

FULL PAPER

Computing M-polynomial and topological indices of TUHRC₄ molecular graph

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Chemical graph theory has an important role in the development of chemical sciences. A graph is produced from certain molecular structure by means of applying several graphical operations. The local graph parameter is valency, which is defined for every vertex as the number associates with other vertices in a graph, for example an atom in a molecule. The demonstration of chemical networks and chemical compounds with the help of M-polynomials is a novel idea. The M-polynomial of different molecular structures help to compute several topological indices. A topological index is a numeric quantity that describes the whole structure of a molecular graph of the chemical compound and clarifies its physical features, chemical reactivities and boiling activities. In this paper we computed M-Polynomial and topological indices of TUHRC₄ Graph, then we recovered numerous topological indices using the M-polynomials.

KEYWORDS

Molecular graph; nanotube; tadpole; M-Polynomial; TUHRC₄; topological indices.

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Introduction

The word "graph" was firstly used by James Joseph Sylvester (1814-1897) in 1878. In mathematics, graph theory is one of the rapidly growing branches now days. Graph theory has also found common application in various fields such as physics, biology, operations research, optimization theory, statistical mechanics, computer science, and engineering and even in chemistry. One of the most important sub field of mathematical chemistry is chemical graph theory which was originated by Ante Graovac, Milan Randić, Alexander Balaban, Haruo Hosoya, Nenad Trinajstić and Ivan Gutman [19-25].

In chemical graph theory, description of molecule is generally characterized by graphs, which are identified by their vertices

and edges. These graphs are set up from chemical molecules in which atoms converted vertices and bonds turn into edges of the graph. The topological index for a molecular graph is the ultimate conclusion of mathematical and logical operations which transform chemical facts of the molecule into suitable number. Topological descriptors are derived from hydrogen-suppressed molecular graphs.

In theoretical chemistry several topological indices are presented to check the properties of molecules which are distributed in three classes distance dependent, degree--dependent and counting related topological indices. A degree depended topological--indices are calculated with the support of degrees of vertices of chemical graph.

The topological indices calculated in this paper are general and inverse Randić index, harmonic index, first, second and modified second Zagreb index, inverse sum index, geometric arithmetic index, augmented Zagreb index.

In this paper all graphs are assumed to be simple and connected. We calculated M-polynomials of graphs, by which we determined topological indices. These graphs are useful to understand the moving behavior of topological indices with respect to structure of a molecule. In this study, a closed form of some degree-based topological indices of $TUHC_4$ was computed by using an M-polynomial.

An algebraic polynomial can also explain the behavior of the molecular structure. M-polynomial is also graph representative mathematical object. With the help of M-polynomial, we computed many degree dependent topological invariant presented in Table 3.

For a graph G , the M-polynomial introduced in 2015 [19] is defined as:

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

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 $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$. M-polynomial of many graphs are introduced [1-15, 17, 18, 23, 24, 26-34] in the past. In this work we computed M-polynomials and topological indices of $St(g; s; t)$.

TUHC₄ nanotubes graph

Nanotubes are formed by rolling up sheets into a tube. The nanotubes have been largely studied in graph theory such as polynomials and topological indices. Carbon nanotubes are composed from sheets of graphite which are rolled up into a tube constitute. In this paper, we focused on the structures of a family of nanostructures called $TUHC_4[S]$

nanotubes. These nanotubes usually are symbolized as $TUC_4(hk)$ for any $h, k \in \mathbb{N}$ in which h is the number of cycles C_4 in the first row and k is the number of cycles C_4 in the first column as depicted in Figure 1.

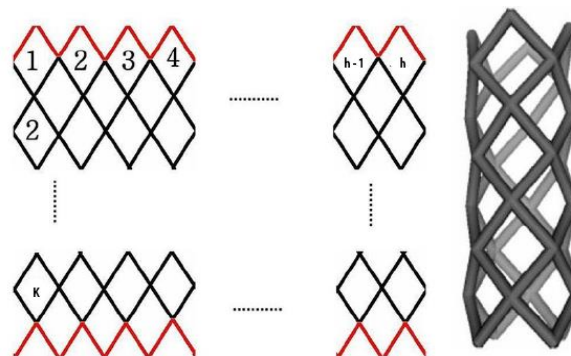


FIGURE 1 2-dimensional lattice of TUHC₄ nanotube($TUC_4(hk)$)

TABLE 1 Edge partition of TUHC₄ nanotube $TUC_4(hk)$. [2]

(d_u, d_v)	Number of edges
(2, 4)	4h
(4, 4)	(4hk-2h)
Total edges	(4hk+2h)

Topological indices

A topological index is a numeric real number related to the topology of the molecular graph. There are many classes of molecular topological invariants but degree dependent topological indices have important role in the field of chemical graph theory. These degree dependent indices are computed on the basis of degrees of vertices of molecular graph. Usually carbon-hydrogen bond is surpassed during the study of topological indices because this bond does not have any effect on the topological properties of the molecular compound. These topological indices have much application in QSAR and QSPR studies. Table 2 shows some important degree-based topological indices.

