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NM-polynomials and Neighborhood Degree Based Topological Indices of Some Benzenoid Systems

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ABSTRACT

Topological indices are numerical descriptors of a chemical structure represented by a graph. Topological indices are used to predict the physical, chemical, and biological properties of chemical structures without experimentation. In this study, the closed forms of the NM-polynomials of and neighborhood degree-based topological indices of the triangular, zigzag, and rhombic benzenoids are calculated. In addition, the topological indices of the studied benzenoids are compared.

Bazı Benzenoid Sistemlerin NM-polinomları ve Komşuluk Derecesine Dayalı Topolojik İndeksleri

Araştırma Makalesi

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Benzenoidler

ÖZ

Topolojik indeksler, bir grafla temsil edilen bir kimyasal yapının sayısal tanımlayıcılarıdır. Topolojik indeksler, kimyasal yapıların fiziksel, kimyasal ve biyolojik özelliklerini deney yapmadan tahmin etmek için kullanılır. Bu çalışmada, üçgen, zikzak ve eşkenar dörtgen benzenoidlerin NM-polinomlarının kapalı formları ve komşu derecesine dayalı topolojiksel indisleri hesaplanmıştır. Ayrıca her bir benzenoid için topolojik indeksleri karşılaştırılmıştır.

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Introduction

Chemical graph theory is a field that studies polynomials and topological indices that predict the properties of chemical structures with graph theory, an area of discrete mathematics. Topological indices are numerical descriptors of the graph representation of a chemical structure. A graph representation of a chemical structure, that is, a chemical graph, is a 2D image of a dehydrogenated chemical. The atoms of the chemical structure are represented as the tops of the graph and the interatomic bonds as the edges of the graph. Topological indices have been used to predict the properties of chemical structures since 1947 (Wiener, 1947). Since then, numerous topological indices have been defined that depend on the topology of the graph (Liu and Singaraj, 2021; Rosary, 2022; Rosary and Fufa, 2022). In some graphs, it can be difficult to calculate topological indices. Therefore, polynomials related to topological indices are defined. One of them is NM-polynomials depending on the neighborhood degree. Havare found that the neighborhood harmonic index for the molar volume property of new cancer drugs is the best predictor index among many topological indices (Havare, 2021). Mondal studied NM-polynomials for Titanium (Mondal et al., 2021). Afzal et al. calculated the NM-polynomials of starphene (Afzal et al., 2022). Çolakoğlu calculated the neighborhood degree-based topological indices of cycle-related graphs (Çolakoğlu, 2022). Sözen and Eryaşar calculated the NM-coindices of potential drug candidates against COVID-19 and obtained QSPR modeling (Sözen and Eryaşar, 2023).

Benzenoids are chemicals with a C_nH_s structure, consisting of hexagons. These chemicals are used in pharmaceutical industry, and food. Akhter and Imran calculated topological indices of triangular benzenoids (Akhter and Imran, 2016). Kwun et al. obtained Zagreb indices and polynomials of benzenoid systems (Kwum et al., 2018a). Afzala calculated the Banhattin indices of zigzag benzenoids (Afzala et al., 2021). Awais et al. studied the irregularity indices of benzenoid graphs (Awais et al., 2023). The M-polynomial and degree-dependent topological indices of some benzenoids were calculated (Ali et al., 2018; Kwun, 2018b; Mumammed et al., 2020). Rosary et al. studied valency-based irregular indices of some benzenoids (Rosary et al., 2023).

In this study, benzenoid systems used in chemistry and industry are discussed with graph theory. The results are intended to be used in QSPR and QSAR modeling for the production of new chemicals. For this purpose, neighborhood polynomials of the zigzag, triangular and rhombic benzenoids are obtained. Using these polynomials, topological indices depending on the neighborhood degree are calculated. The graphics obtained using the MATLAB program are compared.

Material and Methods

If a graph G has $p, q \in V(G)$ vertex set and $pq \in E(G)$ edge set, then the order (size) of vertices (edges) is defined as $|V(G)|$ ($|E(G)|$). The degree of the vertex p of a graph G is denoted by d_p. The neighborhood of a vertex p in a graph G, $N(p)$, is the set of all vertices adjacent to p (Chartrand et al., 2010). Let $\delta_q = \sum_{p \in N(q)} d_p$ and $\tau^*{}_{ij} = \{|\widetilde{NE}_{i,j}|\,|\delta_p = i, \delta_q = j\}$.

