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Calculation of topological indices based on M-polynomial for Polytrimethylene terephthalate

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Abstract. Polytrimethyleneterephthalate is an extensively utilized thermoplastic industrial polymer characterized by a low melting point and minimal water absorption and it follows the general molecular formula $(C_{11}H_{10}O_4)_n$. It is interesting to chemists and engineering researchers due to its application in various industries, especially in textiles and engineering thermoplastics. In this article, the general formulas of some degree-based topological indices are obtained via M-polynomials for Polytrimethylene terephthalate. Calculating indices via these formulas does not require counting the degree of vertices or edge partitioning and can only be calculated by having the number of polytrimethylene terephthalate monomers. The obtained results are displayed numerically and graphically, then the topological indices are graphically compared.

Keywords: polytrimethylene terephthalate, molecular graph, topological index, M-polynomial.
Mathematics Subject Classification (2010): 05C09, 05C31, 05C90, 05C92.

1 Introduction

Natural resource-based approaches to bioengineering plastics are being developed to compete in automobiles, power, and other industries. polytrimethylene terephthalate (PTT) is a particular kind of bioengineering plastic [1]. PTT is a synthesized polyester with the molecular formula $(C_{11}H_{10}O_4)_n$. This polymer is prepared by esterification of $1,3-$propanediol $(HO(CH_2)_3OH)$ with terephthalic acid $(C_6H_4(COOH)_2)$, see Figures 1 and 2. Polyester ac-

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counts for approximately 60 percent of total fiber production. *PTT* fibers are suitable for use in the textile industry due to having advantages such as waterless dyeing, simple dye formulation, reduction of dyeing time, and less energy consumption [2]. *PTT* is also suitable for the carpet industry due to its elasticity, softness, chemical stability, and stain resistance [3].

One of the areas of research in chemical graph theory at the moment is the study of topological indices (TIs) that can be used to predict various chemical and biological characteristics of chemical structures. They encode data on molecular size, shape, and branching in a quantitative way, which is used to evaluate the topological similarity between chemical structures [4]. The American physical chemist Harold Wiener introduced the oldest TI in 1947. He reported the presence of a correlation between this new index and many physicochemical properties of alkanes, including the structural determination of paraffin boiling points. Hosoya defined the Wiener index as the sum of the distances between all unordered pairs of vertices of G. Gutman and Trinajstić introduced the first and second Zagreb index which provides quantitative measures of molecular branching [6–8]. Estrada et al. introduced the Atom-bond connectivity (ABC) index which provides a good model for the stability of linear and branched alkanes [9, 10], some of the degree-based TIs are in Table 1 [11–19].

Topological polynomials are used in mathematical chemistry to calculate TIs, for example, Hosoya, M, MN, and SMP polynomials can be mentioned. Hosoya polynomial admits many chemical applications. Almost all distance-based TIs can be derived from this polynomial [20]. The M-polynomial was introduced in 2015 by Deutsch and Klavžar [21, 22]. The M-polynomial of G is written as:

$$M(G;x,y) = \sum_{\delta \le i \le j \Delta} m_{ij}(G) x^i y^j,$$

where $\delta = min\{d_v | v \in V(G)\}$, $\Delta = max\{d_v | v \in V(G)\}$, and $m_{ij}(G)$ is the number of edges $uv \in E(G)$ such that $\{d_u, d_v\} = \{i, j\}$, and d_u, d_v are the degree of vertices $u, v \in V(G)$.

In this article, general formulas were offered based on the number of monomers for some TIs so these can be obtained without the need to count the degree of vertices and edge partitioning. Notably, no prior studies on this method of calculating the TIs of *PTT* were found in the surveyed literature.

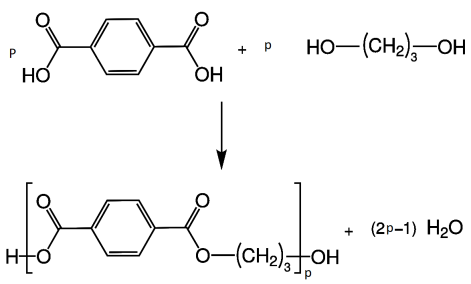

Figure 1 Reaction scheme of PTT-synthesis by esterification.

