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EXPLORING TOPOLOGICAL INDICES OF OLIGOTHIOPHENE DENDRIMER *VIA* NEIGHBORHOOD M-POLYNOMIALS

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Abstract. In this study, we give some theoretical results for studying the structural connectivity of oligothiophene dendrimer by utilizing the neighborhood M-polynomial. The main result of this article presents the closed formula of neighborhood M-polynomial of oligothiophene dendrimer which is used for computing the neighborhood topological indices of the dendrimer. Among the various indices considered, the forgotten index obtained the highest value, followed by the Sanskruti index, first Zagreb index, and second Zagreb index. These topological indices exhibited an increasing trend as the number of generation increases across the dendrimer structure. Conversely, the general Randic index, harmonic index, geometric-arithmetic index and atom bond connectivity index are the least dominant indices, they display minimal increase as the generation increases. The significance of adopting the neighborhood M-polynomial to compute the topological index lies in the fact that it facilitates the analysis of complex molecules in a timely manner and allows pendant vertex to contribute more effectively to the overall degree value of the dendrimer. Furthermore, the dataset resulting from these topological indices serves as a foundation for future studies aimed at predicting the physicochemical properties of the dendrimer.

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1. Introduction

Oligothiophenes are dendrimers obtained *via* combination of multiple thiophenes, a single thiophene structure consists of a planar five member ring which when translated to a chemical graph will become a cycle graph with five vertices, although it is important to note that each thiohene structure considered in this study consists of an additional pendant vertex of trimethyl silyl (TMS) compound which makes the total vertices in a thiophene chemical graph six. A dendrimer consisting of two or more thiophenes is called an oligothiophene. Oligothiophenes posses an interesting electronic properties due to their π-conjugated structure. The π-electrons in the thiophene units can be delocalized along the conjugated backbone allowing for efficient charge transport and interaction with lights, this makes oligothiophenes applicable in different electronic devices including

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organic field-effect transistors (OFETs), organic lights emitting diodes (OLEDs), organic photovoltaics (solar cells) and sensors (for details on oligothiophenes see [19]). Oligothiophene dendrimers exhibit a unique hierarchical structure composed of repeated units, making them highly complex and attractive to explore *via* graph polynomials.

Goli *et al.* [9] explored the computation of structural connectivity of dendrimers *via* the Narumi-Katayama indices in 2021, the theoretical results for the structural connectivity of these dendrimers were discussed (see [8]). Recently, the M-polynomials have emerged as an efficient means to determine a closed formula for a given topological index (TI). The M-polynomial was introduced by Deutsch and Klavžar [6] in 2015 and it provides an easy and efficient way to compute the degree-based TI associated with graphs. A number of studies have been carried out in relation to M-polynomials of graphs and its application in chemical graph theory and other areas of applications (see [3, 4, 7, 12]). A more efficient extension of the degree-based TI was introduced by Mondal [13] in 2019 called the neighborhood degree sum-based TI, it is a more efficient TI with better predictive capability than the degree-based TI, this was further shown in the works of Mondal *et al.* [15] in 2021, where they introduced the neighborhood versions of six existing degree-based TI and demonstrated their efficiency over their degree-based, distance-based, spectral-based and eccentricity-based TI counterparts. A quantitative structure-property relationship (QSPR) model was conducted to establish a relationship between the computed index values and some physical properties of octane isomers. The results obtained showed that the neighborhood reciprocal Randic index modeled the acentric factor of octane isomer with a higher precision compared to other classes of indices considered. (See [1, 11, 13, 15] for more details).

In 2021, Mondal *et al.* [14] introduced the neighborhood M-polynomial (NM-polynomial) as an extension of the traditional M-polynomial. The NM-polynomial offers a faster alternative approach for calculating the neighborhood degree sum-based TI of large chemical graphs such as dendrimers and nanotubes. Mondal *et al.* [14] utilized the NM-polynomial to derive the neighborhood degree sum-based TI for fractal and Cayley tree dendrimers. Through a comparison between the TI computed from NM-polynomial and M-Polynomial, they concluded that the neighborhood degree sum-based TI exhibited superior performance in modeling entropy, acentric factor, and molar refraction compared to the degree-based versions of the first and second Zagreb indices, forgotten index, Randic index, sum connectivity index, and symmetric degree division index. The NM-polynomial distinguishes itself from the classical M-polynomial through its utilization of a neighborhood edge partitioning system to divide the graph's edges allowing for a thorough and compact partitioning of the graph's edges, the partition set allows the extraction of topological information about the graph, such as the distribution of edges within each vertex's neighborhood. The NM-polynomial has recorded a series of applications in different molecular structures and other field of science ranging from pent-heptagonal nanostructures [20], polycyclic aromatic compounds [10], crystallographic structures [16] and machine learning [2] etc. To gain insights into the current state of literature regarding our topic of discussion, we conducted a bibliometric analysis on the NM-polynomials across various fields of study. The findings reveal that NM-polynomials have predominantly been explored in the domains of chemistry, physics/astronomy and material science, other fields includes mathematics, biochemistry, computer science and pharmacology. By presenting this bibliometric analysis, we aim to provide a comprehensive overview of the research direction surrounding NM-polynomials and highlight their relevance in the aforementioned areas of study.