The neighborhood M-polynomial is defined in (Verma et al., 2019) as

$$NM(G,r,s) = \sum_{i \le j} \tau^*{}_{ij} r^i s^j. \quad (1)$$

Neighborhood degree-based topological indices are respectively defined as

$$NTI(G) = \sum_{uv \in E'_{i,J}} \varphi(\delta_u, \delta_v).$$

The formulas of third version of Zagreb ($\acute{M}_1$), neighborhood second modified Zagreb ($\acute{M}_2$), neighborhood forgotten ($\acute{F}$), third NDe (ND_3), fifth NDe (ND_5), neighborhood inverse sum indeg ($I\acute{S}I$), neighborhood harmonic ($\acute{H}$) which are neighborhood degree-based topological indices are given in the following table (see Table 1).

Table 1. The formulas of neighborhood degree-based topological indices.

Topological Indices	Formulas	Derivation From $NM(G,r,s)$
$M_1'(G)$	$\sum_{uv \in E(G)}(\delta_u + \delta_v)$	$\left((D_r + D_s)NM(G,r,s)\right)_{r=s=1}$
$M_2'(G)$	$\sum_{uv \in E(G)}(\delta_u \delta_v)$	$(D_r D_s)\left(NM(G,r,s)\right)_{r=s=1}$
$\acute{F}$	$\sum_{uv \in E(G)}\left({\delta_u}^2 + {\delta_v}^2\right)$	$\left({D_r}^2 + {D_s}^2\right)\left(NM(G,r,s)\right)_{r=s=1}$
NDe_3	$\sum_{uv \in E(G)}(\delta_u \delta_v)(\delta_u + \delta_v)$	$D_r D_s (D_r + D_s)\left(NM(G,r,s)\right)_{r=s=1}$
ND_5	$\sum_{uv \in E(G)}\left(\frac{\delta_u}{\delta_v} + \frac{\delta_v}{\delta_u}\right)$	$(D_r E_s + E_r D_s)\left(NM(G,r,s)\right)_{r=s=1}$
$I\acute{S}I$	$\sum_{uv \in E(G)}\left(\frac{\delta_u \delta_v}{\delta_u + \delta_v}\right)$	$(E_r J D_r D_s)\left(NM(G,r,s)\right)_{r=1}$
$\acute{H}$	$\sum_{uv \in E(G)}\frac{2}{(\delta_u + \delta_v)}$	$(2E_r J)\left(NM(G,r,s)\right)_{r=1}$

Where:

$D_r = r\left(\frac{\partial(NM(G,r,s))}{\partial r}\right)$, $D_s = s\left(\frac{\partial(NM(G,r,s))}{\partial s}\right)$, $E_r = \int_0^r \frac{NM(G,t,r)}{t} dt$, $E_s = \int_0^s \frac{NM(G,r,t)}{t} dt$, $J(\varphi(r,s)) = NM(G,r,r)$.

The graphs of zigzag benzenoids, ZZ_n, have $8n + 2$ vertices and $10n + 1$ edges. Figure 1 shows the zigzag benzenoids with the hydrogen atoms removed (Kwun et al, 2018a).

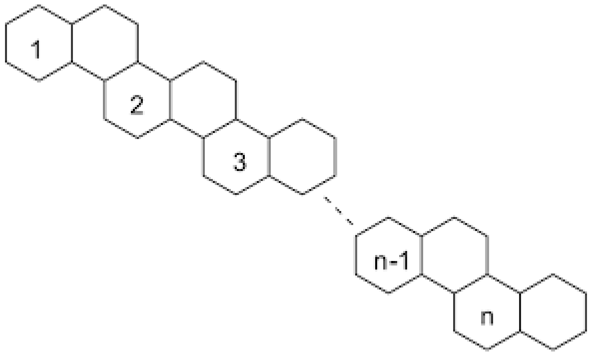

Figure 1. The graph of zigzag benzenoids (Kwun et al, 2018a).

The graphs of triangular benzenoids, $TB(n)$, have $8n + 2$ vertices and $10n + 1$ edges. Figure 2 shows the graph of triangular benzenoids (Kwun et al, 2018a).

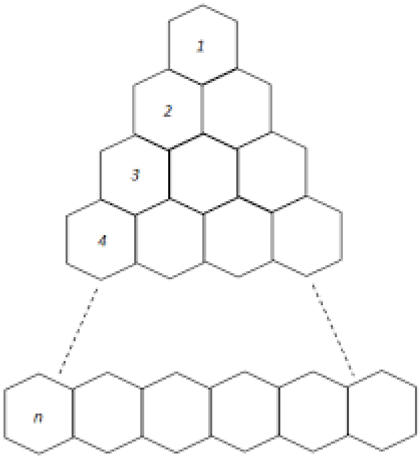

Figure 2. Triangular benzenoids (Kwun et al, 2018a).

