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FULL PAPER

Topological properties of sunscreens using mhr-polynomial of graph

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In this work, M_{hr}- polynomial of oxybenzone, menthyl anthranilate, benzophenone-4, and dimethylamino hydroxybenzoyl hexa benzoate were established. The degree-based topological indices HDR version of Modified Zagreb topological index (HDRM*), HDR version of Modified forgotten topological index (HDRF*), and HDR version of hyper Zagreb index (HDRHM*) were obtained. Accordingly, by using the derivative of M_{hr}- polynomial of sunscreens, the HDRM*, HDRF*, and HDRHM* topological indices of sunscreens were found.

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KEYWORDS

$d_{hr}(v)$ degree; HDR topological indices; M_{hr}-polynomial; oxybenzone; menthyl anthranilate; benzophenone-4; dimethylamino hydroxybenzoyl hexa benzoate.

Introduction

A molecular graph is an undirected graph. It is denoted by G=(V, E), which shows the general properties of the molecular compound, where the vertices of the shovel |V| represent the number of atoms. In contrast, the edges E represent the juxtaposition relationship between those vertices that represent the atoms of the molecular compound [1]. In a molecular graph, the vertices represent atoms, and the edges represent chemical bonds, and they correspond to them. Suppose the G graph represents a chemical compound that contains a set of vertices V(G), and a set of edges is E(G). In that case, the degree of the vertex can be defined as the number of neighbors of the vertex in and is represented define by $d_G(v)$, which is the total number of edges associated with v [2]. Topological indices are essential relationships in modeling quantitative relationships for the structure and activity of chemical graphs [3]; for more didcestion about topological indices [7-30].

Topological indicators are fixed values in a graph by which the real values are assigned, taking the graph as a consistent median and giving similar graphs the same value. Wiener index gave the first topological index [2].

In 1947, for studying boiling points of alkanes, one of the topological indices invented at the preliminary level is the so-called Zagreb index, first provided by [4,5]. They investigated how an electron whole energy relied on the shape of molecules and became discussed. The primary Zagreb indices $M_1(G) = \sum_{uv\in E(G)}[d(u/G) + d(vG)]$., $M_2(G)= \sum_{uv\in E(G)}[d(u/G)d(v/G)]$.[6]

DAlsinai A, at al, [1] define (1):

HDR of Zagreb index version modified of Hyper HDR Zagreb indices modified forgotten topological index of graph G by:

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

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

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

And $\mathbf{d_{hr}(v/G)} = |\{\mathbf{u, v \in V(G)} | \mathbf{d(u/G, v/G)} = \lceil \frac{R}{2} \rceil\}|$And $\mathbf{d(u/G, v/G)}$ is the distance between the nods u and v in V(G), and R is the radius of graph G.

Also, [1] are define(2): the $\boldsymbol{M_{hr}}$ polynomilal for graph

G is $M_{hr}(i,j)(G), i,j \geq 1$, be the |E(G)| such that $\{d_{hr}(u/G); d_{hr}(v/G)\} = \{i,j\}$. *Let* $M_{hr}(i,j) = |M_{hr}(i,j)|$. The M_{hr} −polynomial of a graph as

$$M_{hr}(G,x,y) = \sum_{\delta_{hr}\leq i\leq j\leq \Delta_{hr}} M_{hr}(i,j)x^i y^j.$$

TABLE 1 Derivation of HDR degree-based topological Indices of graph G

Topological Indices	f(x,y)	Derivation From M_{hr} polynomial
$\mathbf{HDRM_1^*(G)}$	(x+y)	$(D_x+D_y)(M_{hr})\|_{x=y=1}$
$\mathbf{HDRHM_1^*(G)}$	$(x+y)^2$	$(D_x+D_y)^2(M_{hr})\|_{x=y=1}$
$\mathbf{HDRF^*(G)}$	X^2+y^2	$(D^2_x+D^2_y)(M_{hr})\|_{x=y=1}$

Materials and methods

Our main results including comuting M_{hr}-polynomial of Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate, the degree-based topological indices HDRM*, HDRF*, and HDRHM* obtained by using the derivative of M_{hr}-polynomial of sunscreens the HDRM*, HDRF*, and HDRHM* topological indices of sunscreens, are found.

Main results

This section includes two subsections computation Mhr- polynomial of Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate, and computation topological indices of sunscreens (Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate).