Given that the existing literature on the application of the NM-polynomial to oligothiophene dendrimers is not yet explored, we are motivated to conduct a comprehensive study of this dendrimer *via* NM-polynomial. By undertaking this study, we aim to contribute to the body of knowledge regarding the NM-polynomial's potential applications and gain insights on the topological indices of oligothiophene dendrimers, thereby expanding the scope of research in this direction.

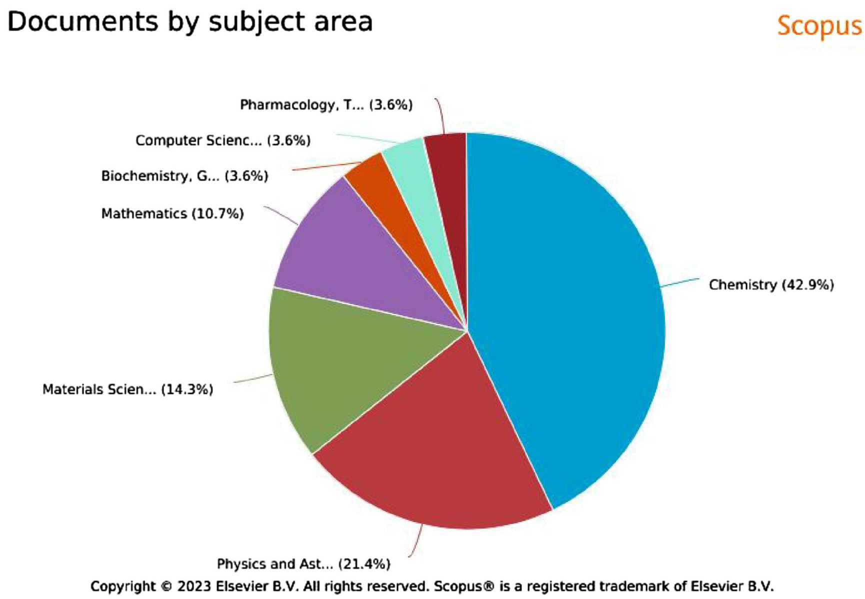

FIGURE 1. Bibliometric analysis of neighbourhoood M-polynomials.

2. Preliminaries

Let $G = (V, E)$ be a simple and connected graph with n vertices and m edges. Let $v \in V$, the degree of v denoted as $d(v)$ is defined as the number of edges connected to v. The neighbors degree of v denoted as $d_N(v)$ is the sum of degree of neigbors of v (we refer the readers to [5, 17, 18] for an extensive introduction to graph theory concepts). Throughout this study, we represent a chemical graph of oligothiophene dendrimers as T_k where k represents the number of thiophenes in the dendrimer. We give a brief review of the M-polynomials below;

[6] Let $m_{ij}(T_k)$, $i, j \geq 1$, be the total number of edges of T_k such that $\{d(u), d(v)\} = \{i, j\}$, the M-polynomial of of T_k is defined as

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

We also recall the definition of NM-polynomial from [10, 14]

$$NM(T_k; x, y) = \sum_{i \leq j} \Gamma]_{ij}(T_k) x^i y^j, \tag{1}$$

where $\Gamma]_{ij}$ is the total number of edges, $uv \in \Gamma](T_k)$ such that $\{d_N(u), d_N(v)\} = \{i, j\}$. The neighborhood degree-based sum TI defined on the collection of a graph T_k is defined as

$$I(T_k; x, y) = \sum_{u,v \in E(T_k)} f(d_N(u), d_N(v)), \tag{2}$$

where $f(d_N(u), d_N(v))$ is the function used to generate the neighbors degree sum of the topological indices. This can further be rewritten as

$$I(T_k; x, y) = \sum_{i \leq j} \Gamma]_{ij} f(i, j). \tag{3}$$

TABLE 1. Some standard neighborhood degree sum-based TI formula derived from NM-polynomial.