The graphs of rhombic benzenoids, $RB(n)$, have $2n(n + 2)$ vertices and $3n^2 + 4n - 1$ edges. Figure 3 shows the rhombic benzenoids and its graph.

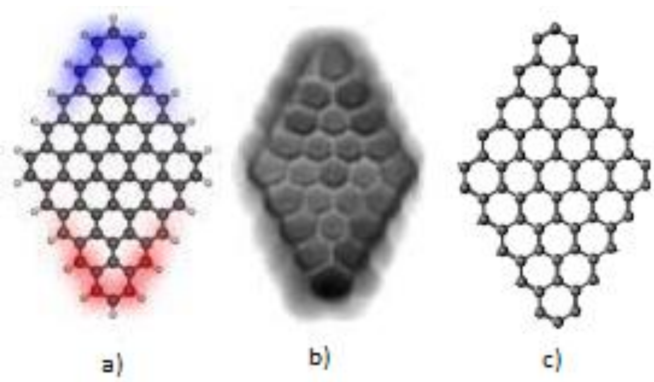

Figure 3. a) [5]-Rhombene (Mishra et al.,2021), b) $C_{70}H_{22}$ open-shell (Mishra et al., 2021) c) its graph, $RB(5)$

Results and Discussion

In this section, the neighborhood M-polynomials of zigzag benzenoids, triangular benzenoids, and rhombic benzenoids are calculated. Using these polynomials, the first and second Zagreb, forgotten, harmonic, inverse sum indices, third NDe and fifth NDe indices based on neighborhood are calculated.

Theorem 1. The neighborhood M-polynomial of ZZ_n is

$$NM(ZZ_n, r, s) = 2r^4s^4 + 4r^4s^5 + 4r^5s^7 + (2n-2)r^5s^5 + (4n-4)r^5s^8 + 2r^7s^8 + (4n-5)r^8s^8.$$

Proof. From Figure 1, $|\widetilde{NE}_{4,4}| = 2$, $|\widetilde{NE}_{4,5}| = 4$, $|\widetilde{NE}_{5,7}| = 4$, $|\widetilde{NE}_{5,5}| = 2n-2$, $|\widetilde{NE}_{5,8}| = 4n-4$, $|\widetilde{NE}_{7,8}| = 2$, $|\widetilde{NE}_{8,8}| = 4n-5$.

From the Equation (1), it is obtained

$$NM(ZZ_n, r, s) = \sum_{4\le 4} \tau^*{}_{44} r^4s^4 + \sum_{4\le 5} \tau^*{}_{45} r^4s^5 + \sum_{5\le 5} \tau^*{}_{55} r^5s^5 + \sum_{5\le 7} \tau^*{}_{57} r^5s^7 + \sum_{5\le 8} \tau^*{}_{58} r^5s^8 + \sum_{7\le 8} \tau^*{}_{78} r^7s^8 + \sum_{8\le 8} \tau^*{}_{88} r^8s^8$$

or

$$NM(ZZ_n, r, s) = 2r^4s^4 + 4r^4s^5 + 4r^5s^7 + (2n-2)r^5s^5 + (4n-4)r^5s^8 + 2r^7s^8 + (4n-5)r^8s^8.$$

Corollary 2. The topological indices based on the neighborhood degree of the ZZ_n graph are

1. $\acute{M}_1(ZZ_n) = 136n - 22.$
2. $\acute{M}_2(ZZ_n) = 466n - 166.$
3. $\acute{F}(ZZ_n) = 968n - 346.$
4. $NDe_3(ZZ_n) = 6676n - 3364.$
5. $ND_5(ZZ_n) = \frac{209}{10}n + \frac{251}{140}.$
6. $I\acute{S}I(ZZ_n) = \frac{433}{13}n - \frac{3092}{585}.$
7. $\acute{H}(ZZ_n) = \frac{197}{130}n + \frac{3191}{4680}.$

