International Journal of Geometric Methods in Modern Physics
Vol. 20, No. 10 (2023) 2350166 (23 pages)

DOI: 10.1142/S0219887823501669

Hosoya polynomials and corresponding indices of aramids

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Received 8 March 2023
Accepted 21 March 2023
Published 4 May 2023

Aramids are man-made high performance fibers admitting useful industrial applications. Aramids can be classified into para-aramids and meta-aramids. Kevlar is a para-aramid and Nomex is a meta-aramid. This work is devoted to compute the empirical formula for the Hosoya polynomial of these aramids. The closed form of a number of distance-related topological indices (TIs) is the famous distance-based Hosoya polynomial. These are Weiner, hyper-Weiner and Tratch–Stankevitch–Zafirov indices. Results exhibit that para-aramid and meta-aramid possess different Hosoya polynomials and corresponding distance-based TIs. Further, distance-related TIs derived from Hosoya polynomial for the para-aramid admit larger values as compared to those of the meta-aramid.

Keywords: Kevlar; Nomex; Hosoya polynomial; Weiner index; hyper-Weiner index; Tratch–Stankevitch–Zafirov index.

Mathematics Subject Classification 2020: 05C12, 05C90, 92E10, 94C15

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1. Introduction

Aramids are aromatic fibers distinguished by rigid polymer chains. They are high performance, strong heat-resistant synthetic fibers. They are utilized for hull strengthening, nautical cordage, and aerospace and military purposes. They are consumed as an asbestos substitute and for the energy storage purposes [1, 2]. Aramids admit high tenacity and high strength-to-weight characteristics. They are significantly resistant to abrasion, cut, tear, bullet/fragment and organic solvents. They possess high melting point, low flammability, integrity, non-conductive and lightweight. They have good integrity under elevated temperatures and sensitive to UV radiations. They are usually non-conductive but degradable under high temperatures (greater than 500°C) [3–5].

Aramids can be characterized as para-aramids and meta-aramids. Para-aramid is a high-strength polyamide, whereas meta-aramid is a heat-resistant polyamide. Para-aramid is crystalline, whereas meta-aramid is semi-crystalline. Furthermore, para-aramid is made using dry-jet wet spinning, whereas meta-aramid is made through wet-spinning. Kevlar is the most prevalent para-aramid, while Nomex is the most frequent meta-aramid.

The mathematical models of molecular structures can be demonstrated as chemical graphs. Atoms and molecular bonds are represented in a chemical graph as the graph's vertices and edges, respectively. A chemical graph leads to the graph invariants (algebraic polynomials or topological indices) in a molecule's topology. A topological index (TI) is a real number used to compute quantitative structure property and structure activity relationships [6]. Distance-based polynomial invariants and TIs have significant applications in chemistry. It is noteworthy that in the recent era the TIs are used to predict the physicochemical properties of the COVID-19 vaccine [7–11]. Moreover, they are also related to the physiochemical properties of fullerenes [12]. Hosoya polynomial is a famous distance-related polynomial serve as a base for many TIs including Weiner, hyper-Weiner and Tratch–Stankevitch–Zafirov (TSZ) indices [13].

The Hosoya polynomial (an algebraic polynomial) is a significant distance-related graph invariant [14] which possesses many chemical applications [15]. Nearly all distance-related TIs can be derived from this polynomial [16,17]. Many distance-related TIs, including the Weiner, hyper-Weiner, and TSZ indices, have a closed form in the Hosoya polynomial. The Wiener index is a measure of the boiling points of alkane molecules [17]. This index links the density, viscosity, critical point, and surface tension of alkane to its liquid transition [18, 19], and the van der Waals surface area of the molecule [20] which are the quantitative structure activity relationships. The Wiener index was a forerunner in the development of other distance-related TIs [21]. The hyper-Wiener index is a number that indicates the subatomic stretching and electronic structures of a particle. The TSZ index is a Wiener index extension.

Hosoya polynomial is widely investigated for distinct chemical structures [22–30]. The distance-related TIs are investigated concerning the applications of molecular structure in medicine, pharmacy and cosmetics, food, biology engineering [31, 32]. A recent investigation of Hosoya polynomial and concerned distance-related indices is made for single wall carbon (n, m) nanotubes, zigzag polyhex nanotube $TUHC_6$, carbon nanotubes TUC_4, capped armchair nanotubes, $C_4C_8(S), C_4C_8, HC_5C_7$ and VC_5C_7 carbon nanosheets [33–38]. The Hosoya and Harary polynomials with the derived TIs are calculated for $TOX(n)$, $RTOX(n)$, $TSL(n)$ and $RTSL(n)$ and hypercube networks [39]. The Hosoya polynomial and Weiner indices of derivatives of Thiazolides have been computed indicating their physiochemical properties. The results confirmed that $RM - 4863$, an effective treatment for viral infections like hepatitis B and C, is a stable physiochemical compound [40]. The Hosoya and the Merrifield–Simmons indices of two benzoid systems R_n and P_n have been calculated for introducing four vectors for each benzoid system [41].

This work deals with the calculations of Hosoya polynomial of two common aramid brands, Kevlar (K) and Nomex (N). The calculations of Hosoya polynomials help us to determine the Weiner, hyper-Weiner and TSZ indices for these aramids. The value of the indices would be graphically computed and compared.

2. Methodology

A molecular graph can be used to display an aramid molecule. Atoms and bonds are, respectively, shown as verticesand edges in a molecular graph. This graph is finite. Take a look at a molecular graph $G = G(V(G), E(G))$ having finite non-empty sets $V(G), E(G)$ that contain the network's vertices and edges, respectively. For any pair of vertices u and v, distance is expressed as $d(u, v)$. The maximum distance between any two vertices in the graph G is shown by the symbol d, and this distance must be calculated in order to determine the Hosoya polynomial of the graph.

A general formula for Hosoya polynomial (in variable x) is given as follows:

$$H(G, x) = |l_1(\mathfrak{n})|x + |l_2(\mathfrak{n})|x^2 + |l_3(\mathfrak{n})|x^3 + |l_4(\mathfrak{n})|x^4 + \cdots + |l_d(\mathfrak{n})|x^d, \tag{1}$$

where the count of pairs of vertices at distance j is $|l_j(\mathfrak{n})|$. We can organize the matrix form for the separation of vertices with a single vertex. It is possible to derive a general form of such matrices. To obtain the jth term coefficient of the Hosoya polynomial, we shall compute the number of vertices with the same distance $|l_j(\mathfrak{n})|$. The TIs, such as the Wiener, hyper-Wiener, and TSZ indices, will be computed applying calculus on Hosoya polynomial.