Neighborhood Degree Sum-Based TI	Derivation from of NM(T_k)	$f(x,y)$
First Zagreb index $ND_1(T_k)$	$(D_x + D_y)(NM(T_k;x,y))x = y = 1$	$x+y$
Second Zagreb index $ND_2(T_k)$	$(D_xD_y)(NM(T_k;x,y))x = y = 1$	xy
Forgotten index $ND_3(T_k)$	$(D_x^2 + D_y^2)(NM(T_k;x,y))x = y = 1$	x^2+y^2
General Randic index $ND_4(T_k)$	$(D_x^\alpha D_y^\alpha)(NM(T_k;x,y))x = y = 1$	$\frac{1}{(xy)^\alpha}$ for $\alpha = 2$
Symmetric division degree index $ND_5(T_k)$	$(D_xS_y + D_yS_x)(NM(T_k;x,y))_{x=y=1}$	$\frac{x^2+y^2}{xy}$
Sanskruti index $ND_6(T_k)$	$S_x^3Q_{-2}JD_x^3D_y^3(NM(T_k;x,y))_{x=1}$	$\left(\frac{xy}{x+y-2}\right)^3$
Harmonic index $ND_7(T_k)$	$2S_xJ(NM(T_k;x,y))_{x=1}$	$\frac{2}{x+y}$
Geometric-arithmetic index $ND_8(T_k)$	$2S_xJ(D_xD_y)^\alpha(NM(T_k;x,y))_{x=1}$	$\frac{2(xy)^\alpha}{x+y}$, for $\alpha \in \frac{1}{2}$
Atom bond connectivity index $ND_9(T_k)$	$S_x^\alpha Q_{-2}JD_x^\alpha D_y^\alpha(NM(T_k;x,y))_{x=1}$	$\left(\frac{x+y-2}{xy}\right)^\alpha$, for $\alpha \in \frac{1}{2}$
Inverse sum index $ND_{10}(T_k)$	$S_xJD_xD_y(NM(T_k;x,y))_{x=1}$	$\frac{xy}{x+y}$

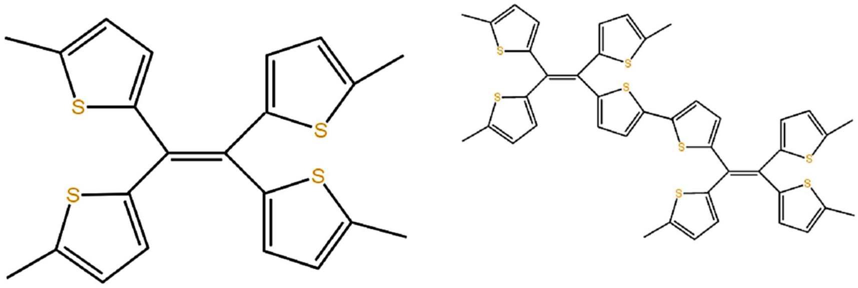

FIGURE 2. First and second generations of oligothiophene dendrimer.

Using operator D_x and D_y defined on differentiable functions of two variables by

$$D_x(f(x,y)) = x\frac{\partial f(x,y)}{\partial x}.$$
$$D_y(f(x,y)) = y\frac{\partial f(x,y)}{\partial y}.$$
$$S_x(NM(T_k;x,y)) = \int_0^x \frac{(NM(T_k))|_{x=z}}{z}dz.$$
$$S_y(NM(T_k;x,y)) = \int_0^y \frac{(NM(T_k))|_{y=z}}{z}dz.$$
$$J(NM(T_k;x,y)) = (NM(T_k))|_{y=x}.$$
$$Q_\alpha = x^\alpha NM(T_k).$$

The NM-polynomial of $20T$-oligothiophene dendrimer will be computed using Table 1 from which a closed formula will be used to compute ten neighbourhood degree sum-based TI of the dendrimer. The dendrimer is named 20T because it contains 20 thiophene components joined together. For the purpose of our study, we will represent a $20T$ chemical graph as T_{20}. The different generations of the dendrimer are illustrated below:

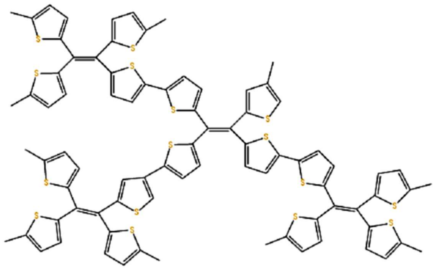

FIGURE 3. Third and fourth generations of oligothiophene dendrimer.

3. Main result

In this section, we establish theoretical results for studying the structural connectivity of oligothiophene dendrimer. We begin by partitioning the edge set of the dendrimer across the different stages of generations based on the sum of neighbor degrees of vertices as illustrated in Figures 2 and 3. This partition serve as a foundation for establishing our theorems and is presented below:

Theorem 3.1. *Let T_{20} be a dendrimer with $n \geq 2$, then the closed form of NM-polynomial is given by*

$$\begin{aligned} NM(T_{20}; x, y) &= (2n+2)x^3y^5 + (6n-4)x^5y^5 + (2n+2)x^5y^6 + (12n-8)x^5y^7 \\ &+ (12n-8)x^6y^7 + 4x^7y^7 + (4n-4)x^7y^9 + (2n-3)x^9y^9. \end{aligned} \tag{4}$$