Evalute the M_{hr}- polynomial of Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate

In this subsection, we compute the M_{hr}Polynomial of the sunscreens structures and we represent Mhr (3D) graphical using MATLAB.

Oxybenzone

Let ***G*** be a graph of oxybenzone, as shown in Figure 1. Then the graph *G* has 17 vertices and 17 edges.

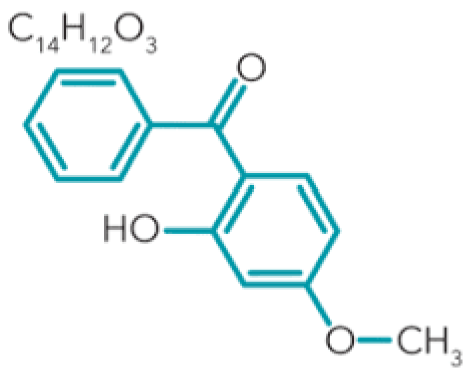

FIGURE 1 Oxybenzone graph with 17 points and17 edges

TABLE 2 |E| of Oxybenzone by $d_{hr}(v)$ degree

$M_{hr}(i,j)$	$Mhr(2,2)$	$Mhr(2,4)$	$Mhr(2,5)$	$Mhr(3,4)$	$M_{hr}(3,5)$	$M_{hr}(4,5)$	$M_{hr}(3,3)$	$M_{hr}(2,3)$	$M_{hr}(1,2)$
no.edge	3	1	1	2	3	1	2	2	2

Theorem 1. Let G be a graph of oxybenzone. Then

$M_{hr}(G,x,y) = 2xy^2 + 3x^2x^2 + x^2y^4 + x^2y^5 + 2x^3y^4 + 3x^3y^5 + x^4y^5 + 2x^3y^3 + 2x^2y^3$.

Proof. Let G a graph of Oxybenzone as in Figure 1. Then by using Table 2 and Definition2, we have:

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \le i \le j \le \Delta_{hr}} M_{hr}(i,j)x^i y^j$$
$$= M_{hr}(1,2)xy^2 + M_{hr}(2,2)x^2 y^2 + M_{hr}(2,4)x^2y^4 + M_{hr}(2,5)x^2y^5 + M_{hr}(3,4)x^3x^4 + M_{hr}(3,5)x^3y^5 + M_{hr}(4,5)x^4y^5 + M_{hr}(3,3)x^3y^3 + M_{hr}(2,3)x^2y^3$$
$$= 2xy^2 + 3x^2y^2 + x^2y^4 + x^2y^5 + 2x^3y^4 + 3x^3y^5 + x^4y^5 + 2x^3y^3 + 2x^2y^3.$$

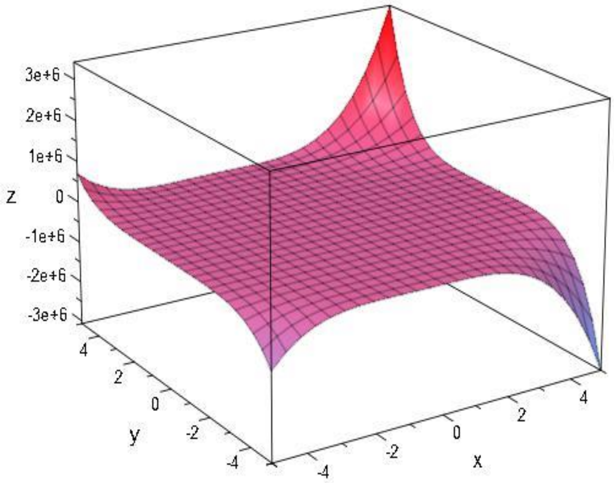

FIGURE 2 M_{hr} –polynomial of oxybenzon

Menthyl anthranilate

Let G be a graph of Menthyl Anthranilate, as shown in Figure 3. The graph G contain 18 vertices and 19 edges.