The Wiener (W), hyper-Weiner (HW) and TSZ indices can be derived from the Hosoya index using the following formulas:

$$W(G) = \frac{d}{dx} H(G, x)|_{x=1}, \tag{2}$$

$$\mathrm{HW}(G) = \frac{1}{2}\frac{d^2}{dx^2}(xH(G,x))|_{x=1}, \tag{3}$$

$$\mathrm{TSZ}(G) = \frac{1}{6}\frac{d^3}{dx^3}(x^2H(G,x))|_{x=1}, \tag{4}$$

where $\frac{d}{dx}, \frac{d^2}{dx^2}, \frac{d^3}{dx^3}$, respectively, represent the first three derivatives corresponding to variable x. The limit $x = 1$ gives the value at specific value 1 of the variable x.

The following steps should be adopted to perform the research:

Step 1: The molecular graph of the aramid (Kevlar and Nomax) will be drawn.
Step 2: The vertices and the distances between all the pair of vertices will be identified to derive empirical distance formulae for them.
Step 3: The Hosoya polynomial will be computed for the aramid using the empirical formulae.
Step 4: The distance-related TIs (Weiner, hyper-Weiner and TSZ indices) will be computed using Software MAPLE on the basis of Hosoya polynomial derived for the aramid.
Step 5: The graphs of Hosoya polynomial and concerning distance-related TIs will be computed and analyzed.

3. Computational Results

This section contains the chemical graphs of the two aramids, Kevlar and Nomax are shown to understand theirstructure. The distance-related calculations lead to the Hosoya polynomial. The expression of Hosoya polynomial leads to the distance-related TIs including Weiner, hyper-Weiner and TSZ indices. All these indices are calculated using the Software Maple.

4. Distance-Based Graph Invariants of Kevlar

Kevlar are fibers with high tenacity, elongation, performance, and modulus. They have a high moisture sorption capacity and are resistant to hydrolysis. They are synthetic fibers with a strong abrasion resistance and a highly orientated structure. They are more flexible and resistant to chemicals. The graph of Kevlar is shown in Fig. 1.

Theorem 1. *The Hosoya polynomial of Kevlar* $K_{\mathfrak{n}}$ (*where* $\mathfrak{n}$ *is the length*) *for* $n \geq 2$ *can be computed as*

$$\begin{aligned} H(K_{\mathfrak{n}}) &= (20\mathfrak{n} - 14)x^1 + (28\mathfrak{n} - 22)x^2 + (30\mathfrak{n} - 27)x^3 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 14)x^{6m-2} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 15)x^{6m-1} + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 17)x^{6m} \end{aligned}$$

$$+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-18)x^{6m+1}+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-22)x^{6m+2}$$
$$+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-25)x^{6m+3}. \tag{5}$$

Proof. The distance matrix D corresponding to the molecular graph of Kevlar $K_{\mathfrak{n}}$ is

$$D=\begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 & \dots & A_{2\mathfrak{n}-2} & C_{2\mathfrak{n}-1}\\ A_1^T & A_0 & A_1 & A_2 & A_3 & A_4 & \dots & A_{2\mathfrak{n}-3} & C_{2\mathfrak{n}-2}\\ A_2^T & A_1^T & A_0 & A_1 & A_2 & A_3 & \dots & A_{2\mathfrak{n}-4} & C_{2\mathfrak{n}-3}\\ A_3^T & A_2^T & A_1^T & A_0 & A_1 & A_2 & \dots & A_{2\mathfrak{n}-5} & C_{2\mathfrak{n}-4}\\ A_4^T & A_3^T & A_2^T & A_1^T & A_0 & A_1 & \dots & A_{2\mathfrak{n}-6} & C_{2\mathfrak{n}-5}\\ A_5^T & A_4^T & A_3^T & A_2^T & A_1^T & A_o & \dots & A_{2\mathfrak{n}-7} & C_{2\mathfrak{n}-6}\\ . & . & . & . & . & . & . & . & \\ . & . & . & . & . & . & . & . & \\ . & . & . & . & . & . & . & . & \\ A_{2\mathfrak{n}-2}^T & A_{2\mathfrak{n}-3}^T & A_{2\mathfrak{n}-4}^T & A_{2\mathfrak{n}-5}^T & A_{2\mathfrak{n}-6}^T & A_{2\mathfrak{n}-7}^T & \dots & A_0 & C_1\\ C_{2\mathfrak{n}-1}^T & C_{2\mathfrak{n}-2}^T & C_{2\mathfrak{n}-3}^T & C_{2\mathfrak{n}-4}^T & C_{2\mathfrak{n}-5}^T & C_{2\mathfrak{n}-6}^T & \dots & C_1^T & C_0 \end{bmatrix}_{1\le m\le 2\mathfrak{n}-1},$$

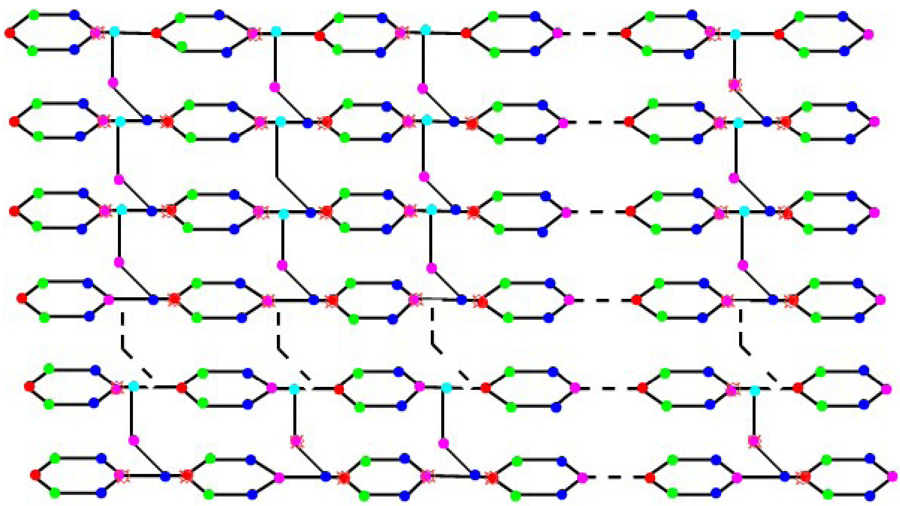

Fig. 1. Graph of para-aramid Kevlar.