Proof. From (1) and Table 1, we obtain

$$NM(T_{20}; x, y) = \sum_{i \leq j} \Gamma]_{ij}(T_k)x_iy_j \tag{5}$$

$$\begin{aligned} &= \Gamma]_{3,5}x^3y^5 + \Gamma]_{5,5}x^5y^5 + \Gamma]_{5,6}x^5y^6 + \Gamma]_{5,7}x^5y^7 \\ &+ \Gamma]_{6,7}x^6y^7 + \Gamma]_{7,7}x^7y^7 + \Gamma]_{7,9}x^7y^9 + \Gamma]_{9,9}x^9y^9 \\ &= (2n+2)x^3y^5 + (6n-4)x^5y^5 + (2n+2)x^5y^6 + (12n-8)x^5y^7 \\ &+ (12n-8)x^6y^7 + 4x^7y^7 + (4n-4)x^7y^9 + (2n-3)x^9y^9. \end{aligned} \tag{6}$$

□

In the subsequent results, we will utilize Theorem 3.1 to derive the formulas for computing the neighborhood degree sum-based TI of oligothiophene dendrimer.

Theorem 3.2. *Let T_{20} be a dendrimer with $n \geq 2$, then the neighborhood first and second Zagreb indices and neighborhood forgotten index are given by*

(i) $ND_1(T_{20} = 498n - 264$
(ii) $ND_2(T_{20}) = 1578n - 925$
(iii) $ND_3(T_{20}) = 2842n - 1496$.

Proof. From Theorem 3.1, Tables 1 and 2, we obtain the following neighborhood TI

TABLE 2. Neighborhood edge partition set across the different stages of generation.

$(d_N(u), d_N(v))$ where $u, v \in E(T_k)$	Total number of edges $\lvert\Gamma]\rvert$
$(3,5)$	$2n+2$
$(5,5)$	$6n-4$
$(5,6)$	$2n+2$
$(5,7)$	$12n-8$
$(6,7)$	$12n-8$
$(7,7)$	4
$(7,9)$	$4n-4$
$(9,9)$	$2n-3$

(i) For first Zagreb index

$$(D_x + D_y)[NM(T_k; x, y)] = 8(2n+2)x^3y^5 + 10(6n-4)x^5y^5 + 11(2n+2)x^5y^6 + 12(2n-8)x^5y^7 \\ + 13(12n-8)x^6y^7 + 56x^7y^7 + 16(4n-4)x^7y^9 + 18(2n-3)x^9y^9.$$

At $x = y = 1$, we obtain

$$(D_x + D_y)[NM(T_k; x, y)] = 498n - 264. \tag{7}$$

(ii) For second Zagreb,

$$(D_x \cdot D_y)[NM(T_k; x, y)] = (30n+30)x^3y^5 + (150n-100)x^5y^5 + (60n+60)x^5y^6 + (420n-280)x^5y^7 \\ + (504n-336)x^6y^7 + 196x^7y^7 + (252n-252)x^7y^9 + (162n-243)x^9y^9.$$

At $x = y = 1$, we obtain

$$(D_x \cdot D_y)[NM(T_k; x, y)] = 1578n - 925. \tag{8}$$

(iii) For forgotten index, we obtain

$$(D_x^2 + D_y^2)[NM(T_n; x, y)] = 34(2n+2)x^3y^5 + 50(6n-4)x^5y^5 + 61(2n+2)x^5y^6 + 74(12n-8)x^5y^7 \\ + 85(12n-8)x^6y^7 + 392x^7y^7 + 130(4n-4)x^7y^9 + 162(2n-3)x^9y^9.$$

At $x = y = 1$, we obtain

$$(D_x^2 + D_y^2)[NM(T_n; x, y)] = 2842n - 1496. \tag{9}$$

□

Theorem 3.3. *The neighborhood general Randic index of a T_{20} dendrimer with $n \geq 2$, is given by*

$$ND_4(T_{20}) = \frac{1}{(15)^\alpha}(2n+2) + \frac{1}{(25)^\alpha}(6n-4) + \frac{1}{(30)^\alpha}(2n+2) + \frac{1}{(35)^\alpha}(12n-8) \\ + \frac{1}{(42)^\alpha}(12n-8) + \frac{4}{(49)^\alpha} + \frac{1}{(63)^\alpha}(4n-4) + \frac{1}{(81)^\alpha}(2n-3).$$

