y^5\\
&\quad +7x^4y^6+(4s-10)x^5y^5+(4s+2t-12)x^5y^6\\
&\quad +(2t-4)x^5y^7+(2t-2)x^6y^7+(4s-3)x^6y^8\\
&\quad +(2t-4)x^7y^8+(6st-8t-10s+12)x^8y^8.
\end{aligned}$$

Then

(1). $HDRM_1^*(L(G))=96st-20s-8t-58.$

(2). $HDRM_2(L(G))=384st-328s-146t-106.$

(3). $HDRM_2(L(G))=24576st-29244s-23518t-30598.$

(4). $HDRF(L(G))=768st-436s-276t-478$

Proof. Let

$$\begin{aligned}
M_{hr}(L(G),x,y)=f(x,y) &= 2x^3y^3+2x^3y^4+2x^3y^5+8x^4y^4+(2t-2)x^4y^5\\
&\quad +7x^4y^6+(4s-10)x^5y^5+(4s+2t-12)x^5y^6\\
&\quad +(2t-4)x^5y^7+(2t-2)x^6y^7+(4s-3)x^6y^8\\
&\quad +(2t-4)x^7y^8+(6st-8t-10s+12)x^8y^8.\\
(D_x+D_y)(f(x,y)) &= 12x^3y^3+14x^3y^4+16x^3y^5+64x^4y^4+9(2t-2)x^4y^5
\end{aligned}$$

$$
\begin{aligned}
&+ 70x^4y^6 + 10(4s-10)x^5y^5 + 11(4s+2t-12)x^5y^6 \\
&+ 12(2t-4)x^5y^7 + 13(2t-2)x^6y^7 + 14(4s-3)x^6y^8 \\
&+ 15(2t-4)x^7y^8 + 16(6st-8t-10s+12)x^8y^8. \\
D_xD_y(f(x,y)) &= 18x^3y^3 + 24x^3y^4 + 30x^3y^5 + 128x^4y^4 + 20(2t-2)x^4y^5 \\
&+ 168x^4y^6 + 25(4s-10)x^5y^5 + 30(4s+2t-12)x^5y^6 \\
&+ 35(2t-4)x^5y^7 + 42(2t-2)x^6y^7 + 48(4s-3)x^6y^8 \\
&+ 56(2t-4)x^7y^8 + 64(6st-8-10s+12)x^8y^8. \\
(D_xD_y)^2(f(x,y)) &= 162x^3y^3 + 288x^3y^4 + 450x^3y^5 + 2048x^4y^4 + 400(2t-2)x^4y^5 \\
&+ 4032x^4y^6 + 625(4s-10)x^5y^5 + 900(4s+2t-12)x^5y^6 \\
&+ 1225(2t-4)x^5y^7 + 1764(2t-2)x^6y^7 + 2304(4s-3)x^6y^8 \\
&+ 336(2t-4)x^7y^8 + 4096(6st-8-10s+12)x^8y^8. \\
(D_x^2 + D_y^2)(f(x,y)) &= 36x^3y^3 + 50x^3y^4 + 68x^3y^5 + 256x^4y^4 + 41(2t-2)x^4y^5 \\
&+ 364x^4y^6 + 50(4s-10)x^5y^5 + 61(4s+2t-12)x^5y^6 \\
&+ 74(2t-4)x^5y^7 + 85(2t-2)x^6y^7 + 100(4s-3)x^6y^8 \\
&+ 113(2t-4)x^7y^8 + 128(6st-8t-10s+12)x^8y^8.
\end{aligned}
$$

The required result can obtain by using Table 1. □

3.2 Computing the M_{hr}-polynomial and Degree Based Topological Indices of Graphene

The Graphene with t rows and s benzene rings in each row. Ammar et al. [1] computed M_2-polynomial of Graphene and honeycomb network, where $G_{s,t}$ is the graph of Graphene with t rows and s Columns. In this part, we compute the first, second and third leap Zagreb indices of Graphene, also we compute the first and second leap hyper-Zagreb indices, and leap forgotten topological index of Graphene, by the derivative of the ψ_2-polynomial of Graphene.