where $A_0, A_1, A_2, A_3, A_4, A_5, \ldots, A_{2\mathfrak{n}-2}$ and $C_0, C_1, C_2, C_3, C_4, C_5, \ldots, C_{2\mathfrak{n}-1}$ are the submatrices. These matrices are calculated as follows ($\clubsuit = 6\mathfrak{n}$):

$$A_0 = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 3 \\ 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 4 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 5 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 4 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 1 \\ 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 2 \\ 3 & 4 & 5 & 4 & 3 & 2 & 1 & 2 & 0 \end{bmatrix},$$

$$A_k = \begin{bmatrix} \clubsuit & \clubsuit-1 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 & \clubsuit+3 \\ \clubsuit+1 & \clubsuit & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 & \clubsuit+4 & \clubsuit+4 \\ \clubsuit+2 & \clubsuit+1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 & \clubsuit+4 & \clubsuit+5 & \clubsuit+5 \\ \clubsuit+1 & \clubsuit & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 & \clubsuit+4 & \clubsuit+4 \\ \clubsuit & \clubsuit-1 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 & \clubsuit+3 \\ \clubsuit-1 & \clubsuit-2 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+2 \\ \clubsuit-2 & \clubsuit-3 & \clubsuit-4 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+1 \\ \clubsuit-1 & \clubsuit-2 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+2 \\ \clubsuit-3 & \clubsuit-4 & \clubsuit-5 & \clubsuit-4 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit \end{bmatrix}_{1 \le k \le \frac{\clubsuit}{3}-2},$$

$$C_0 = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix},$$

$$C_k = \begin{bmatrix} \clubsuit & \clubsuit-1 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 \\ \clubsuit+1 & \clubsuit & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 \\ \clubsuit+2 & \clubsuit+1 & \clubsuit & \clubsuit+1 & \clubsuit+2 & \clubsuit+3 \\ \clubsuit+1 & \clubsuit & \clubsuit-1 & \clubsuit & \clubsuit+1 & \clubsuit+2 \\ \clubsuit & \clubsuit-1 & \clubsuit-2 & \clubsuit-1 & \clubsuit & \clubsuit+1 \\ \clubsuit-1 & \clubsuit-2 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit \\ \clubsuit-2 & \clubsuit-3 & \clubsuit-4 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 \\ \clubsuit-1 & \clubsuit-2 & \clubsuit-3 & \clubsuit-2 & \clubsuit-1 & \clubsuit \\ \clubsuit-3 & \clubsuit-4 & \clubsuit-5 & \clubsuit-4 & \clubsuit-3 & \clubsuit-2 \end{bmatrix}_{1 \le k \le \frac{\clubsuit}{3}-1}.$$

The calculations for $|l_k(\mathfrak{n})|$ (k is the distance between the pairs) are as follows:

$$\begin{aligned} l_1(\mathfrak{n}) &= [\#1 \in A_0] \times [\#A_0] + [\#1 \in A_1] \times [\#A_1] \\ &\quad + [\#1 \in C_0] \times [\#C_0] + [\#1 \in C_1] \times [\#C_1], \\ &= 9(2\mathfrak{n} - 2) + 1(2\mathfrak{n} - 3) + 6(1) + 1(1), \\ &= 18\mathfrak{n} - 18 + 2\mathfrak{n} - 3 + 7, \\ &= 20\mathfrak{n} - 14. \end{aligned}$$

Similarly

$$\begin{aligned} |l_2(\mathfrak{n})| &= 28\mathfrak{n} - 22, \\ |l_3(\mathfrak{n})| &= 30\mathfrak{n} - 27, \\ |l_{6m-2}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 14(2\mathfrak{n} - m) - 14, \\ |l_{6m-1}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 14(2\mathfrak{n} - m) - 15, \\ |l_{6m}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 14(2\mathfrak{n} - m) - 17, \\ |l_{6m+1}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 13(2\mathfrak{n} - m) - 18, \\ |l_{6m+2}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 13(2\mathfrak{n} - m) - 22, \\ |l_{6m+3}(\mathfrak{n})| &= \Sigma_{m=1}^{\mathfrak{n}} 13(2\mathfrak{n} - m) - 25. \end{aligned}$$

The above values when substituted into Eq. (1) lead to the following form of Hosoya polynomial for Kevlar turn out to be

$$\begin{aligned} H(K_{\mathfrak{n}}) &= (20\mathfrak{n} - 14)x^1 + (28\mathfrak{n} - 22)x^2 + (30\mathfrak{n} - 27)x^3 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 14)x^{6m-2} + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 15)x^{6m-1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (14(2\mathfrak{n} - m) - 17)x^{6m} + \sum_{m=1}^{\mathfrak{n}} (13(2\mathfrak{n} - m) - 18)x^{6m+1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (13(2\mathfrak{n} - m) - 22)x^{6m+2} + \sum_{m=1}^{\mathfrak{n}} (13(2\mathfrak{n} - m) - 25)x^{6m+3}. \end{aligned}$$

□

Corollary 1. *The Wiener, hyper-Weiner and TSZ indices of Kevlar $K_{\mathfrak{n}}$ can be found using as*

$$W(K_{\mathfrak{n}}) = -2232 - \frac{51729}{5}\mathfrak{n} - 16830\mathfrak{n}^2 - 5598\mathfrak{n}^3 + 8019\mathfrak{n}^4 + \frac{26244}{5}\mathfrak{n}^5, \quad (6)$$

$$\mathrm{HW}(K_{\mathfrak{n}}) = \frac{1}{2}(-484 - 1788\mathfrak{n} - 1761\mathfrak{n}^2 + 738\mathfrak{n}^3 + 1215\mathfrak{n}^4), \quad (7)$$

$$\mathrm{TSZ}(K_{\mathfrak{n}}) = \frac{1}{6}(-139 - 360\mathfrak{n} - 36\mathfrak{n}^2 + 324\mathfrak{n}^3). \quad (8)$$

Proof. The Wiener index of Kevlar $K_{\mathfrak{n}}$ is computed taking the first derivative of Hosoya polynomial at $x = 1$. The first derivative of Eq. (5) with respect to x gives

$$\begin{aligned}\frac{dH(K_{\mathfrak{n}})}{dx} &= (20\mathfrak{n} - 14) + 2(28\mathfrak{n} - 22)x + 3(30\mathfrak{n} - 27)x^2 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m-2)(14(2\mathfrak{n} - m) - 14)x^{6m-3} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m-1)(14(2\mathfrak{n} - m) - 15)x^{6m-2} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m)(14(2\mathfrak{n} - m) - 17)x^{6m-1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m+1)(13(2\mathfrak{n} - m) - 18)x^{6m} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m+2)(13(2\mathfrak{n} - m) - 22)x^{6m+1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (6m+3)(13(2\mathfrak{n} - m) - 25)x^{6m+2}.\end{aligned}$$