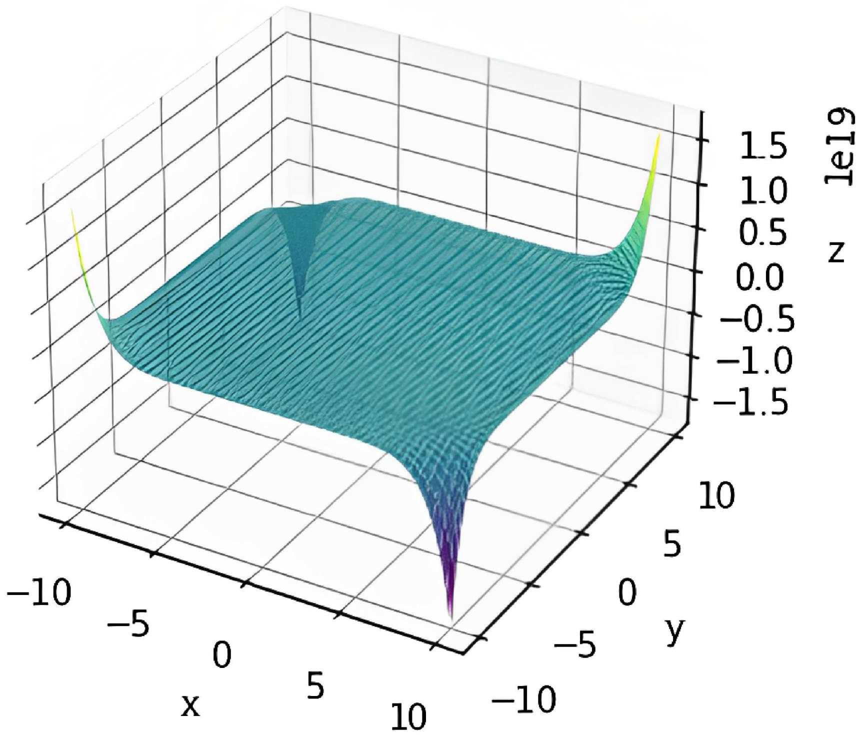

FIGURE 4. 3D plot of NM-polynomial $NM(T_{20}; x, y)$.

Proof. From Theorem 3.1, Tables 1 and 2,

$$\begin{aligned}(S_x^\alpha S_y^\alpha)[NM(T_{20};x,y)] &= \frac{1}{(15)^\alpha}(2n+2)x^3y^5 + \frac{1}{(25)^\alpha}(6n-4)x^5y^5 + \frac{1}{(30)^\alpha}(2n+2)x^5y^6 \\ &+ \frac{1}{(35)^\alpha}(12n-8)x^5y^7 + \frac{1}{(42)^\alpha}(12n-8)x^6y^7 + \frac{1}{(49)^\alpha}(4)x^7y^7 \\ &+ \frac{1}{(63)^\alpha}(4n-4)x^7y^9 + \frac{1}{(81)^\alpha}(2n-3)x^9y^9.\end{aligned}$$

At $x = y = 1$, we obtain

$$\begin{aligned}(S_x^\alpha S_y^\alpha)[NM(T_{20};x,y)] &= \frac{1}{(15)^\alpha}(2n+2) + \frac{1}{(25)^\alpha}(6n-4) + \frac{1}{(30)^\alpha}(2n+2) \\ &+ \frac{1}{(35)^\alpha}(12n-8) + \frac{1}{(42)^\alpha}(12n-8) \\ &+ \frac{4}{(49)^\alpha} + \frac{1}{(63)^\alpha}(4n-4) + \frac{1}{(81)^\alpha}(2n-3).\end{aligned}$$

□

Theorem 3.4. *Let T_{20} be a dendrimer with $n \geq 2$, we define the neighborhood symmetric division degree index as*

$$ND_5(T_{20}) = 82.508n - 44.756. \tag{10}$$

Proof. From Theorem 3.1, Tables 1 and 2, we obtain the neighborhood symmetric division degree index

$$\begin{aligned}(D_xS_y + D_yS_x)[NM(T_k; x, y)] = &\frac{34}{15}(2n+2)x^3y^5 + 2(6n-4)x^5y^5 + \frac{61}{30}(2n+2)x^5y^6\\ &+ \frac{74}{35}(12n-8)x^5y^7 + \frac{85}{42}(12n-8)x^6y^7 + 8x^7y^7\\ &+ \frac{130}{63}(4n-4)x^7y^9 + 2(2n-3)x^9y^9.\end{aligned}$$

At $x = y = 1$, we obtain

$$(D_xS_y + D_yS_x)[NM(T_k; x, y)] = 82.508n - 44.756. \tag{11}$$

□

Theorem 3.5. *The neighborhood Sanskruti index of T_{20} dendrimer with $n \geq 2$, is given by*

$$ND_6(T_{20}) = 2094.884n - 1286.454. \tag{12}$$

Proof. From Theorem 3.1, Tables 1 and 2, we obtain the Sanskruti index

$$\begin{aligned}(S_x^3Q_{-2}JD_x^3D_y^3)[NM(T_{20}, x, y)] = &\left(\frac{15}{6}\right)^3(2n+2)x^6 + \left(\frac{25}{8}\right)^3(6n-4)x^8 + \left(\frac{30}{9}\right)^3(2n+2)x^9\\ &+ \left(\frac{35}{10}\right)^3(12n-8)x^{10} + \left(\frac{42}{11}\right)^3(12n-8)x^{11}\\ &+ 4\left(\frac{49}{12}\right)^3x^{12} + \left(\frac{63}{14}\right)^3(4n-4)x^{14} + \left(\frac{81}{16}\right)^3(2n-3)x^{16}.\end{aligned}$$