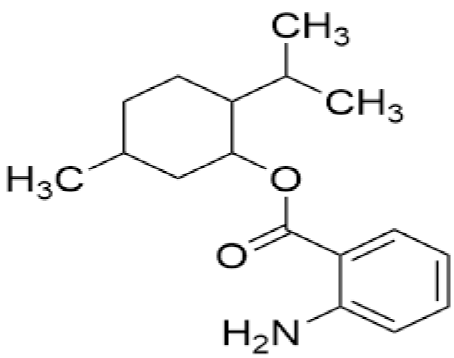

FIGURE 3 The graph of menthyl anthranilate with 19 points and 20 edge

TABLE 3 The |E(G)| of menthyl anthranilate using $d_{hr}(u)$ degree

$M_{hr}(i,j)$	$Mhr(2,2)$	$Mhr(2,3)$	$Mhr(3,3)$	$Mhr(3,5)$	$Mhr(5,4)$	$Mhr(2,4)$
no.edge	5	4	3	3	3	2

Theorem 2. Let G be a graph of menthyl anthranilate. Then

$$M_{hr}(G,x,y) = 5x^2y^2 + 4x^2y^3 + 3x^2y^4 + 3x^3y^3 + 3x^3y^5 + 2x^4y^5$$

Proof. Let G be a graph of Menthyl Anthranilate as in Figure3. Then by using Table 3 and Definition 2, we have

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \le i \le j \le \Delta_{hr}} M_{hr}(i,j)x^i y^j = M_{hr}(2,2)\, x^2y^2 + M_{hr}(2,3)x^2y^3 + M_{hr}(2,4)x^2y^4 + M_{hr}(3,3)x^3y^3 + M_{hr}(3,5)x^3y^5 + M_{hr}(4,5)x^4y^5$$
$$= 5x^2y^2 + 4x^2y^3 + 3x^2y^4 + 3x^3y^3 + 3x^3y^5 + 2x^4y^5.$$

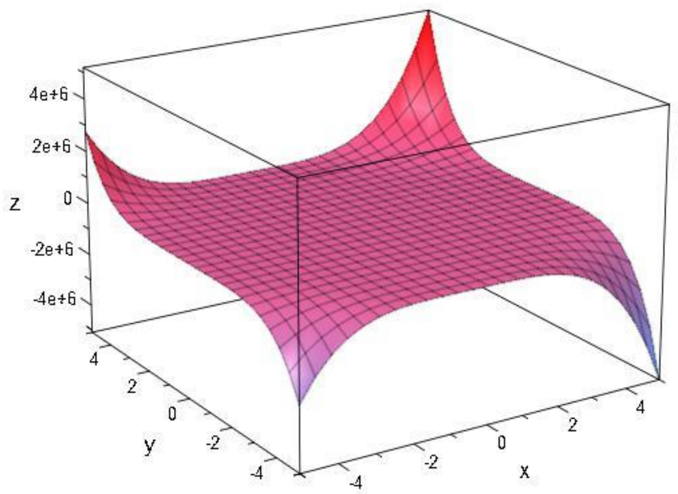

FIGURE 4 M_{hr} −polynomial of menthyl anthranilate

Benzophenone-4

Let G be a graph of Benzophenone-4, as shown in Figure 5. Then the graph G contain 21 points and 22 edges and

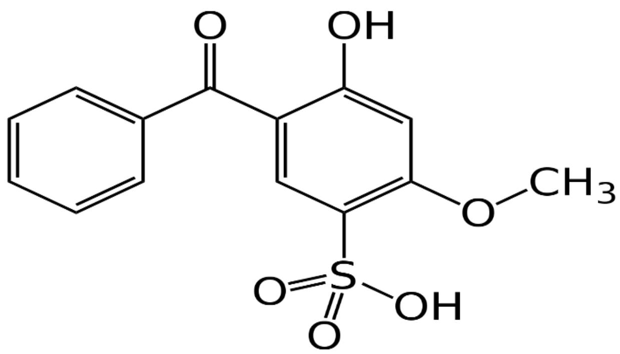

FIGURE 5 The graph of benzophenone-4 contains 22vertices and 21 edges

TABLE 4 The number of edges of benzophenone-4 using $d_{hr}(v)$ degree

$M_{hr}(i,j)$	$M_{hr}(2,3)$	$M_{hr}(3,3)$	$M_{hr}(3,8)$	$M_{hr}(3,5)$	$M_{hr}(4,8)$	$M_{hr}(4,4)$
no.edge	6	3	1	3	1	2
$M_{hr}(i,j)$	$M_{hr}(4,5)$	$M_{hr}(3,4)$	$M_{hr}(1,2)$			
no.edge	3	1	2			

Theorem 3. Let G be the graph of benzophenone-4. Then

$$M_{hr}(G,x,y) = 6x^2y^3 + 3x^3y^3 + x^3y^8 + 3x^3y^5 + x^4y^8 + 2x^4y^4 + 3x^4y^5 + x^3y^4 + 2\,xy^2$$