Taking limit $x = 1$ gives

$$\begin{aligned}W(K_{\mathfrak{n}}) = \frac{dH(K_{\mathfrak{n}})}{dx}\bigg|_{x=1} &= (20\mathfrak{n} - 14) + 2(28\mathfrak{n} - 22) + 3(30\mathfrak{n} - 27) \\ &+ \sum_{m=1}^{\mathfrak{n}} (6m-2)(14(2\mathfrak{n} - m) - 14) + \sum_{m=1}^{\mathfrak{n}} (6m-1)(14(2\mathfrak{n} - m) - 15) \\ &+ \sum_{m=1}^{\mathfrak{n}} (6m)(14(2\mathfrak{n} - m) - 17) + \sum_{m=1}^{\mathfrak{n}} (6m+1)(13(2\mathfrak{n} - m) - 18) \\ &+ \sum_{m=1}^{\mathfrak{n}} (6m+2)(13(2\mathfrak{n} - m) - 22) + \sum_{m=1}^{\mathfrak{n}} (6m+3)(13(2\mathfrak{n} - m) - 25).\end{aligned}$$

The simplification leads to the following expression of Wiener index:

$$W(K_{\mathfrak{n}}) = -2232 - \frac{51729}{5}\mathfrak{n} - 16830\mathfrak{n}^2 - 5598\mathfrak{n}^3 + 8019\mathfrak{n}^4 + \frac{26244}{5}\mathfrak{n}^5.$$

The hyper-Wiener index of Kevlar $K_{\mathfrak{n}}$ is calculated taking product of x and Hosoya polynomial, and then finding the value of second derivative at $x = 1$.

Taking product of Eq. (5) with x leads to

$$\begin{aligned}xH(K_{\mathfrak{n}},x) &= (20\mathfrak{n}-14)x^2+(28\mathfrak{n}-22)x^3+(30\mathfrak{n}-27)x^4\\&\quad+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-14)x^{6m-1}+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-15)x^{6m}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-17)x^{6m+1}+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-18)x^{6m+2}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-22)x^{6m+3}+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-25)x^{6m+4}.\end{aligned}$$

Twice differentiation with respect to x implies

$$\begin{aligned}\frac{d^2(xH(K_{\mathfrak{n}},x))}{dx^2} &= 2(20\mathfrak{n}-14)+6(28\mathfrak{n}-22)x+12(30\mathfrak{n}-27)x^2\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m-1)(6m-2)(14(2\mathfrak{n}-m)-14)x^{6m-3}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m)(6m-1)(14(2\mathfrak{n}-m)-15)x^{6m-2}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+1)(6m)(14(2\mathfrak{n}-m)-17)x^{6m-1}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+2)(6m+1)(13(2\mathfrak{n}-m)-18)x^{6m}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+3)(6m+2)(13(2\mathfrak{n}-m)-22)x^{6m+1}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+4)(6m+3)(13(2\mathfrak{n}-m)-25]x^{6m+2}).\end{aligned}$$

Taking limit at $x=1$ gives

$$\begin{aligned}HW(K_{\mathfrak{n}}) = \left.\frac{d^2(xH(K_{\mathfrak{n}},x))}{dx^2}\right|_{x=1} &= 2(20\mathfrak{n}-14)+6(28\mathfrak{n}-22)+12(30\mathfrak{n}-27)\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m-1)(6m-2)(14(2\mathfrak{n}-m)-14)\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m)(6m-1)(14(2\mathfrak{n}-m)-15)\end{aligned}$$

$$+\sum_{m=1}^{\mathfrak{n}}(6m+1)(6m)(14(2\mathfrak{n}-m)-17)$$
$$+\sum_{m=1}^{\mathfrak{n}}(6m+2)(6m+1)(13(2\mathfrak{n}-m)-18)$$
$$+\sum_{m=1}^{\mathfrak{n}}(6m+3)(6m+2)(13(2\mathfrak{n}-m)-22)$$
$$+\sum_{m=1}^{\mathfrak{n}}(6m+4)(6m+3)(13(2\mathfrak{n}-m)-25).$$

The simplification leads to the following expression for hyper-Wiener index:

$$\mathrm{HW}(K_{\mathfrak{n}})=\frac{1}{2}(-484-1788n-1761n^2+738n^3+1215n^4).$$

The TSZ index of Kevlar $K_{\mathfrak{n}}$ is calculated taking product of x^2 and Hosoya polynomial, and then finding the value of third derivative at $x=1$. Taking product of Eq. (5) with x^2 gives

$$\begin{aligned}x^2H(K_{\mathfrak{n}},x)&=(20\mathfrak{n}-14)x^3+(28\mathfrak{n}-22)x^4+(30\mathfrak{n}-27)x^5\\&\quad+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-14)x^{6m}+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-15)x^{6m+1}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(14(2\mathfrak{n}-m)-17)x^{6m+2}+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-18)x^{6m+3}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-22)x^{6m+4}+\sum_{m=1}^{\mathfrak{n}}(13(2\mathfrak{n}-m)-25)x^{6m+5}.\end{aligned}$$

Taking third derivative with respect to x gives

$$\begin{aligned}\frac{d^3(x^2H(K_{\mathfrak{n}},x))}{dx^3}&=6(20\mathfrak{n}-14)+24(28\mathfrak{n}-22)x+60(30\mathfrak{n}-27)x^2\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m)(6m-1)(6m-2)(14(2\mathfrak{n}-m)-14)x^{6m-3}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+1)(6m)(6m-1)(14(2\mathfrak{n}-m)-15)x^{6m-2}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+2)(6m+1)(6m)(14(2\mathfrak{n}-m)-17)x^{6m-1}\\&\quad+\sum_{m=1}^{\mathfrak{n}}(6m+3)(6m+2)(6m+1)(13(2\mathfrak{n}-m)-18)x^{6m}\end{aligned}$$

$$+\sum_{m=1}^{\mathfrak{n}}(6m+4)(6m+3)(6m+2)(13(2\mathfrak{n}-m)-22)x^{6m+1}$$

$$+\sum_{m=1}^{\mathfrak{n}}(6m+5)(6m+4)(6m+3)(13(2\mathfrak{n}-m)-25)x^{6m+2}.$$

Taking limit $x=1$ implies

$$\begin{aligned}\mathrm{TSZ}(K_{\mathfrak{n}}) = {} & \left.\frac{d^3(x^2H(K_{\mathfrak{n}},x))}{dx^3}\right|_{x=1} = 6(20\mathfrak{n}-14)+24(28\mathfrak{n}-22)\\ & +60(30\mathfrak{n}-27)+\sum_{m=1}^{\mathfrak{n}}(6m)(6m-1)(6m-2)(14(2\mathfrak{n}-m)-14)\\ & +\sum_{m=1}^{\mathfrak{n}}(6m+1)(6m)(6m-1)(14(2\mathfrak{n}-m)-15)\\ & +\sum_{m=1}^{\mathfrak{n}}(6m+2)(6m+1)(6m)(14(2\mathfrak{n}-m)-17)\\ & +\sum_{m=1}^{\mathfrak{n}}(6m+3)(6m+2)(6m+1)(13(2\mathfrak{n}-m)-18)\\ & +\sum_{m=1}^{\mathfrak{n}}(6m+4)(6m+3)(6m+2)(13(2\mathfrak{n}-m)-22)\\ & +\sum_{m=1}^{\mathfrak{n}}(6m+5)(6m+4)(6m+3)(13(2\mathfrak{n}-m)-25).\end{aligned}$$