At $x = 1$, we obtain

$$(S_x^3Q_{-2}JD_x^3D_y^3)[NM(T_{20}, x, y)] = 2094.884n - 1286.454. \tag{13}$$

□

Theorem 3.6. *Let T_{20} be a dendrimer with $n \geq 2$, the neighborhood harmonic index is given by*

$$ND_7(T_{20}) = 6.632n - 2.763. \tag{14}$$

Proof. From Theorem 3.1, Tables 1 and 2

$$\begin{aligned}(2S_xJ)[NM(T_{20}; x, y)] = &\frac{1}{4}(2n+2)x^8 + \frac{1}{5}(6n-4)x^{10} + \frac{2}{11}(2n+2)x^{11}\\ &+ \frac{1}{6}(12n-8)x^{12} + \frac{2}{13}(12n-8)x^{13} + \frac{4}{7}x^7y^7 + \frac{1}{8}(4n-4)x^{16}\\ &+ \frac{1}{9}(2n-3)x^{18}.\end{aligned}$$

At $x = 1$, we obtain

$$(2S_xJ)[NM(T_{20}; x, y)] = 6.632n - 2.763. \tag{15}$$

□

Theorem 3.7. *Let T_{20} be a dendrimer with $n \geq 2$, the GA index is given by*

$$ND_8(T_{20}) = \frac{(15)^\alpha}{4}(2n+2) + \frac{(25)^\alpha}{5}(6n-4) + \frac{2(30)^\alpha}{11}(2n+2) + \frac{(35)^\alpha}{6}(12n-8) \tag{16}$$

$$+ \frac{2(42)^\alpha}{13}(12n-8) + \frac{4(49)^\alpha}{7} + \frac{(63)^\alpha}{8}(4n-4) + \frac{(81)^\alpha}{9}(2n-3). \tag{17}$$

Proof. From Theorem 3.1, Tables 1 and 2

$$\begin{aligned}2S_xJ(D_xD_y)^\alpha[NM(T_{20};x,y)] &= \frac{(215)^\alpha}{8}(2n+2)x^8 + \frac{2(25)^\alpha}{10}(6n-4)x^{10} + \frac{2(30)^\alpha}{11}(2n+2)x^{11}\\ &+ \frac{2(35)^\alpha}{12}(12n-8)x^{12} + \frac{2(42)^\alpha}{13}(12n-8)x^{13} + \frac{8(49)^\alpha}{14}x^{14}\\ &+ \frac{2(63)^\alpha}{16}(4n-4)x^{16} + \frac{2(81)^\alpha}{18}(2n-3)x^{18}.\end{aligned}$$

At $x = 1$, we have have that

$$\begin{aligned}2S_xJ(D_xD_y)^\alpha[NM(T_{20};x,y)] &= \frac{(15)^\alpha}{4}(2n+2) + \frac{(25)^\alpha}{5}(6n-4) + \frac{2(30)^\alpha}{11}(2n+2) + \frac{(35)^\alpha}{6}(12n-8)\\ &+ \frac{2(42)^\alpha}{13}(12n-8) + \frac{4(49)^\alpha}{7} + \frac{(63)^\alpha}{8}(4n-4) + \frac{(81)^\alpha}{9}(2n-3).\end{aligned}$$

$\square$

Theorem 3.8. *Let T_{20} be a dendrimer with $n \geq 2$, the NABC index is given by*

$$\begin{aligned}ND_9(T_{20}) &= \left(\frac{2}{5}\right)^\alpha(2n+2) + \left(\frac{8}{25}\right)^\alpha(6n-4) + \left(\frac{3}{10}\right)^\alpha(2n+2) + \left(\frac{2}{7}\right)^\alpha(12n-8)\\ &+ \left(\frac{11}{42}\right)^\alpha(12n-8) + \left(\frac{12}{49}\right)^\alpha + \left(\frac{14}{63}\right)^\alpha(4n-4) + \left(\frac{16}{81}\right)^\alpha(2n-3).\end{aligned}$$

Proof. From Theorem 3.1, Tables 1 and 2

$$\begin{aligned}(S^\alpha Q_{-2}JD_x^\alpha D_y^\alpha)[NM(T_{20};x,y)] &= \left(\frac{6}{15}\right)^\alpha(2n+2)x^6 + \left(\frac{8}{25}\right)^\alpha(6n-4)x^8 + \left(\frac{9}{30}\right)^\alpha(2n+2)x^9\\ &+ \left(\frac{10}{35}\right)^\alpha(12n-8)x^{10} + \left(\frac{11}{42}\right)^\alpha(12n-8)x^{11} + \left(\frac{12}{49}\right)^\alpha x^{12}\\ &+ \left(\frac{14}{63}\right)^\alpha(4n-4)x^{14} + \left(\frac{16}{81}\right)^\alpha(2n-3)x^{16}.\end{aligned}$$