Proof. Let G be the graph of Benzophenone-4, as seen in Figure 5. Then by using Table 4 and Definition 2, we have:

$$\begin{aligned} M_{hr}(G,x,y) &= \sum_{\delta_{hr}\le i\le j\le \Delta_{hr}} M_{hr}(i,j)x^i y^j \\ &= M_{hr}(1,2)xy^2 + M_{hr}(2,3)x^2y^3 + M_{hr}(2,2)x^2y^2 + M_{hr}(3,3)x^3y^3 + M_{hr}(3,8)x^3y^8 \\ &\quad + M_{hr}(3,5)x^3y^5 + M_{hr}(4,8)x^4y^8 + M_{hr}(4,4)x^4y^4 + M_{hr}(4,5)x^4y^5 + M_{hr}(3,4)x^3y^4 \\ &= 6x^2y^3 + 3x^3y^3 + x^3y^8 + 3x^3y^5 + x^4y^8 + 2x^4y^4 + 3x^4y^5 + x^3y^4 + 2\,xy^2 \end{aligned}$$

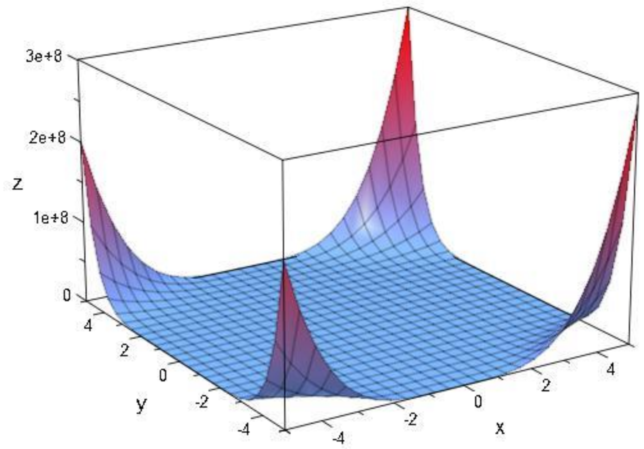

FIGURE 6 M_{hr} −polynomial of benzophenone-4

Dimethylamino hydroxybenzoyl hexa benzoate

Let G be the graph of Dimethylamino hydroxybenzoyl hexa benzoate, as shown in Figure 7. The graph G contains 21 points and 22 edges.

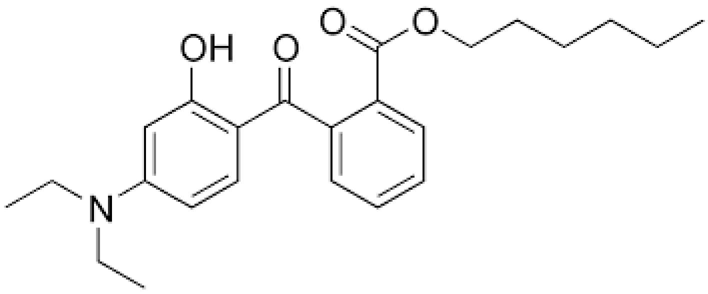

FIGURE 7 The graph of dimethylamino hydroxybenzoyl hexa benzoate with 27 vertices and 29 edges

TABLE 5 The number of edges of Dimethylamino hydroxybenzoyl hexa benzoate, using $d_{hr}(v)$ degree

$\boldsymbol{M_{hr}(i,j)}$	$\boldsymbol{Mhr(1,1)}$	$\boldsymbol{Mhr(2,2)}$	$\boldsymbol{Mhr(2,4)}$	$\boldsymbol{Mhr(4,4)}$	$\boldsymbol{Mhr(3,4)}$	$\boldsymbol{Mhr(3,3)}$
no.edge	4	4	2	1	4	3
$M_{hr}(i,j)$	$Mhr(2,3)$	$Mhr(2,5)$	$Mhr(5,5)$	$Mhr(1,2)$		
no.edge	2	3	2	4		

Theorem 4. Let Gbe a moleculargraph of Dimethylamino hydroxybenzoyl hexa benzoate, then

$$M_{hr}(G,x,y) = 4xy + 4xy^2 + 4x^2y^2 + 2x^2y^4 + x^4y^4 + 4x^3y^4 + 3x^3y^3 + 2x^2y^3 + 3x^2y^5 + 3x^5y^5$$