Proof. Using Theorem 1 and Table 1, the following equations are obtained

$$D_r(NM(ZZ_n, r, s) = 8r^4s^4 + 16r^4s^5 + 20r^5s^7 + 5(2n-2)r^5s^5 + 5(4n-4)r^5s^8 + 14r^7s^8 + 8(4n-5)r^8s^8,$$

$$D_s(NM(ZZ_n, r, s)) = 8r^4s^4 + 20r^4s^5 + 28r^5s^7 + 5(2n-2)r^5s^5 + 8(4n-4)r^5s^8 + 16r^7s^8 + 8(4n-5)r^8s^8,$$

$$D_rD_s(NM(ZZ_n, r, s)) = 32r^4s^4 + 80r^4s^5 + 140r^5s^7 + 25(2n-2)r^5s^5 + 40(4n-4)r^5s^8 + 112r^7s^8 + 64(4n-5)r^8s^8,$$

$D_r^{\,2}(NM(ZZ_n,r,s)) = 32r^4s^4 + 64r^4s^5 + 100r^5s^7 + 25(2n-2)r^5s^5 + 25(4n-4)r^5s^8 + 98r^7s^8 + 64(4n-5)r^8s^8$,

$D_s^{\,2}\big(NM(ZZ_n,r,s)\big) = 32r^4s^4 + 100r^4s^5 + 196r^5s^7 + 25(2n-2)r^5s^5 + 64(4n-4)r^5s^8 + 128r^7s^8 + 64(4n-5)r^8s^8$,

$D_rD_s(D_r+D_s)\big(NM(ZZ_n,r,s)\big) = 256r^4s^4 + 720r^4s^5 + 1680r^5s^7 + 250(2n-2)r^5s^5 + 520(4n-4)r^5s^8 + 1680r^7s^8 + 1024(4n-5)r^8s^8$,

$(D_rE_s + E_rD_s)\big(NM(ZZ_n,r,s)\big) = 4r^4s^4 + \frac{41}{5}r^4s^5 + \frac{296}{35}r^5s^7 + 2(2n-2)r^5s^5 + \frac{89}{40}(4n-4)r^5s^8 + \frac{113}{28}r^7s^8 + 2(4n-5)r^8s^8$,

$(E_rJD_rD_s)\big(NM(ZZ_n,r,s)\big) = 4r^8 + \frac{80}{9}r^9 + \frac{35}{3}r^{12} + 5(n-1)r^{10} + \frac{40}{13}(4n-4)r^{13} + \frac{112}{15}r^{15} + 4(4n-5)r^{16}$,

$(2E_rJ)\big(NM(ZZ_n,r,s)\big) = \frac{1}{2}r^8 + \frac{8}{9}r^9 + \frac{2}{3}r^{12} + \frac{(2n-2)}{5}r^{10} + \frac{2(4n-4)}{13}r^{13} + \frac{4}{15}r^{15} + \frac{(4n-5)}{8}r^{16}$,

The following results are obtained:

1. $\acute{M}_1(ZZ_n) = (16r^4s^4 + 36r^4s^5 + 48r^5s^7 + 10(2n-2)r^5s^5 + 13(4n-4)r^5s^8 + 30r^7s^8 + 16(4n-5)r^8s^8)(1,1) = 136n - 22.$
2. $\acute{M}_2(ZZ_n) = (32r^4s^4 + 80r^4s^5 + 140r^5s^7 + 25(2n-2)r^5s^5 + 40(4n-4)r^5s^8 + 112r^7s^8 + 64(4n-5)r^8s^8)(1,1) = 466n - 116.$
3. $\acute{F}(ZZ_n) = (64r^4s^4 + 164r^4s^5 + 296r^5s^7 + 50(2n-2)r^5s^5 + 89(4n-4)r^5s^8 + 226r^7s^8 + 128(4n-5)r^8s^8)(1,1) = 968n - 346.$
4. $NDe_3(ZZ_n) = (256r^4s^4 + 720r^4s^5 + 1680r^5s^7 + 250(2n-2)r^5s^5 + 520(4n-4)r^5s^8 + 1680r^7s^8 + 1024(4n-5)r^8s^8)(1,1) = 6676n - 3364.$
5. $ND_5(ZZ_n) = \left(4r^4s^4 + \frac{41}{5}r^4s^5 + \frac{296}{35}r^5s^7 + 2(2n-2)r^5s^5 + \frac{89}{40}(4n-4)r^5s^8 + \frac{113}{28}r^7s^8 + 2(4n-5)r^8s^8\right)(1,1) = \frac{209}{10}n + \frac{251}{140}.$
6. $I\acute{S}I(ZZ_n) = \left(4r^8 + \frac{80}{9}r^9 + \frac{35}{3}r^{12} + 5(n-1)r^{10} + \frac{40}{13}(4n-4)r^{13} + \frac{112}{15}r^{15} + 4(4n-5)r^{16}\right)(1) = \frac{433}{13}n - \frac{3092}{585}.$
7. $\acute{H}(ZZ_n) = \left(\frac{1}{2}r^8 + \frac{8}{9}r^9 + \frac{2}{3}r^{12} + \frac{(2n-2)}{5}r^{10} + \frac{2(4n-4)}{13}r^{13} + \frac{4}{15}r^{15} + \frac{(4n-5)}{8}r^{16}\right)(1) = \frac{197}{130}n - \frac{3191}{4680}.$