At $x = 1$, we have that

$$\begin{aligned}(S^\alpha Q_{-2}JD_x^\alpha D_y^\alpha)[NM(T_{20};x,y)] &= \left(\frac{2}{5}\right)^\alpha(2n+2) + \left(\frac{8}{25}\right)^\alpha(6n-4) + \left(\frac{3}{10}\right)^\alpha(2n+2)\\ &+ \left(\frac{2}{7}\right)^\alpha(12n-8) + \left(\frac{11}{42}\right)^\alpha(12n-8) + \left(\frac{12}{49}\right)^\alpha\\ &+ \left(\frac{14}{63}\right)^\alpha(4n-4) + \left(\frac{16}{81}\right)^\alpha(2n-3).\end{aligned}$$

$\square$

Theorem 3.9. *The neighborhood inverse sum index for a T_{20} dendrimer with $n \geq 2$, is*

$$ND_{10}(T_{20};x,y) = 122.72n - 65.23.$$

Proof. From Theorem 3.1, Tables 1 and 2,

$$\begin{aligned}(S_xJD_xD_y)[NM(T_{20};x,y)] &= \frac{15}{8}(2n+2)x^8 + \frac{25}{10}(6n-4)x^{10} + \frac{30}{11}(2n+2)x^{11} + \frac{35}{12}(12n-8)x^{12}\\ &+ \frac{42}{13}(12n-8)x^{13} + \frac{196}{14}x^{14} + \frac{63}{16}(4n-4)x^{16} + \frac{81}{18}(2n-3)x^{18}.\end{aligned}$$

TABLE 3. The computed values of neighborhood TI of T_{20} oligothiophene dendrimer.

$I(T_{20})$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
$ND_1(T_{20})$	732	1230	1728	2226	2724
$ND_2(T_{20})$	2231	3809	5387	6965	8543
$ND_3(T_{20})$	4188	7030	9872	12714	15556
$ND_4(T_{20})$	0.07	0.11	0.15	0.19	0.23
$ND_5(T_{20})$	120.26	202.77	285.27	367.78	450.29
$ND_6(T_{20})$	2903.33	4998.20	7093.08	9187.97	11282.85
$ND_7(T_{20})$	10.50	17.13	23.77	30.40	37.03
$ND_8(T_{20})$	60.48	100.18	139.87	179.56	219.26
$ND_9(T_{20})$	38.33	64.43	90.52	116.62	142.72
$ND_{10}(T_{20})$	180.19	302.91	425.63	548.35	671.07

At $x=1$, we obtain

$$(S_xJD_xD_y)[NM(T_{20};x,y)] = 122.72n - 65.23. \tag{18}$$

□

In summary, this section establishes a theorem for the computation of closed form of NM-polynomial (see Thm. 3.1) which is then used to determine the formulas for neighborhood degree sum-based TI of the dendrimer, such as the first and second Zagreb index, forgotten index, atom bond connectivity index, geometric arithmetic index etc. The derived neighborhood degree sum-based TI formulas will be employed to determine the numerical parameters associated with the dendrimer in the next subsection of this article.

3.1. Numerical result

In this subsection, we present the numerical values of the TI obtained *via* the derived NM-polynomial expressions. Here, n is the number of generations of the dendrimer. These parameters are particularly important in QSPR models, they allow for easy quantitative comparison and ranking of molecules according to their properties. This is particularly useful when assessing the similarity or dissimilarity between different compounds in a large dataset.

Next, we visualize the data in Table 3 on a 3D bar chart. Visualization of this nature enable easy comparison between the different TI. By visualizing the data side by side, researchers can quickly identify similarities or differences in the values of TI and understand how they relate to each other. This facilitates comparative analysis and helps in identifying the most influential or significant TI in respect of this dendrimer.

4. DISCUSSION

To compute the neighborhood degree sum-based TI of oligothiophene dendrimer *via* NM-polynomial, we followed a step-by-step approach. Initially, we partitioned the dendrimer into four stages of generations, this was done to make partitioning of the edge set easier. Next, we partitioned the edge set based on the sum of neighbor degrees of vertices across each generation. The obtained neighbor degrees for the four generations of the dendrimer were as follows: $(d_N(u), d_N(v)) = (3,5),(5,5),(5,6),(5,7),(6,7),(7,7),(7,9),(9,9)$. Partitioning the edge set based on the sum of neighbor degrees offers a significant advantage in handling pendant vertices. It allows the pendant vertex to contribute more effectively to the overall degree value, providing a more accurate representation of its connectivity, instead of being assigned a degree value of only one. Additionally, the sum of degree of neighbors of vertex provides a measure of the structural importance of every vertex in the dendrimer. Vertices with a higher sum of neighbor degrees tend to play a more crucial role in maintaining the connectivity and overall structure of the dendrimer. The edge partitioning set, which is detailed in Table 2, was instrumental