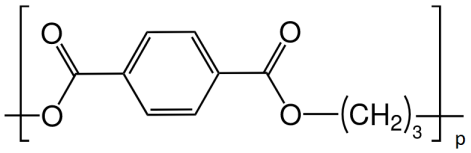

Figure 2 polytrimethylene terephthalate structure.

2 Results and Discussion

The base graph of polytrimethylene terephthalate $PTT(p)$, presented in Figure 3, can be considered a structure with p number of monomers, which is a simple molecular graph with $15p$ vertices and $16p-1$ edges. The number of vertices, edges, and monomers are denoted by n, m, and p, respectively. Edge partitioning of the $PTT(p)$ graph is given in Table 1. Table 2 shows the mathematical formula for the degree-based TIs used in this article and Table 3 includes some degree-based topological indices computed via M-polynomial, where operators used are defined as:

$$D_xM(x,y)=x\frac{\partial M}{\partial x}, \qquad D_yM(x,y)=y\frac{\partial M}{\partial y},$$

$$S_xM(x,y)=\int_0^x \frac{M(t,y)}{t}d_t, \qquad S_yM(x,y)=\int_0^y \frac{M(x,t)}{t}d_t,$$

$$JM(x,y)=M(x,x), \qquad Q_\alpha M(x,y)=x^\alpha M(x,y),$$

$$D_x^{\frac{1}{2}}M(x,y)=\sqrt{x\frac{\partial M(x,y)}{\partial x}}.\sqrt{M(x,y)}, \qquad D_y^{\frac{1}{2}}M(x,y)=\sqrt{y\frac{\partial M(x,y)}{\partial y}}.\sqrt{M(x,y)},$$

$$S_x^{\frac{1}{2}}M(x,y)=\sqrt{\int_0^x \frac{M(t,y)}{t}dt}.\sqrt{M(x,y)}, \qquad S_y^{\frac{1}{2}}M(x,y)=\sqrt{\int_0^y \frac{M(x,t)}{t}dt}.\sqrt{M(x,y)}.$$

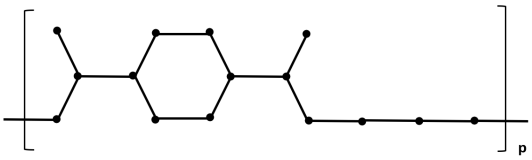

Figure 3 Base graph of polytrimethylene terephthalate.

Table 1 Edge partition of PTT.

(d_u, d_v)	$(1,2)$	$(1,3)$	$(2,2)$	$(2,3)$	$(3,3)$	Total edges
Number of Edges	1	$2p+1$	$6p-2$	$6p-1$	$2p$	$16p-1$

Table 2 Some degree-based topological indices.

Topological index	Mathematical formula
First Zagreb	$FZ(G) = \Sigma_{uv \in E(G)} (d_u + d_v)$
Second Zagreb	$SZ(G) = \Sigma_{uv \in E(G)} (d_u d_v)$
Hyper Zagreb	$HZ(G) = \Sigma_{uv \in E(G)} (d_u + d_v)^2$
Modified Zagreb	$MZ(G) = \Sigma_{uv \in E(G)} \frac{1}{d_u d_v}$
Harmonic	$H(G) = \Sigma_{uv \in E(G)} \frac{2}{d_u + d_v}$
Symmetric Division Deg	$SDD(G) = \Sigma_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v}$
Inverse sum	$I(G) = \Sigma_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$
Forgotten	$F(G) = \Sigma_{uv \in E(G)} d_u^2 + d_v^2$
Sigma	$\sigma(G) = \Sigma_{uv \in E(G)} (d_u - d_v)^2$
First Gourava	$Go_1(G) = \Sigma_{uv \in E(G)} (d_u + d_v + d_u d_v)$
Second Gourava	$Go_2(G) = \Sigma_{uv \in E(G)} (d_u^2 d_v + d_v^2 d_u)$
Atom Band Connectivity	$ABC(G) = \Sigma_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$

Table 3 Derivation of degree-based topological indices via M-polynomial.