Theorem 2. The neighborhood M-polynomial of TB_n is

$$NM(TB_n, r, s) = 6r^4s^5 + 6r^5s^7 + (6n - 12)r^6s^7 + (3n - 3)r^7s^9 + \frac{3}{2}(3n^2 + n)r^9s^9.$$

Proof. From Figure 2, $|\widetilde{NE}_{4,5}| = 6$, $|\widetilde{NE}_{5,7}| = 6$, $|\widetilde{NE}_{6,7}| = 6n - 12$, $|\widetilde{NE}_{7,9}| = 3n - 3$, $|\widetilde{NE}_{9,9}| = \frac{3}{2}(3n^2 + n)$.

From the Equation (1), it is obtained

$NM(TB_n, r, s) = \sum_{4\le 5} \tau^*{}_{45} r^4s^5 + \sum_{5\le 7} \tau^*{}_{57} r^5s^7 + \sum_{6\le 7} \tau^*{}_{67} r^6s^7 + \sum_{7\le 9} \tau^*{}_{79} r^7s^9 + \sum_{9\le 9} \tau^*{}_{99} r^9s^9$

or

$$NM(TB_n, r, s) = 6r^4s^5 + 6r^5s^7 + (6n - 12)r^6s^7 + (3n - 3)r^7s^9 + \frac{3}{2}(3n^2 + n)r^9s^9$$

Corollary 2. The topological indices based on the neighborhood degree of the TB_n graph are

1. $\acute{M}_1(TB_n) = 81n^2 + 153n - 78.$
2. $\acute{M}_2(TB_n) = \frac{729}{2}n^2 + \frac{1125}{2}n - 363.$
3. $\acute{F}(TB_n) = 729n^2 + 1143n - 720.$
4. $NDe_3(TB_n) = 6561n^2 + 8487n - 5976$
5. $ND_5(TB_n) = 9n^2 + \frac{64}{3}n - \frac{1153}{210}$
6. $I\acute{S}I(TB_n) = \frac{81}{4}n^2 + \frac{7893}{208}n - \frac{12323}{624}$
7. $\acute{H}(TB_n) = \frac{n^2}{4} + \frac{457}{312}n + \frac{35}{312}$

Proof. Using Theorem 2 and Table 1, the following results are obtained

1. $\acute{M}_1(TB_n) = (54r^4s^5 + 72r^5s^7 + 13(6n - 12)r^6s^7 + 16(3n - 3)r^7s^9 + 27(3n^2 + n)r^9s^9)(1,1) = 81n^2 + 153n - 78.$
2. $\acute{M}_2(TB_n) = \left(120r^4s^5 + 210r^5s^7 + 42(6n - 12)r^6s^7 + 63(3n - 3)r^7s^9 + \frac{243}{2}(3n^2 + n)r^9s^9\right)(1,1) = \frac{729}{2}n^2 + \frac{1125}{2}n - 363.$
3. $\acute{F}(TB_n) = (246r^4s^5 + 444r^5s^7 + 85(6n - 12)r^6s^7 + 144(3n - 3)r^7s^9 + 243(3n^2 + n)r^9s^9)(1,1) = 729n^2 + 1185n - 762.$
4. $NDe_3(TB_n) = (1080r^4s^5 + 2520r^5s^7 + 546(6n - 12)r^6s^7 + 1008(3n - 3)r^7s^9 + 2187(3n^2 + n)r^9s^9)(1,1) = 6561n^2 + 8487n - 5976.$

5. $ND_5(TB_n) = \left(\frac{123}{10}r^4s^5 + \frac{444}{35}r^5s^7 + \frac{85}{42}(6n-12)r^6s^7 + \frac{130}{63}(3n-3)r^7s^9 + 3(3n^2+n)r^9s^9\right)(1,1) = 9n^2 + \frac{64}{3}n - \frac{1153}{210}$.