Theorem 3.7. *Let $G_{s,t}$ be a graph of Graphene with $s = t = 1$ and $M_{hr}(G_{s,t}, x, y) = 6x^2y^2$. Then*

(1). $HDRM_1^*(G_{s,t}) = 24.$

(2). $HDRM_2(G_{s,t}) = 24.$

(3). $HM_1(G_{s,t}) = 96.$

(4). $HDRHM_2(G_{s,t}) = 196.$

(5). $HDRF(G_{s,t}) = 48.$

Proof. Let $M_{hr}(G_{s,t}, x, y) = f(x,y) = 6x^2y^2$. Then we have

$$D_x + D_y(f(x,y)) = 24x^2y^2.$$

$$D_xD_y(f(x,y)) = 24x^2y^2.$$
$$(D_x + D_y)^2(f(x,y)) = 96x^2y^2.$$
$$(D_xD_y)^2 = 196x^2y^2.$$
$$(D_x^2 + D_y^2)(f(x,y)) = 48x^2y^2.$$

The required result can obtain by using Table 1. □

Theorem 3.8. *Let $G_{s,t}$ be a graph of Graphene with $t = 1$ and $s > 1$, with*

$$M_{hr}(G_{s,t}, x, y) = 2x^2y^2 + 4x^2y^3 + 4x^3y^4 + (5s - 9)x^4y^4.$$

Then

(1). $HDRM_1^*(G_{s,t}) = 40s - 16.$

(2). $HDRM_2(G_{s,t}) = 80s - 64.$

(3). $HDRHM_1(G_{s,t}) = 330s - 248.$

(4). $HDRHM_2(G_{s,t}) = 1280s - 1552.$

(5). $HDRF(G_{s,t}) = 160s - 120.$

Proof. Let $M_2(G_{s,t}) = f(x,y) = 2x^2y^2 + 4x^2y^3 + 4x^3y^4 + (5s - 9)x^4y^4$. Then, we have

$$(D_x + D_y)(f(x,y)) = 8x^2y^2 + 20x^2y^3 + 28x^3y^4 + 8(5s - 9)x^4y^4.$$
$$D_xD_y(f(x,y)) = 8x^2y^2 + 24x^2y^3 + 48x^3y^4 + 16(5s - 9)x^4y^4.$$
$$(D_x + D_y)^2(f(x,y)) = 32x^2y^2 + 100x^2y^3 + 196x^3y^4 + 64(5s - 9)x^4y^4.$$
$$(D_xD_y)^2(f(x,y)) = 32x^2y^2 + 144x^2y^3 + 576x^3y^4 + 256(5s - 9)x^4y^4.$$
$$(D_x^2 + D_y^2)(f(x,y)) = 16x^2y^2 + 52x^2y^3 + 100x^3y^4 + 32(5s - 9)x^4y^4.$$

The required result can obtain by using Table 1. □

Theorem 3.9. *Let $G_{s,t}$ be a graph of Graphene, with $s = 1$, $t > 1$ and*

$$M_2(G_{s,t}, x, y) = 2x^2y^2 + 4x^2y^3 + (t - 2)x^3y^3 + 4x^3y^4 + (2t - 4)x^3y^5 + 2x^4y^5 + (2t - 5)x^5y^5.$$

Then

(1). $HDRM_1^*(G_{s,t}) = 42t - 20.$

(2). $HDRM_2(G_{s,t}) = 89t - 83.$

(3). $HDRHM_1(G_{s,t}) = 364t - 388.$

(4). $HDRHM_2(G_{s,t}) = 1556t - 2827.$

(5). $HDRF(G_{s,t}) = 168ts - 172.$

Proof. Let

$$M_2(G_{s,t}, x, y) = f(x,y) = 2x^2y^2 + 4x^2y^3 + (t-2)x^3y^3 + 4x^3y^4 + (2t-4)x^3y^5 + 2x^4y^5 + (2t-5)x^5y^5$$