The simplification leads to the following expression for TSZ index of Kevlar $K_{\mathfrak{n}}$

$$\mathrm{TSZ}(K_{\mathfrak{n}}) = \frac{1}{6}(-139-360\mathfrak{n}-36\mathfrak{n}^2+324\mathfrak{n}^3). \qquad \square$$

The distance-related indices, Weiner, hyper-Weiner and TSZ indices of para-aramid Kevlar are presented in Fig. 2. It is visible that all the indices are directly proportional to n. All the indices increase with the increase in n. The Weiner index possesses the minimum values whereas the TSZ index admits the maximum values.

5. Distance Based Graph Invariants of Nomex

Nomex fibers are fire, heat, and flame resistant. They are infusible and admit hydrolytic stability against organic and inorganic liquids. Their tensile qualities are comparable to those of high-performance polyester and nylon fibers. The graph of Nomex is shown in Fig. 2.

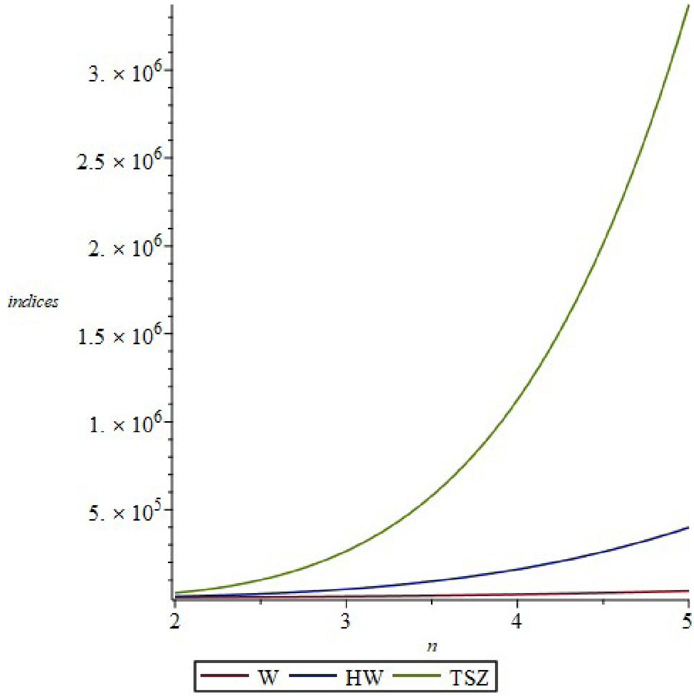

Fig. 2. Weiner, hyper-Weiner and TSZ indices of para-aramid Kevlar.

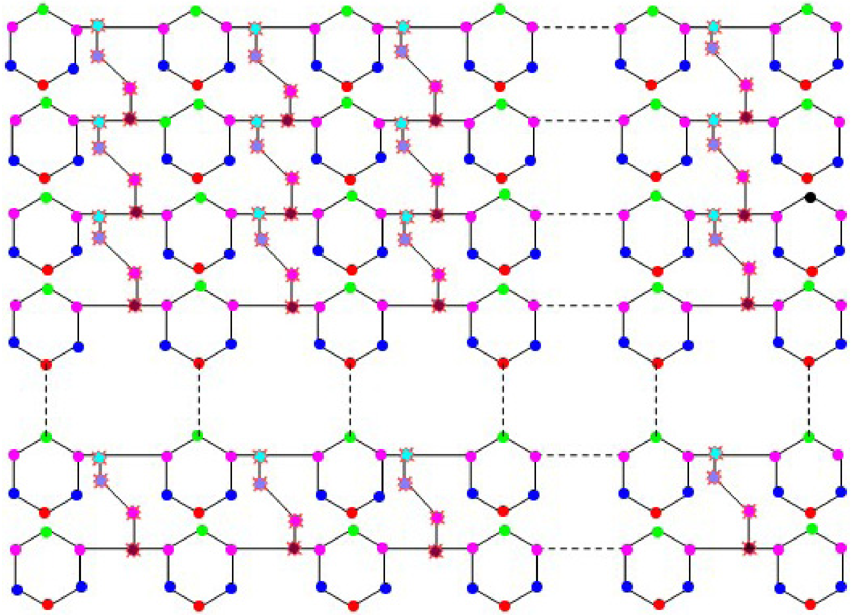

Fig. 3. Graph of meta-aramid Nomex.

Theorem 2. *The Hosoya Polynomial of Nomex $N_{\mathfrak{n}}$ (where $\mathfrak{n}$ is the length) for $n \geq 2$ can be computed as*

$$\begin{aligned} H(N_{\mathfrak{n}}) &= (22\mathfrak{n}-16)x^1 + (30\mathfrak{n}-24)x^2 + (34\mathfrak{n}-31)x^3 + (36\mathfrak{n}-37)x^4 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-23)x^{5m} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-26)x^{5m+1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-31)x^{5m+2} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-36)x^{5m+3} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-40)x^{5m+4}. \end{aligned} \tag{9}$$

Proof. The distance matrix D corresponding to the molecular graph of Nomex $N_{\mathfrak{n}}$ is

$$D = \begin{bmatrix} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 & \dots & A_{2\mathfrak{n}-2} & B_{2\mathfrak{n}-1} \\ A_1^T & A_0 & A_1 & A_2 & A_3 & A_4 & \dots & A_{2\mathfrak{n}-3} & B_{2\mathfrak{n}-2} \\ A_2^T & A_1^T & A_0 & A_1 & A_2 & A_3 & \dots & A_{2\mathfrak{n}-4} & B_{2\mathfrak{n}-3} \\ A_3^T & A_2^T & A_1^T & A_0 & A_1 & A_2 & \dots & A_{2\mathfrak{n}-5} & B_{2\mathfrak{n}-4} \\ A_4^T & A_3^T & A_2^T & A_1^T & A_0 & A_1 & \dots & A_{2\mathfrak{n}-6} & B_{2\mathfrak{n}-5} \\ A_5^T & A_4^T & A_3^T & A_2^T & A_1^T & A_o & \dots & A_{2\mathfrak{n}-7} & B_{2\mathfrak{n}-6} \\ . & . & . & . & . & . & . & . & \\ . & . & . & . & . & . & . & . & \\ . & . & . & . & . & . & . & . & \\ A_{2\mathfrak{n}-2}^T & A_{2\mathfrak{n}-3}^T & A_{2\mathfrak{n}-4}^T & A_{2\mathfrak{n}-5}^T & A_{2\mathfrak{n}-6}^T & A_{2\mathfrak{n}-7}^T & \dots & A_0 & B_1 \\ B_{2\mathfrak{n}-1}^T & B_{2\mathfrak{n}-2}^T & B_{2\mathfrak{n}-3}^T & B_{2\mathfrak{n}-4}^T & B_{2\mathfrak{n}-5}^T & B_{2\mathfrak{n}-6}^T & \dots & B_1^T & B_0 \end{bmatrix}_{1\leq i\leq 2\mathfrak{n}-1},$$