6. $\acute{ISI}(TB_n) = \left(\frac{40}{3}r^9 + \frac{35}{2}r^{12} + \frac{42}{13}(6n-12)r^{13} + \frac{63}{16}(3n-3)r^{16} + \frac{27}{4}(3n^2 + n)r^{18}\right)(1) = \frac{81}{4}n^2 + \frac{7893}{208}n - \frac{12323}{624}$.

7. $\acute{H}(TB_n) = \left(\frac{4}{3}r^9 + r^{12} + \frac{2}{13}(6n-12)r^{13} + \frac{1}{8}(3n-3)r^{16} + \frac{1}{6}(3n^2+n)r^{18}\right)(1) = \frac{n^2}{2} + \frac{457}{312}n + \frac{35}{312}$.

Theorem 3. The neighborhood M-polynomial of RB_n is

$$NM(RB_n, r, s) = 4r^4s^5 + 2r^5s^5 + 8r^5s^7 + (8n-16)r^6s^7 + (4n-4)r^7s^9 + (3n^2 - 8n + 5)r^9s^9.$$

Proof. From Fig. 3, $|\widetilde{NE}_{4,5}| = 4$, $|\widetilde{NE}_{5,5}| = 2$, $|\widetilde{NE}_{5,7}| = 8$, $|\widetilde{NE}_{6,7}| = 8n-16$, $|\widetilde{NE}_{7,9}| = 4n-4$, $|\widetilde{NE}_{9,9}| = 3n^2 - 8n + 5$.

From the Equation (1), it is obtained

$NM(RB_n, r, s) = \sum_{4\le 5} \tau^*{}_{45} r^4s^5 + \sum_{5\le 5} \tau^*{}_{55} r^5s^5 + \sum_{5\le 7} \tau^*{}_{57} r^5s^7 + \sum_{6\le 7} \tau^*{}_{67} r^6s^7 + \sum_{7\le 9} \tau^*{}_{79} r^7s^9 + \sum_{9\le 9} \tau^*{}_{99} r^9s^9$

or

$$NM(RB_n, r, s) = 4r^4s^5 + 2r^5s^5 + 8r^5s^7 + (8n-16)r^6s^7 + (4n-4)r^7s^9 + (3n^2 - 8n + 5)r^9s^9$$

Corollary 3. The topological indices based on the neighborhood degree of the RB_n graph are

1. $\acute{M}_1(RB_n) = 54n^2 + 24n - 30$.
2. $\acute{M}_2(RB_n) = 243n^2 - 60n - 109$.
3. $\acute{F}(RB_n) = 486n^2 - 168n - 142$.
4. $ND_3(RB_n) = 4374n^2 - 3264n - 7463$
5. $ND_5(RB_n) = 6n^2 + \frac{76}{9}n - \frac{479}{315}$
6. $\acute{ISI}(RB_n) = \frac{27}{2}n^2 + \frac{291}{52}n - \frac{3613}{468}$
7. $\acute{H}(RB_n) = \frac{n^2}{3} + \frac{197}{234}n + \frac{253}{1170}$.

Proof. Using Theorem 3 and Table 1, the following results are obtained

1. $\acute{M}_1(RB_n) = (36r^4s^5 + 20r^5s^5 + 96r^5s^7 + 13(8n - 16)r^6s^7 + 16(4n - 4)r^7s^9 + 18(3n^2 - 8n + 5)r^9s^9)(1,1) = 54n^2 + 24n - 30.$

2. $\acute{M}_2(RB_n) = (80r^4s^5 + 50r^5s^5 + 280r^5s^7 + 42(8n - 16)r^6s^7 + 63(4n - 4)r^7s^9 + 81(3n^2 - 8n + 5)r^9s^9)(1,1) = 243n^2 - 60n - 109.$

3. $\acute{F}(RB_n) = (164r^4s^5 + 100r^5s^5 + 592r^5s^7 + 85(8n - 16)r^6s^7 + 112(4n - 4)r^7s^9 + 162(3n^2 - 8n + 5)r^9s^9)(1,1) = 486n^2 - 168n - 142.$

4. $ND_3(RB_n) = (720r^4s^5 + 500r^5s^5 + 3360r^5s^7 + 546(8n - 16)r^6s^7 + 1008(4n - 4)r^7s^9 + 1458(3n^2 - 8n + 5)r^9s^9)(1,1) = 4374n^2 - 3264n - 7463.$