Topological index	Derivative from $M(G;x,y)$
First Zagreb	$(D_x + D_y)M(PTT;x,y)\|_{x=y=1}$
Second Zagreb	$D_x D_y M(PTT;x,y)\|_{x=y=1}$
Hyper Zagreb	$D_x^2 J M(PTT;x,y)\|_{x=1}$
Modified Zagreb	$S_x S_y M(PTT;x,y)\|_{x=y=1}$
Harmonic	$2S_x J M(PTT;x,y)\|_{x=y=1}$
Symmetric Division Deg	$(D_x S_y + D_y S_x)M(PTT;x,y)\|_{x=y=1}$
Inverse sum	$S_x J D_x D_y M(PTT;x,y)\|_{x=1}$
Forgotten	$(D_x^2 + D_y^2)M(PTT;x,y)\|_{x=y=1}$
Sigma	$(D_x^2 + D_y^2 - 2D_x D_y)M(PTT;x,y)\|_{x=y=1}$
First Gourava	$(D_x + D_y + D_x D_x)M(PTT;x,y)\|_{x=y=1}$
Second Gourava	$(D_x^2 D_y + D_y^2 D_x)M(PTT;x,y)\|_{x=y=1}$
Atom Band Connectivity	$D_x^{\frac{1}{2}} Q_{-2} J S_x^{\frac{1}{2}} S_y^{\frac{1}{2}} M(PTT;x,y)\|_{x=y=1}$

Theorem 2.1. *Consider PTT with p number of monomers. Then its M-polynomial is as follows:*

$$M(PTT;x,y) = xy^2 + (2p+1)xy^3 + (6p-2)x^2y^2 + (6p-1)x^2y^3 + (2p)x^3y^3.$$

Proof. We can calculate the M-polynomial of PTT using Figure 3 and Table 1 as follows:

$$\begin{aligned}
M(G;x,y) &= \sum_{\delta \le i \le j \Delta} m_{ij}(G) x^i y^j \\
&= \sum_{1 \le 2} m_{12}(G) xy^2 + \sum_{1 \le 3} m_{13}(G) xy^3 \\
&+ \sum_{2 \le 2} m_{22}(G) x^2y^2 + \sum_{2 \le 3} m_{23}(G) x^2y^3 \\
&+ \sum_{3 \le 3} m_{33}(G) x^3y^3 = |E_{(1,2)}| xy^2 + |E_{(1,3)}| xy^3 \\
&+ |E_{(2,2)}| x^2y^2 + |E_{(2,3)}| x^2y^3 + |E_{(3,3)}| x^3y^3 \\
&= xy^2 + (2p+1)xy^3 + (6p-2)x^2y^2 + (6p-1)x^2y^3 + (2p)x^3y^3.
\end{aligned}$$

□

Theorem 2.2. *Let $PTT(p)$, where $p \ge 1$. Then the following hold:*

(i) $FZ(PTT) = 74p - 6$,

(ii) $SZ(PTT) = 84p - 9$,

(iii) $SDD(PTT) = \frac{146}{3}p - \frac{5}{2}$,

(iv) $MZ(PTT) = \frac{61}{18}p + \frac{1}{6}$,

(v) $H(PTT) = \frac{212p-7}{30}$,

(vi) $I(PTT) = 17.7p - 1.78$,

(vii) $ABC(PTT) = \sqrt{2}(\frac{1}{\sqrt{3}} - 1) + p(\frac{2\sqrt{2}}{\sqrt{3}} + 6\sqrt{2} + \frac{4}{3})$,

(viii) $\sigma(PTT) = 14p + 4$,

(ix) $F(PTT) = 182p - 14$,

(x) $HZ(PTT) = 350p - 32$,

(xi) $GO_1(PTT) = 128p + 15$,

(xii) $GO_2(PTT) = 408p - 44$.

Proof. Let $M(PTT;x,y) = xy^2 + (2p+1)xy^3 + (6p-2)x^2y^2 + (6p-1)x^2y^3 + (2p)x^3y^3$. The following results are obtained by applying the operators on the M-polynomial.