where $A_0, A_1, A_2, A_3, A_4, A_5, \dots, A_{2\mathfrak{n}-2}$ and $B_0, B_1, B_2, B_3, B_4, B_5, \dots, B_{2\mathfrak{n}-1}$ are the submatrices. These matrices are calculated as follows ($\spadesuit = 5\mathfrak{n}$):

$$A_0 = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 \\ 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 1 \\ 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 3 \\ 3 & 4 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 0 \end{bmatrix},$$

$$A_k = \begin{bmatrix} \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+3 \\ \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+5 & \spadesuit+4 \\ \spadesuit+2 & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+3 & \spadesuit+4 & \spadesuit+5 & \spadesuit+6 & \spadesuit+5 \\ \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+5 & \spadesuit+4 \\ \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+3 \\ \spadesuit-1 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 \\ \spadesuit-2 & \spadesuit-3 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 \\ \spadesuit-1 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 \\ \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+3 \\ \spadesuit-3 & \spadesuit-4 & \spadesuit-3 & \spadesuit-2 & \spadesuit-1 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit \end{bmatrix}_{1\le k\le 2(\frac{\spadesuit}{5}-1)},$$

$$B_0 = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix},$$

$$B_k = \begin{bmatrix} \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 \\ \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 \\ \spadesuit+2 & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+4 & \spadesuit+3 \\ \spadesuit+1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+3 & \spadesuit+2 \\ \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 \\ \spadesuit-1 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit \\ \spadesuit-2 & \spadesuit-3 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit-1 \\ \spadesuit-1 & \spadesuit-2 & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit \\ \spadesuit & \spadesuit-1 & \spadesuit & \spadesuit+1 & \spadesuit+2 & \spadesuit+1 \\ \spadesuit-3 & \spadesuit-4 & \spadesuit-3 & \spadesuit-2 & \spadesuit-1 & \spadesuit-2 \end{bmatrix}_{1\le k\le 2(\frac{\clubsuit}{5})-1},$$

The calculations for $|l_k(\mathfrak{n})|$ (k is the distance between the pairs) are as follows:

$$\begin{aligned} l_1(\mathfrak{n}) &= [\#1 \in A_0] \times [\#A_0] + [\#1 \in A_1] \times [\#A_1] \\ &\quad + [\#1 \in B_0] \times [\#B_0] + [\#1 \in B_1] \times [\#B_1], \\ &= 10(2\mathfrak{n}-2) + 1(2\mathfrak{n}-3) + 6(1) + 1(1), \\ &= 20\mathfrak{n} - 20 + 2\mathfrak{n} - 3 + 7, \\ &= 22\mathfrak{n} - 16. \end{aligned}$$

Similarly

$$|l_2(\mathfrak{n})| = 30\mathfrak{n} - 24,$$

$$|l_3(\mathfrak{n})| = 34\mathfrak{n} - 31,$$

$$|l_4(\mathfrak{n})| = 36\mathfrak{n} - 37,$$

$$|l_{5m}(\mathfrak{n})| = \Sigma_{m=1}^{\mathfrak{n}} 20(2\mathfrak{n}-m)-23,$$
$$|l_{5m+1}(\mathfrak{n})| = \Sigma_{m=1}^{\mathfrak{n}} 20(2\mathfrak{n}-m)-26,$$
$$|l_{5m+2}(\mathfrak{n})| = \Sigma_{m=1}^{\mathfrak{n}} 20(2\mathfrak{n}-m)-31,$$
$$|l_{5m+3}(\mathfrak{n})| = \Sigma_{m=1}^{\mathfrak{n}} 20(2\mathfrak{n}-m)-36,$$
$$|l_{5m+4}(\mathfrak{n})| = \Sigma_{m=1}^{\mathfrak{n}} 20(2\mathfrak{n}-m)-40.$$

The above values when substituted into Eq. (1) lead to the following form of Hosoya polynomial for Nomex that can be calculated as

$$\begin{aligned} H(N_{\mathfrak{n}}) &= (22\mathfrak{n}-16)x^1 + (30\mathfrak{n}-24)x^2 + (34\mathfrak{n}-31)x^3 + (36\mathfrak{n}-37)x^4 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-23)x^{5m} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-26)x^{5m+1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-31)x^{5m+2} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-36)x^{5m+3} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n}-m)-40)x^{5m+4}. \end{aligned} \tag{10}$$

Hence proved. □

Corollary 2. *The Wiener, hyper-Weiner and TSZ indices of Nomex N_n can be found as*

$$W(N_{\mathfrak{n}}) = -305 - \frac{1804}{3}\mathfrak{n} + 160\mathfrak{n}^2 + \frac{1000}{3}\mathfrak{n}^3, \tag{11}$$

$$W(N_{\mathfrak{n}}) = \frac{1}{2}\left(-1288 - \frac{11264}{3}\mathfrak{n} - \frac{4385}{3}\mathfrak{n}^2 + \frac{4850}{3}\mathfrak{n}^3 + \frac{3125}{3}\mathfrak{n}^4\right), \tag{12}$$

$$TSZ(N_{\mathfrak{n}}) = \frac{1}{6}(-6972 - 25873\mathfrak{n} - 22375\mathfrak{n}^2 + 1450\mathfrak{n}^3 + 10750\mathfrak{n}^4 + 3750\mathfrak{n}^5). \tag{13}$$