5. $ND_5(RB_n) = \left(\frac{41}{5}r^4s^5 + 4r^5s^5 + \frac{592}{35}r^5s^7 + \frac{85}{42}(8n - 16)r^6s^7 + \frac{130}{63}(4n - 4)r^7s^9 + 2(3n^2 - 8n + 5)r^9s^9\right)(1,1) = 6n^2 + \frac{76}{9}n - \frac{479}{315}.$

6. $I\acute{S}I(RB_n) = \left(\frac{80}{9}r^9 + 5r^{10} + \frac{70}{3}r^{12} + \frac{42}{13}(8n - 16)r^{13} + \frac{63}{16}(4n - 4)r^{16} + \frac{9}{2}(3n^2 - 8n + 5)r^{18}\right)(1) = \frac{27}{2}n^2 + \frac{291}{52}n - \frac{3613}{468}.$

7. $\acute{H}(RB_n) = \left(\frac{8}{9}r^9 + \frac{2}{5}r^{10} + \frac{4}{3}r^{12} + \frac{2(8n-16)}{13}r^{13} + \frac{(4n-4)}{8}r^{16} + \frac{(3n^2-8n+5)}{9}r^{18}\right)(1) = \frac{n^2}{3} + \frac{197}{234}n + \frac{253}{1170}.$

The graphs of the topological indices depending on the neighborhood of the zigzag benzenoid graphs are given in Figure 4.

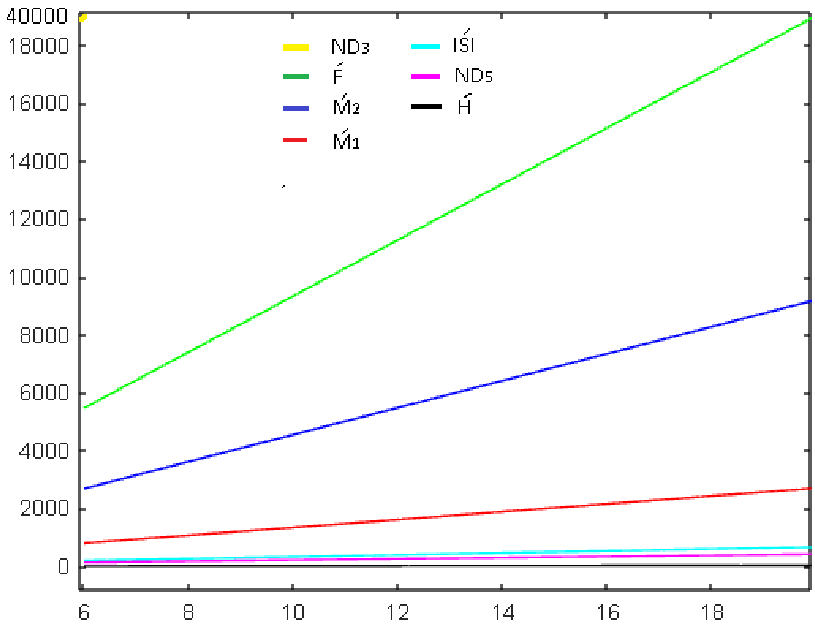

Figure 4. The topological indices of zigzag benzenoid graphs

The fastest growing topological index for zigzag benzenoids is the ND_3 index from Figure 4. It was observed that $ND_3, \acute{F}, \acute{M}_2, \acute{M}_1, I\acute{S}I, ND_5, and\ \acute{H}$, from largest to smallest, respectively. Figure 5 shows the graph of the topological indices depending on the degree of neighborhood of the triangular benzenoid graphs.