$$D_xM(PTT;x,y) = xy^2 + (2p+1)xy^3 + 2(6p-2)x^2y^2 + 2(6p-1)x^2y^3 + 6px^3y^3,$$
$$D_yM(PTT;x,y) = 2xy^2 + 3(2p+1)xy^3 + 2(6p-2)x^2y^2 + 3(6p-1)x^2y^3 + 6px^3y^3,$$
$$S_xM(PTT;x,y) = xy^2 + (2p+1)xy^3 + \frac{(6p-2)}{2}x^2y^2 + \frac{(6p-1)}{2}x^2y^3 + \frac{2p}{3}x^3y^3,$$
$$S_yM(PTT;x,y) = \frac{xy^2}{2} + \frac{(2p+1)}{3}xy^3 + \frac{(6p-2)}{2}x^2y^2 + \frac{6p-1}{3}x^2y^3 + \frac{2}{3}px^3y^3,$$
$$S_xS_yM(PTT;x,y) = \frac{1}{2}xy^2 + \frac{2p+1}{3}xy^3 + \frac{6p-2}{4}x^2y^2 + \frac{6p-1}{6}x^2y^3 + \frac{2}{9}x^3y^3,$$
$$JM(PTT;x,y) = x^3 + (8p-1)x^4 + (6p-1)x^5 + 2px^6,$$
$$S_xJM(PTT;x,y) = \frac{x^3}{3} + (8p-1)\frac{x^4}{4} + (6p-1)\frac{x^5}{5} + 2p\frac{x^6}{6},$$
$$Q_\alpha M(PTT;x,y) = x^{\alpha+1}y^2 + (2p+1)x^{\alpha+1}y^3 + (6p-2)x^{\alpha+2}y^2 + (6p-1)x^{\alpha+2}y^3 + 2px^{\alpha+3}y^3,$$
$$D_y^\alpha M(PTT;x,y) = 2^\alpha xy^2 + 3^\alpha(2p+1)xy^3 + 2^\alpha(6p-2)x^2y^2 + 3^\alpha(6p-1)x^2y^3 + 2(3)^\alpha px^3y^3,$$
$$D_x^\alpha D_y^\beta M(PTT;x,y) = 1^\alpha 2^\beta xy^2 + 1^\alpha 3^\beta(2p+1)xy^3 + 2^\alpha 2^\beta(6p-2)x^2y^2 + 2^\alpha 3^\beta(6p-1)x^2y^3$$
$$+ (2)3^\alpha 3^\beta px^3y^3,$$
$$S_y^\alpha M(PTT;x,y) = \frac{1}{2^\alpha}xy^2 + \frac{2p+1}{3^\alpha}xy^3 + \frac{6p-2}{2^\alpha}x^2y^2 + \frac{6p-1}{3^\alpha}x^2y^3 + \frac{2}{3^\alpha}px^3y^3,$$
$$S_x^\alpha(S_y^\alpha)M(PTT;x,y) = \frac{xy^2}{1^\alpha 2^\alpha} + \frac{(2p+1)}{1^\alpha 3^\alpha}xy^3 + \frac{(6p-2)}{2^\alpha 2^\alpha}x^2y^2 + \frac{(6p-1)}{2^\alpha 3^\alpha}x^2y^3 + \frac{2p}{3^\alpha 3^\alpha}x^3y^3,$$
$$D_x^2D_y + D_y^2D_xM(PTT;x,y) = 6xy^2 + 12(2p+1)xy^3 + 16(6p-2)x^2y^2 + 30(6p-1)x^2y^3$$
$$+ 108x^3y^3.$$

Then due to Table 3, we conclude that

(i) $FZ(PTT) = (D_x + D_y)M(PTT;x,y)|_{x=y=1} = 74p - 6,$
(ii) $SZ(PTT) = D_xD_yM(PTT;x,y)|_{x=y=1} = 84p - 9,$
(iii) $SDD(PTT) = (D_xS_y + D_yS_x)M(PTT;x,y)|_{x=y=1} = \frac{146}{3}p - \frac{5}{2},$
(iv) $MZ(PTT) = S_xS_yM(PTT;x,y)|_{x=y=1} = \frac{61}{18}p + \frac{1}{6},$
(v) $H(PTT) = 2S_xJM(PTT;x,y)|_{x=y=1} = \frac{212p-7}{30},$
(vi) $I(PTT) = S_xJD_xD_yM(PTT;x,y)|_{x=1} = 17.7p - 1.78,$
(vii) $ABC(PTT) = D_x^{\frac{1}{2}}Q_{-2}JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}M(PTT;x,y)_{x=y=1} = \sqrt{2}(\frac{1}{\sqrt{3}} - 1) + p(\frac{2\sqrt{2}}{\sqrt{3}} + 6\sqrt{2} + \frac{4}{3}),$
$(viii)$ $\sigma(PTT) = (D_x^2 + D_y^2 - 2D_xD_y)M(PTT;x,y)|_{x=y=1} = 14p + 4,$
(ix) $F(PTT) = (D_x^2 + D_y^2)M(PTT;x,y)|_{x=y=1} = 182p - 14,$
(x) $HZ(PTT) = D_X^2JM(PTT;x,y)|_{x=1} = 350p - 32,$
(xi) $GO_1(PTT) = (D_x + D_y + D_xD_y)M(PTT;x,y)|_{x=y=1} = 128p + 15,$
(xii) $GO_2(PTT) = (D_x^2D_y + D_y^2D_x)M(PTT;x,y)|_{x=y=1} = 408p - 44.$