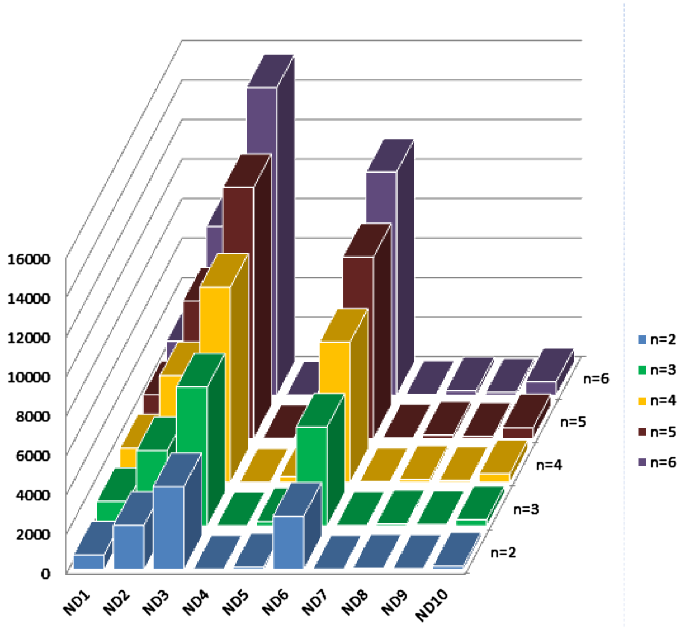

FIGURE 5. Visualization of the computed values of TI on a 3D bar chart.

in computing the general form of the NM-polynomial and subsequent formulas for the neighborhood degree sum-based TI of the dendrimer. These formulas were then utilized to generate the dataset presented in Table 3.

Figure 5 visually represents the dataset of the neighborhood degree sum-based TI in Table 3. Among all the TIs, the Forgotten index (ND_3) stands out as the most dominant index. It exhibits a similar behavior to the Sanskruti index (ND_6), second Zagreb index (ND_2), and first Zagreb index (ND_1), as they all increase with an increase in the value of n. Following the Forgotten index (ND_3), the Sanskruti index (ND_6) emerges as the second most dominant index, followed by the second Zagreb index (ND_2) and the first Zagreb index (ND_1). Although, symmetric division degree index (ND_5) and inverse sum index (ND_{10}) tend to show a little increase with an increase in the value of n. On the other hand, the general Randic index (ND_4), harmonic index (ND_7), geometric-arithmetic index (ND_8) and atom bond connectivity index (ND_9) are the least dominant indices among all. Interestingly, these indices show very little or almost no increase with an increase in the value of n. It is worth noting that despite their numeric values, all the obtained indices are important in their respective roles within the QSPR modeling process. An index may have a low value but can still be highly effective within a QSPR model. These data is important in modeling the physicochemical and electrochemical properties associated with the dendrimer.

5. CONCLUSIONS

In this study, our main objective was to explore the structural connectivity of oligothiophene dendrimer. We conducted a mathematical analysis by calculating the general form of its NM-polynomial, which allowed us to derive closed formulas for computing the neighborhood degree sum-based TI of the dendrimer. Among the various indices considered, the forgotten index obtained the highest value, followed by the Sanskruti index, first Zagreb index, and second Zagreb index. These TI exhibited an increasing trend as the number of generation, denoted by n, increases throughout the dendrimer. This implies that the index values will generally rise as the number of generation across the dendrimer increases. Conversely, the general Randic index, harmonic index, geometric-arithmetic index and atom bond connectivity index are the least dominant indices, they display minimal increase as the generation increases.

The significance of adopting the NM-polynomial to compute the neighborhood degree sum-based TI is twofold. Firstly, it provides a faster and more efficient method for calculating the TI of chemical graphs. This computational advantage facilitates the analysis of complex molecules in a timely manner. Secondly, the application of the NM-polynomial enhances the efficiency of predicting the physicochemical properties of dendrimers during the QSPR modeling process. This is possible because NM-polynomial provides a measure of the structural importance of every vertex in the dendrimer through the neighborhood edge partitioning system where vertices with a higher sum of neighbor degrees tend to play a more crucial role in maintaining the connectivity and overall structure of the dendrimer.

The data obtained from this computation possesses broader implications across various fields such as materials science, chemistry, and drug design. This dataset can be utilized in predictive modeling and QSPR analysis to predict the physicochemical properties of oligothiophene dendrimer. Such predictions can guide the design and development of dendrimers for specific applications, including drug delivery systems, optoelectronic devices, and sensing platforms. In the future, researchers can investigate the analysis of the physicochemical properties of this dendrimer using QSPR models.

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The authors declare that they have no competing interests.

Data availability statement

The manuscript contains all the data relevant to this study.

Ethics Statement

This research does not include studies on human subjects, human data or tissue, or animals.

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