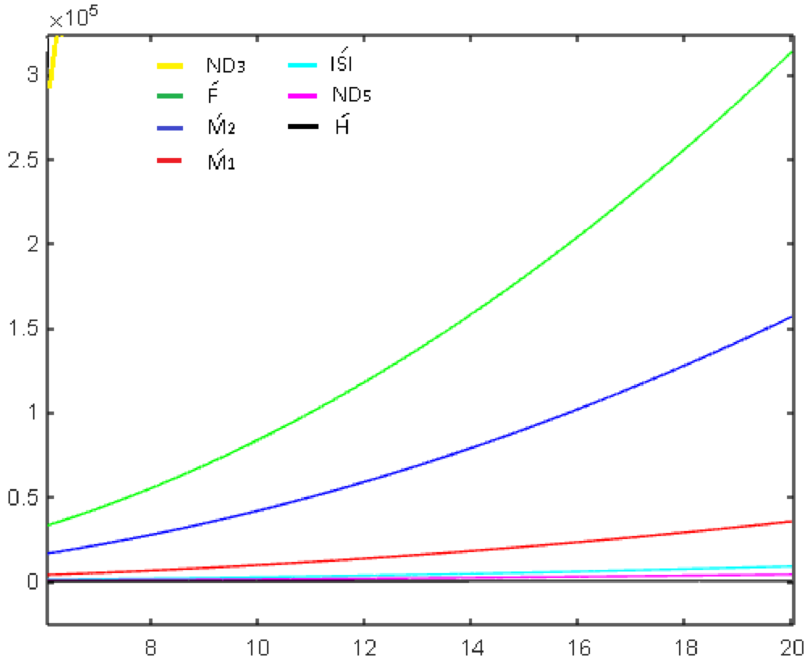

Figure 5. The topological indices of triangular benzenoid graphs

The fastest growing index for triangular benzenoid graphs from Figure 5 is ND_3. The topological indices of triangular benzenoid graphs are $ND_3, \acute{F}, \acute{M}_2, \acute{M}_1, I\acute{S}I, ND_5, and\ \acute{H}$ respectively, from the largest to the smallest values. Figure 6 is a plot of topological indices depending on the degree of adjacency of rhombic benzenoid graphs.

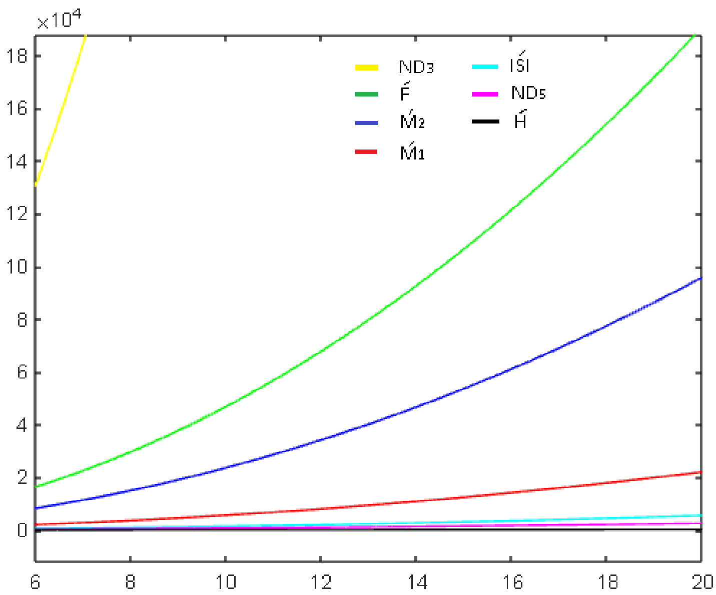

Figure 6. The plots of topological indices for rhombic benzenoid graphs

It is seen from Figure 6 that values of the topological indices depending on the neighborhood of the rhombic benzenoid graphs are $\boldsymbol{ND_3, \acute{F}, \acute{M}_2, \acute{M}_1, I\acute{S}I, ND_5, and\ \acute{H}}$, from the largest to the smallest, respectively.

Conclusion

Recently, it has been important to predict the properties of chemicals for rapid chemical production unexperimented. Therefore, topological indices and studies on this subject have increased. In this study, zigzag benzenoids, triangular benzenoids, and rhombic benzenoids are considered. The neighborhood polynomials of the graphs of these chemicals are found and the topological indices depending on the neighborhood degree are calculated via these polynomials. The neighborhood degree based on first and second Zagreb indices, the neighborhood degree based forgotten, harmonic, inverse sum indices, third NDe and fifth NDe indices are studied.

While the topological indices values of zigzag benzenoids increase linearly, the values of the indices of triangular and rhombic benzenoids increase curvilinearly. For all of these benzenoids, the order of values of the topological indices is the same and the ND_3 index has the largest values, the $\acute{H}$ index has the smallest values. The order of the values of the topological indexes is $ND_3 > \acute{F} > \acute{M}_2 > \acute{M}_1 > I\acute{S}I > ND_5 > \acute{H}$.

The results of this study can be used to predict the properties of new chemicals with the benzenoid system. It will shed light on the fields of chemistry, pharmaceutical industry, mathematical chemistry. These results can be used in QSPR and QSAR studies.

Author’s Contributions

The author declares that she has contributed 100% to the article.

Conflict of Interest

The author has declared that that there are no competing interests.

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