□

The general formulas of some degree-based TIs of PTT were obtained according to the number of their monomers. The numerical values of these TIs for $PTT(p)$ with the values of the variable p ranging from 1 to 10 are shown in Table 4. Considering that the value of p increases gradually, it can be seen from Figures 4, 5, and 6 that all indices are increasing. This increasing trend of p shows that the TIs values increase accordingly in Table 4. Among the investigated indices for PTT, Modified Zagreb has the lowest value, and the Second Gourava has the highest value.

Table 4 Computation of TIs of PTT.

p	FZ	SZ	SDD	MZ	H	I	ABC	σ	F	HZ	GO_1	GO_2
1	68	75	46.16	3.55	6.83	15.92	10.8	18	168	318	143	364
2	142	159	94.83	6.94	13.9	33.62	22.17	32	350	668	271	772
3	216	243	143.5	10.33	20.96	51.32	33.54	46	532	1018	399	1180
4	290	327	192.16	13.72	28.03	69.02	44.91	60	714	1368	527	1588
5	364	411	240.83	17.11	35.1	86.72	56.28	74	896	1718	655	1996
6	438	495	289.5	20.5	42.16	104.42	67.65	88	1078	2068	783	2404
7	512	579	338.16	23.88	49.23	122.12	79.02	102	1260	2418	911	2812
8	586	663	386.83	27.27	56.3	139.82	90.39	116	1442	2768	1039	3220
9	660	747	435.50	30.66	63.36	157.52	101.76	130	1624	3118	1167	3628
10	734	831	484.66	34.05	70.43	175.22	113.13	144	1806	3468	1295	4036

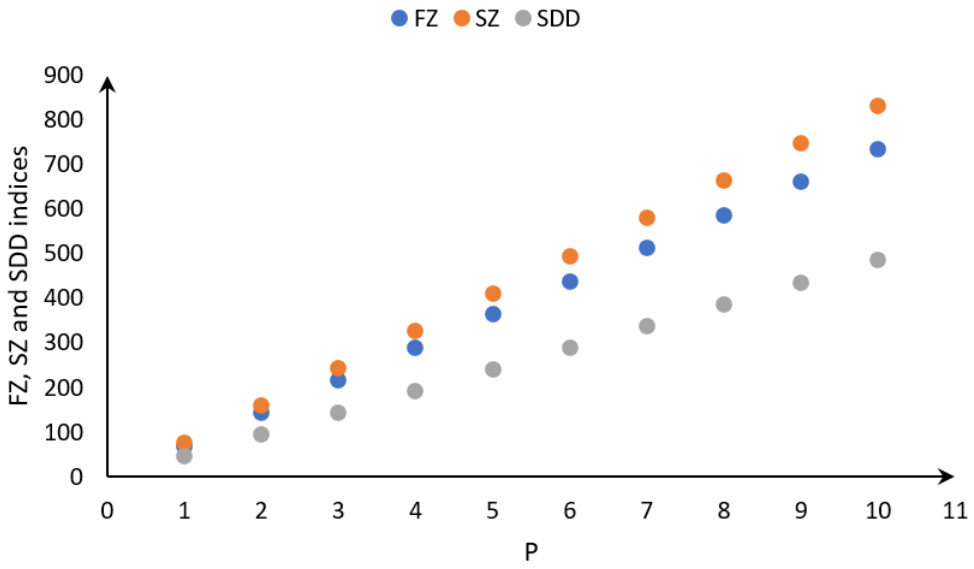

Figure 4 Comparison of FZ, SZ and SDD.