Then we have,

$$\begin{aligned}
(D_x + D_y)(f(x,y)) &= 8x^2y^2 + 20x^2y^3 + 6(t-2)x^3y^3 + 28x^3y^4 \\
&\quad + 8(2t-4)x^3y^5 + 18x^4y^5 + 10(2t-5)x^5y^5. \\
D_xD_y(f(x,y)) &= 8x^2y^2 + 24x^2y^3 + 9(t-2)x^3y^3 + 48x^3y^4 \\
&\quad + 15(2t-4)x^3y^5 + 40x^4y^5 + 25(2t-5)x^5y^5. \\
(D_x + D_y)^2(f(x,y)) &= 32x^2y^2 + 100x^2y^3 + 36(t-2)x^3y^3 + 196x^3y^4 \\
&\quad + 64(2t-4)x^3y^5 + 162x^4y^5 + 100(2t-5)x^5y^5. \\
(D_xD_y)^2(f(x,y)) &= 32x^2y^2 + 144x^2y^3 + 81(t-2)x^3y^3 \\
&\quad + 384x^3y^4 + 225(t-4)x^3y^5 + 800x^4y^5 + 625x^5y^5. \\
(D_x^2 + D_y^2)(f(x,y)) &= 16x^2y^2 + 52x^2y^3 + 18(t-2)x^3y^3 + 100x^3y^4 \\
&\quad + 34(2t-4)x^3y^5 + 82x^4y^5 + 50(2t-5)x^5y^5.
\end{aligned}$$

The required result can obtain by using Table 1. □

Theorem 3.10. *Let $G_{s,t}$ be a graph of Graphene, with $s > 1, t > 1$ and*

$$\begin{aligned}
M_2(G_{s,t}, x, y) &= 4x^2y^3 + tx^3y^3 + 8x^3y^4 + (2t-4)x^3y^5 + (4s-8)x^4y^4 \\
&\quad + 2sx^4y^6 + (2t-4)x^5y^6 + (t-2)x^5y^5 + (3st - 4s - 4t + 5)x^6y^6.
\end{aligned}$$

Then

(1). $HDRM_1^*(G_{s,t}) = 36st + 4s + 6t - 24.$

(2). $HDRM_2(G_{s,t}) = 108st - 32s - 20t - 58.$

(3). $HDRHM_1(G_{s,t}) = 5328st - 6864s - 5098t - 760$

(4). $HDRHM_2(G_{s,t}) = 648st - 416s - 262t - 126.$

(5). $HDRF(G_{s,t}) = 2016st + 56s - 120t - 123.$

Proof. Let

$$M_2(G_{s,t},x,y) = f(x,y) = 4x^2y^3 + tx^3y^3 + 8x^3y^4 + (2t-4)x^3y^5 + (4s-8)x^4y^4 \\ + 2sx^4y^6 + (2t-4)x^5y^6 + (t-2)x^5y^5 + (3st-4s-4t+5)x^6y^6.$$