Proof. The Wiener index of Nomex $N_{\mathfrak{n}}$ is computed taking the first derivative of Hosoya polynomial at $x = 1$. The firstderivative of Eq. (9) with respect to x gives

$$\begin{aligned} \frac{dH(N_{\mathfrak{n}})}{dx} &= (22\mathfrak{n}-16) + 2(30\mathfrak{n}-24)x + 3(34\mathfrak{n}-31)x^2 + 4(36\mathfrak{n}-37)x^3 \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (5m)(20(2\mathfrak{n}-m)-23)x^{5m-1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}} (5m+1)(20(2\mathfrak{n}-m)-26)x^{5m} \end{aligned}$$

$$+\sum_{m=1}^{\mathfrak{n}}(5m+2)(20(2\mathfrak{n}-m)-31)x^{5m+1}$$
$$+\sum_{m=1}^{\mathfrak{n}}(5m+3)(20(2\mathfrak{n}-m)-36)x^{5m+2}$$
$$+\sum_{m=1}^{\mathfrak{n}}(5m+4)(20(2\mathfrak{n}-m)-40)x^{5m+3}. \tag{14}$$

Taking limit $x=1$ gives

$$\begin{aligned}W(N_{\mathfrak{n}}) &= \left.\frac{dH(N_{\mathfrak{n}},x)}{dx}\right|_{x=1}\\ &= (22\mathfrak{n}-16)+2(30\mathfrak{n}-24)+3(34\mathfrak{n}-31)+4(36\mathfrak{n}-37)\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(5m)(20(2\mathfrak{n}-m)-23)+\sum_{m=1}^{\mathfrak{n}}(5m+1)(20(2\mathfrak{n}-m)-26)\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(5m+2)(20(2\mathfrak{n}-m)-31)+\sum_{m=1}^{\mathfrak{n}}(5m+3)(20(2\mathfrak{n}-m)-36)\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(5m+4)(20(2\mathfrak{n}-m)-40).\end{aligned}$$

The simplification leads to the following expression of Wiener index:

$$W(N_{\mathfrak{n}}) = -305-\frac{1804}{3}\mathfrak{n}+160\mathfrak{n}^2+\frac{1000}{3}\mathfrak{n}^3.$$

The hyper-Wiener index of Nomex $N_{\mathfrak{n}}$ is calculated taking product of x and Hosoya polynomial, and then finding the value of second derivative at $x=1$. Taking product of Eq. (9) with x leads to

$$\begin{aligned}xH(N_{\mathfrak{n}},x) &= (22\mathfrak{n}-16)x^2+(30\mathfrak{n}-24)x^3+(34\mathfrak{n}-31)x^4+(36\mathfrak{n}-37)x^5\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(20(2\mathfrak{n}-m)-23)x^{5m+1}+\sum_{m=1}^{\mathfrak{n}}(20(2\mathfrak{n}-m)-26)x^{5m+2}\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(20(2\mathfrak{n}-m)-31)x^{5m+3}+\sum_{m=1}^{\mathfrak{n}}(20(2\mathfrak{n}-m)-36)x^{5m+4}\\ &\quad+\sum_{m=1}^{\mathfrak{n}}(20(2\mathfrak{n}-m)-40)x^{5m+5}].\end{aligned}$$

Twice differentiation with respect to x implies

$$\begin{aligned}\frac{d^2(xH(N_{\mathfrak{n}},x))}{dx^2} &= 2(22\mathfrak{n}-16)+6(30\mathfrak{n}-24)x \\ &\quad + 12(34\mathfrak{n}-31)x^2 + 20(36\mathfrak{n}-37)x^3 \\ &\quad + \sum_{m=1}^{\mathfrak{n}}(5m+1)(5m)(20(2\mathfrak{n}-m)-23)x^{5m-1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}}(5m+2)(5m+1)(20(2\mathfrak{n}-m)-26)x^{5m} \\ &\quad + \sum_{m=1}^{\mathfrak{n}}(5m+3)(5m+2)(20(2\mathfrak{n}-m)-31)x^{5m+1} \\ &\quad + \sum_{m=1}^{\mathfrak{n}}(5m+4)(5m+3)(20(2\mathfrak{n}-m)-36)x^{5m+2} \\ &\quad + \sum_{m=1}^{\mathfrak{n}}(5m+5)(5m+4)(20(2\mathfrak{n}-m)-40)x^{5m+3}].\end{aligned}$$

Taking limit at $x=1$ gives

$$\begin{aligned}HW(N_{\mathfrak{n}}) = \left.\frac{d^2(xH(N_{\mathfrak{n}},x))}{dx^2}\right|_{x=1} &\Bigg(2(22\mathfrak{n}-16)+6(30\mathfrak{n}-24)+12(34\mathfrak{n}-31) \\ &+ 20(36\mathfrak{n}-37) + \sum_{m=1}^{\mathfrak{n}}(5m+1)(5m)[20(2\mathfrak{n}-m)-23\Bigg) \\ &+ \sum_{m=1}^{\mathfrak{n}}(5m+2)(5m+1)(20(2\mathfrak{n}-m)-26) \\ &+ \sum_{m=1}^{\mathfrak{n}}(5m+3)(5m+2)(20(2\mathfrak{n}-m)-31) \\ &+ \sum_{m=1}^{\mathfrak{n}}(5m+4)(5m+3)(20(2\mathfrak{n}-m)-36) \\ &+ \sum_{m=1}^{\mathfrak{n}}(5m+5)(5m+4)(20(2\mathfrak{n}-m)-40).\end{aligned}$$

The simplification leads to the following expression for hyper-Wiener index:

$$HW(N_{\mathfrak{n}}) = \frac{1}{2}\left(-1288-\frac{11264}{3}\mathfrak{n}-\frac{4385}{3}\mathfrak{n}^2+\frac{4850}{3}\mathfrak{n}^3+\frac{3125}{3}\mathfrak{n}^4\right).$$

The TSZ index of Nomex $N_{\mathfrak{n}}$ is calculated taking product of x^2 and Hosoya polynomial, and then finding the value of third derivative at $x = 1$. Taking product of Eq. (9) with x^2 gives

$$\begin{aligned}x^2 H(N_{\mathfrak{n}}, x) = (22\mathfrak{n} - 16)x^3 + (30\mathfrak{n} - 24)x^4\\ + (34\mathfrak{n} - 31)x^5 + (36\mathfrak{n} - 37)x^6 + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n} - m) - 23)x^{5m+2}\\ + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n} - m) - 26)x^{5m+3} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n} - m) - 31)x^{5m+4}\\ + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n} - m) - 36)x^{5m+5} + \sum_{m=1}^{\mathfrak{n}} (20(2\mathfrak{n} - m) - 40)x^{5m+6}.\end{aligned}$$