Proof. Let Ga molecular graph of Dimethylamino hydroxybenzoyl hexa benzoate, as seen in Figure 7. Then by using Table 5 and Definition 2, we have

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \le i \le j \le \Delta_{hr}} M_{hr}(i,j)x^i y^j$$
$$= Mhr(1,1)xy + Mhr(1,2)x^2y^2 + Mhr(2,2)x^2y^2 + Mhr(2,4)x^2y^4 + M_{hr}(4,4)x^4y^4 + M_{hr}(3,4)x^3y^4 + M_{hr}(3,3)x^3y^3 + M_{hr}(2,3)x^2y^3 + M_{hr}(2,5)x^2y^5 + M_{hr}(5,5)x^5y^5$$
$$= 4xy + 4xy^2 + 4x^2y^2 + 2x^2y^4 + x^4y^4 + 4x^3y^4 + 3x^3y^3 + 2x^2y^3 + 3x^2y^5 + 3x^5y^5$$

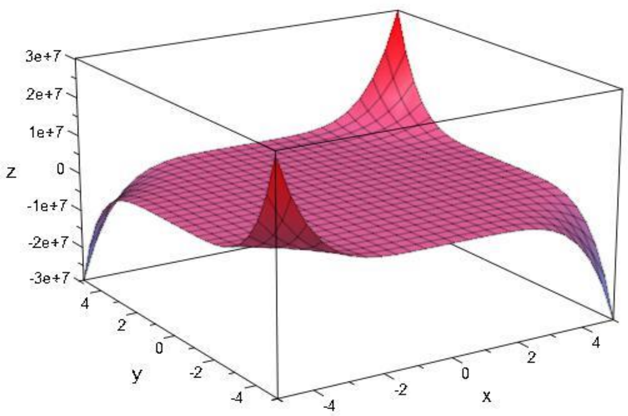

FIGURE 8 M_{hr} –polynomial of dimethylamino hydroxybenzoyl hexa benzoate

Compution HDR topological indices of sunscreens (Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate)

In this subsection, we computed HDR indices of Modified Zagreb topological index (HDRM*), (HDRF*), and (HDRHM*) by using the derivative of Mhr- polynomial of sunscreens

Theorem 5. Let G be the graph of Oxybenzone, and

$M_{hr}(G,x,y) = 2xy^2 + 3x^2y^2 + x^2y^4 + x^2y^5 + 2x^3y^4 + 3x^3y^5 + x^4y^5 + 2x^3y^3 + 2x^2y^3$. Then.

$\mathbf{HDRM_1^*(G)} = 102$.
$\mathbf{HDRF^*(G)} = 383$.
$\mathbf{HDRHM_1^*(G)} = \mathbf{408}$.

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

$(D_x + D_y)f(x,y) = 11x^4y^5 + 24x^3y^5 + 14x^3y^4 + 12x^3y^3 + 7x^2y^5 + 6x^2y^4 + 10x^2y^3 + 12x^2y^2 + 6xy^2$.

$(D_x^2 + D_y^2)f(x,y) = 41x^4y^5 + 102x^3y^5 + 50x^3y^4 + 36x^3y^3 + 29x^2y^5 + 20x^2y^4 + 26x^2y^3 + 24x^2y^2 + 10xy^2$.

$(D_x + D_y)^2f(x,y) = 51x^4y^5 + 114x^3y^5 + 62x^3y^4 + 48x^3y^3 + 27x^2y^5 + 22x^2y^4 + 34x^2y^3 + 36x^2y^2 + 14xy^2$.

Using Table 1, we find the outcome.■

Theorem 6. Let G be a molecular graph of Menthyl Anthranilate, and

$M_{hr}(G,x,y) = 5x^2y^2 + 4x^2y^3 + 3x^2y^4 + 3x^3y^3 + 3x^3y^5 + 2x^4y^5$. Then

$\mathbf{HDRM_1^*(G)} = 118$.
$\mathbf{HDRF^*(G)} = 390$
$\mathbf{HDRHM_1^*(G)} = \mathbf{750}$.

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

$(D_x + D_y)f(x,y) = 20x^2y^2 + 20x^2y^3 + 18x^2y^4 + 18x^3y^3 + 24x^3y^5 + 18x^4y^5$.

$(D_x^2 + D_y^2)f(x,y) = 41x^4y^5 + 102x^3y^5 + 50x^3y^4 + 36x^3y^3 + 29x^2y^5 + 20x^2y^4 + 26x^2y^3 + 24x^2y^2 + 10xy^2$.