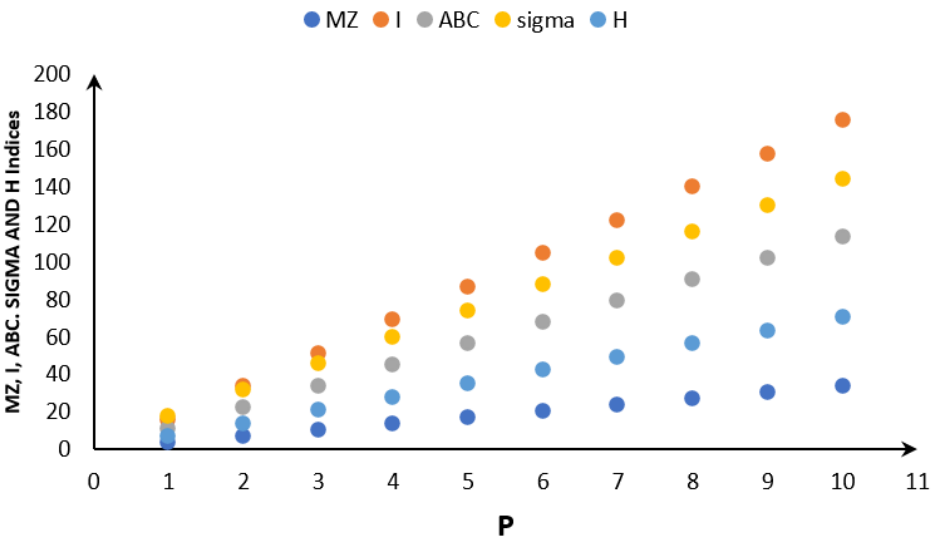

Figure 5 Comparison of MZ, H, I, ABC and σ.

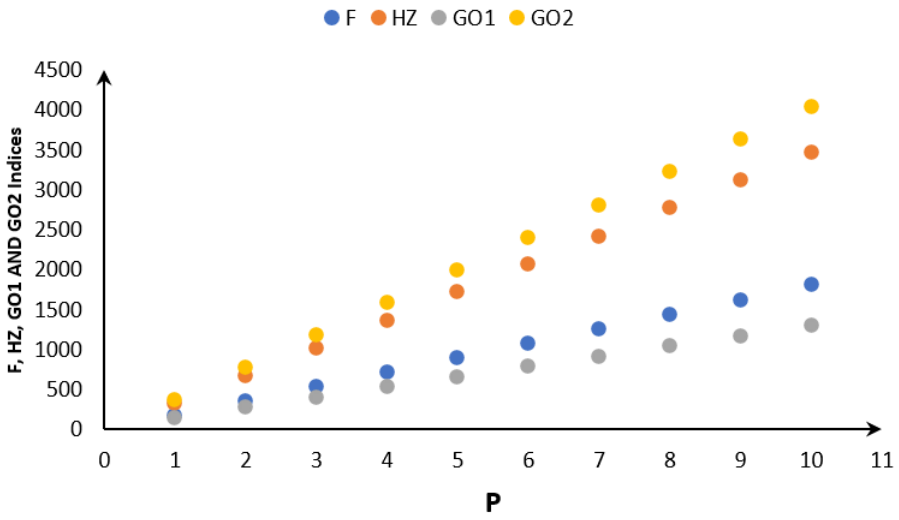

Figure 6 Comparison of F, HZ, GO_1 and GO_2.

3 Conclusion

In this article, the M-polynomial of the chemical structure of polytrimethylene terephthalate was calculated and general formulas were obtained based on the number of its monomers for some degree-based topological indices. Using these formulas, there is no need to count the edge and calculate the vertex degree to calculate the mentioned topological indices. These

indices can be used to study chemical structures and better understand their physical and chemical properties. The obtained results are presented both graphically and numerically. Considering that the value of p increases gradually, all indices are increasing. Among the investigated indices for polytrimethylene terephthalate, modified Zagreb has the lowest value, and the second Gourava has the highest value. The general conclusion of the above calculations is that according to the linear trend between the electronic properties of polytrimethylene terephthalate and topological indices with the number of monomers, the electronic properties of polytrimethylene terephthalate can be estimated with any number of monomers. The numerical values of this manuscript are valuable to the industry, and quality is easily measured by these numerical values in production evaluation. These results are suitable for other studies because no polynomials are involved. In the next studies, formulas for the topological indices of polyethylene terephthalate can be obtained. Structures of polytrimethylene terephthalate and polyethylene terephthalate can be compared and determined.

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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