Taking third derivative with respect to x gives

$$\begin{aligned}\frac{d^3(x^2 H(N_{\mathfrak{n}}, x))}{dx^3} &= 6(22\mathfrak{n} - 16) + 24(30\mathfrak{n} - 24)x + 60(34\mathfrak{n} - 31)x^2\\ &+ 120(36\mathfrak{n} - 37)x^3\\ &+ \sum_{m=1}^{\mathfrak{n}} (5m+2)(5m+1)(5m)(20(2\mathfrak{n} - m) - 23)x^{5m-1}\\ &+ \sum_{m=1}^{\mathfrak{n}} (5m+3)(5m+2)(5m+1)(20(2\mathfrak{n} - m) - 26)x^{5m}\\ &+ \sum_{m=1}^{\mathfrak{n}} (5m+4)(5m+3)(5m+2)(20(2\mathfrak{n} - m) - 31)x^{5m+1}\\ &+ \sum_{m=1}^{\mathfrak{n}} (5m+5)(5m+4)(5m+3)(20(2\mathfrak{n} - m) - 36)x^{5m+2}\\ &+ \sum_{m=1}^{\mathfrak{n}} (5m+6)(5m+5)(5m+4)(20(2\mathfrak{n} - m) - 40)x^{5m+3}.\end{aligned}$$

Taking limit $x = 1$ implies

$$\begin{aligned}TSZ(N_{\mathfrak{n}}) = \left.\frac{d^3(x^2 H(N_{\mathfrak{n}}, x))}{dx^3}\right|_{x=1} = 6(22\mathfrak{n} - 16) + 24(30\mathfrak{n} - 24) + 60(34\mathfrak{n} - 31)\\ + 120(36\mathfrak{n} - 37) + \sum_{m=1}^{\mathfrak{n}} (5m+2)(5m+1)(5m)(20(2\mathfrak{n} - m) - 23)\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{m=1}^{\mathfrak{n}} (5m+3)(5m+2)(5m+1)(20(2\mathfrak{n}-m)-26)\\
&+ \sum_{m=1}^{\mathfrak{n}} (5m+4)(5m+3)(5m+2)(20(2\mathfrak{n}-m)-31)\\
&+ \sum_{m=1}^{\mathfrak{n}} (5m+5)(5m+4)(5m+3)(20(2\mathfrak{n}-m)-36)\\
&+ \sum_{m=1}^{\mathfrak{n}} (5m+6)(5m+5)(5m+4)(20(2\mathfrak{n}-m)-40).
\end{aligned}
$$

The simplification leads to the following expression for TSZ index of Nomex $N_{\mathfrak{n}}$:

$$TSZ(N_{\mathfrak{n}}) = \frac{1}{6}[-6972 - 25873n - 22375n^2 + 1450n^3 + 10750n^4 + 3750n^5]. \qquad \square$$

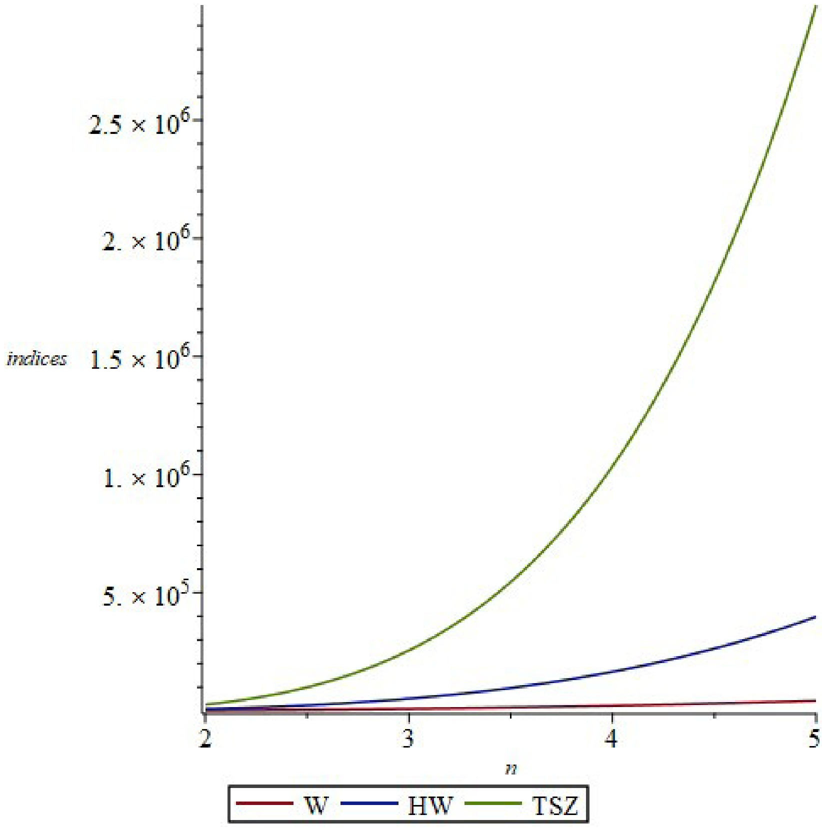

Fig. 4. Weiner, hyper-Weiner and TSZ indices of meta-aramid Nomex.

The distance-related indices, Weiner, hyper-Weiner and TSZ indices of Nomex are shown in Fig. 4. It is visible that all the indices are directly proportional to n. All the indices increase with the increase in n. The Weiner index possesses the minimum values whereas the TSZ index admits the maximum values.

6. Conclusion

We have computed the Hosoya polynomials concerning the two aramids, the para-aramid Kevlar and meta-aramid Nomex of finite length $\mathfrak{n}$. We revealed that different expressions are found as Hosoya polynomial for both aramids. The Hosoya polynomial leads to the distance-related Wiener, hyper-Wiener, and TSZ indices. We also derived the concerned the distance-related TIs including Wiener, hyper-Wiener and TSZ indices. These indices admit several physical applications including, the branching and surface area of a molecule. They are also related to physical properties like saturation capacity of hydrocarbons, ultrasonic velocities for alkane and alcohol, cyclicity, electroreduction, vaporization, carbonization, molecular density, critical points including melting and boiling points and heat of formation. Because of these qualities, these indices are useful for creating novel drugs [42, 43]. These indices present the sub-atomic stretching in electronic structures, discuss the physiochemical properties of organic compounds in pharmacology and create an increase in hardware security of computer lattice [44].

The different expressions computed as the Hosoya polynomial for Kevlar and Nomex gives different values for distance-related TIs including Wiener, hyper-Wiener and TSZ indices. Moreover, the behavior of indices for the two structures is different for $2 \leq n \leq 5$. It is noteworthy that all the three distance-related TIs admit larger values for Kevlar as compared to Nomex. This may lead to the generalized result that the para-aramids possess higher values of Wiener, hyper-Wiener and TSZ indices when compared to the meta-aramids.

Acknowledgments

The work was partially funded by Slovak Grant Agency for Science VEGA under the grant number VEGA 2/0076/23. Moreover, the authors acknowledge the support of HEC Pakistan, National Textile University Faisalabad and University of Education, Lahore for their administrative and technical support.

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