$(D_x + D_y)^2f(x,y) = 80x^2y^2 + 100x^2y^3 + 108x^2y^4 + 108x^3y^3 + 192x^3y^5 + 162x^4y^5$

Using Table 1, we find the outcome .■

Theorem 7. Let G be a molecular graph of Benzophenone-4, and

$M_{hr}(G,x,y) = 6x^2y^3 + 3x^3y^3 + x^3y^8 + 3x^3y^5 + x^4y^8 + 2x^4y^4 + 3x^4y^5 + x^3y^4 + 2\,xy^2$. Then

$\mathbf{HDRM_1^*(G)} = 148$
$\mathbf{HDRF^*(G)} = 390$
$\mathbf{HDRHM_1^*(G)} = \mathbf{1137}$.

Proof. Let $M_{hr}(G,x,y) = f(x,y) = 6x^2y^3 + 3x^3y^3 + x^3y^8 + 3x^3y^5 + x^4y^8 + 2x^4y^4 + 3x^4y^5 + x^3y^4 + 2\,xy^2$. Then

Then we have,

$(D_x + D_y)f(x,y) = 30x^2y^3 + 15x^3y^3 + 11x^3y^8 + 24x^3y^5 + 12x^4y^8 + 16x^4y^4 + 27x^4y^5 + 7x^3y^4 + 6\,xy^2$. Then

$$(D_x^2 + D_y^2)f(x,y) = 78x^2y^3 + 45x^3y^3 + 73x^3y^8 + 102x^3y^5 + 80x^4y^8 + 64x^4y^4 + 168x^4y^5 + 25x^3y^4 + 10\,xy^2$$

$$(D_x + D_y)^2f(x,y) = 150x^2y^3 + 99x^3y^3 + 121x^3y^8 + 192x^3y^5 + 128x^4y^8 + 128x^4y^4 + 288x^4y^5 + 49x^3y^4 + 18\,xy^2$$

Using Table 1, we find the outcome .■

Theorem 8. Let G be a molecular graph of Dimethylamino hydroxybenzoyl hexa benzoate, and

$M_{hr}(G,x,y) = 4xy + 4xy^2 + 4x^2y^2 + 2x^2y^4 + x^4y^4 + 4x^3y^4 + 3x^3y^3 + 2x^2y^3 + 3x^2y^5 + 3x^5y^5$. Then

$\mathbf{HDRM_1^*(G)} = 163.$
$\mathbf{HDRF^*(G)} = 549.$
$\mathbf{HDRHM_1^*(G)} = \mathbf{1055}.$

Proof. Let $M_{hr}(G,x,y) = f(x,y) = 4xy + 4xy^2 + 4x^2y^2 + 2x^2y^4 + x^4y^4 + 4x^3y^4 + 3x^3y^3 + 2x^2y^3 + 3x^2y^5 + 3x^5y^5$. Then

Then we have,

$(D_x + D_y)f(x,y) = 8xy + 12xy^2 + 16x^2y^2 + 12x^2y^4 + 8x^4y^4 + 28x^3y^4 + 18x^3y^3 + 10x^2y^3 + 21x^2y^5 + 30x^5y^5$. Then

$$(D_x^2 + D_y^2)f(x,y) = 8xy + 20xy^2 + 32x^2y^2 + 40x^2y^4 + 32x^4y^4 + 100x^3y^4 + 54x^3y^3 + 26x^2y^3 + 87x^2y^5 + 150x^5y^5$$

$(D_x + D_y)^2 f(x,y) = 16xy + 36xy^2 + 64x^2y^2 + 72x^2y^4 + 64x^4y^4 + 198x^3y^4 + 108x^3y^3 + 50x^2y^3 + 147x^2y^5 + 300x^5y^5$.■

FIGURE 6 The structure of Benzophenone-4

Conclusion

We found Mhr- polynomial of Oxybenzone, Menthyl Anthranilate, Benzophenone-4, and Dimethylamino hydroxybenzoyl hexa benzoate, the degree-based topological indices HDRM*, HDRF*, HDRHM* obtained. By using the derivative of Mhr- polynomial of sunscreens the HDRM*, HDRF*, and HDRHM* topological indices of sunscreens, were found. The results of the HDRM*, HDRF*, and HDRHM* of sunscreens are better than the leap indices and Zagreb Indices.

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