Then we have,

$$\begin{aligned}
(D_x+D_y)(f(x,y)) &= 20x^2y^3 + 6tx^3y^3 + 56x^3y^4 + 8(2t-4)x^3y^5 \\
&\quad + 8(4s-8)x^4y^4 + 20sx^4y^6 + 11(2t-4)x^5y^6 \\
&\quad + 10(t-2)x^3y^5 + 12(3st-4s-4t+5)x^6y^6. \\
D_xD_y(f(x,y)) &= 24x^2y^3 + 9tx^3y^3 + 96x^3y^4 + 15(2t-4)x^3y^5 \\
&\quad + 16(4s-8)x^4y^4 + 48sx^4y^6 + 30(2t-4)x^5y^6 \\
&\quad + 25(t-2)x^5y^5 + 36(3st-4s-4t+5)x^6y^6. \\
(D_x+D_y)^2(f(x,y) &= 340x^2y^3 + 180tx^3y^3 + 668x^3y^4 + 484(2t-4)x^3y^5 \\
&\quad + 544(4s-8)x^4y^4 + 1616sx^4y^6 + 1555(2t-4)x^5y^6 \\
&\quad + 1300(t-2)x^3y^5 + 2664(3st-4s-4t+5)x^6y^6. \\
(D_xD_y)^2(f(x,y)) &= 144x^2y^3 + 81tx^3y^3 + 1152x^3y^4 + 225(2t-4)x^3y^5 \\
&\quad + 256(4s-8)x^4y^4 + 768sx^4y^6 + 750(2t-4)x^5y^6 \\
&\quad + 625(t-2)x^5y^5 + 1296(3st-4s-4t+5)x^6y^6. \\
(D_x^2+D_y^2)(f(x,y)) &= 52x^2y^3 + 18tx^3y^3 + 200x^3y^4 + 34(2t-4)x^3y^5 \\
&\quad + 32(4s-8)x^4y^4 + 80sx^4y^6 + 55(2t-4)x^5y^6 \\
&\quad + 50(t-2)x^3y^5 + 72(3st-4s-4t+5)x^6y^6..
\end{aligned}$$

The required result can obtain by using Table 1. □

Theorem 3.11. *Let $HN(n)$ be the graph of honeycomb network of n hexagon, with $n \geq 2$ and*

$$M_2(HN(n),x,y) = 6x^3y^3 + 12x^3y^4 + (12n-24)x^4y^4 + 6(n-1)x^4y^6 + 9n^2 - 21n + 12)x^6y^6$$

Then

(1). $HDRM_1^*(HN(n)) = 108n^2 - 96n - 108.$

(2). $HDRM_2(HN(n)) = 324n^2 - 336n + 102.$

(3). $HDRHM_1(HN(n)) = 324n^2 - 164n + 170$

(4). $HDRHM_2(HN(n)) = 11664n^2 - 21840n - 9318.$

(5). $HDRF(HN(n)) = 468n^2 - 472n + 46.$

Proof. Let

$$M_2(HN(n), x, y) = f(x, y) = 6x^3y^3 + 12x^3y^4 + (12n - 24)x^4y^4 + 6(n-1)x^4y^6 + 9n^2 - 21n + 12)x^6y^6.$$

Then we have

$$\begin{aligned}
(D_x + D_y)(f(x,y)) &= 36x^3y^3 + 84x^3y^4 + 8(12n - 24)x^4y^4 \\
&\quad + 60(n-1)x^4y^6 + 12(9n^2 - 21n + 12)x^6y^6. \\
D_xD_y(f(x,y)) &= 54x^3y^3 + 144tx^3y^4 + 16(12n - 24)x^4y^4 \\
&\quad + 144(n-1)x^4y^6 + 36(9n^2 - 121n + 12)x^6y^6. \\
(D_x + D_y)^2(f(x,y) &= 270x^3y^3 + 756x^3y^4 + 80(12n - 24)x^4y^4 \\
&\quad + 616(n-1)x^4y^6 + 140(9n^2 - 21n + 12)x^6y^6. \\
(D_xD_y)^2(f(x,y)) &= 486x^3y^3 + 1728x^3y^4 + 256(12n - 2n)x^4y^4 \\
&\quad + 2304(n-1)x^4y^6 + 1296(9n^2 - 21n + 12). \\
(D_x^2 + D_y^2)(f(x,y)) &= 102x^3y^3 + 306x^3y^4 + 32(12n - 24)x^4y^4 \\
&\quad + 236(n-1)x^4y^6 + 52(9n^2 - 21n + 12)x^6y^4.
\end{aligned}$$

The required result can obtain by using Table 1. □

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