Table 3 relates some well-known degree based topological indices computed via M-Polynomial.

TABLE 2 Degree-based topological indices [1,13,14,15]

First Zagreb index [22]	$M_1[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} (d_u + d_v)$
Second Zagreb index[22]	$M_2[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} (d_u \cdot d_v)$
Randić Index[25]	$R_{-\frac{1}{2}}[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \frac{1}{\sqrt{d_u \cdot d_v}}$
General Randić Index[25]	$R_\alpha[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} (d_u \cdot d_v)^\alpha$
Inverse Randić Index[25]	$RR_\alpha[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \left(\frac{1}{d_u \cdot d_v}\right)^\alpha$
Harmonic index[20]	$H[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \left(\frac{2}{d_u + d_v}\right)$
Symmetric division index	$SSD[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u}\right)$
Inverse sum index[16]	$I[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \left(\frac{d_u \cdot d_v}{d_u + d_v}\right)$
Augmented Zagreb index[21]	$A[TUC_4(hk)] = \sum_{uv \in E(TUC_4(hk))} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$

TABLE 3 Degree dependent topological indices.[1,13,14,15]

Topological index	Derivation from $M(G;x,y)$
First Zagreb index[22]	$M_1[TUC_4(hk)] = (D_x + D_y)[f(x, y)]_{x=y=1}$
Second Zagreb index[22]	$M_2[TUC_4(hk)] = (D_x D_y)[f(x, y)]_{x=y=1}$
Modified second Zagreb index	${}^m M_2[TUC_4(hk)] = (S_x S_y)[f(x, y)]_{x=y=1}$
General Randić Index[25]	$R_\alpha[TUC_4(hk)] = (D_x^\alpha D_y^\alpha)[f(x, y)]_{x=y=1}$
Inverse Randić Index[25]	$RR_\alpha[TUC_4(hk)] = (S_x^\alpha S_y^\alpha)[f(x, y)]_{x=y=1}$
Harmonic index	$H[TUC_4(hk)] = 2S_x J[f(x, y)]_{x=1}$
Symmetric division index	$SSD[TUC_4(hk)] = (D_x S_y + S_x D_y)[f(x, y)]_{x=y=1}$
Inverse sum index	$I[TUC_4(hk)] = S_x J D_x D_y [f(x, y)]_{x=1}$
Augmented Zagreb index	$A[TUC_4(hk)] = S_x^3 Q_{-2} J D_x^3 D_y^3 [f(x, y)]_{x=1}$

Where the operator used are defined as

$$D_x f(x, y) = x \frac{\partial(f(x, y))}{\partial x}, D_y f(x, y) = y \frac{\partial(f(x, y))}{\partial y},$$

$$L_x f(x, y) = f(x^2, y), L_y f(x, y) = f(x, y^2),$$

$$S_x f(x, y) = \int_0^x \frac{f(t, y)}{t} dt, S_y f(x, y) = \int_0^y \frac{f(x, t)}{t} dt,$$

$$Jf(x, y) = f(x, x), Q_\alpha f(x, y) = x^\alpha f(x, y),$$

$$S_x^{\frac{1}{2}} f(x, y) = \sqrt{\int_0^x \frac{f(t, y)}{t} dt \cdot \sqrt{f(x, y)}},$$

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

M-Polynomial of TUHRC₄ nanotube

Theorem 5.1. Let $TUC_4(hk)$ be a TUHRC₄ nanotube then for $h, k > 1$, M-polynomial of $TUC_4(hk)$ is

$$M[TUC_4(hk); x; y] = 4hx^2y^4 + (4hk - 2h)x^4y^4$$

Proof. Let $TUC_4(hk)$ be a nanotube then by using Figure 1 we have the following vertex partition.

$$V_2 = \{u \in TUC_4(hk) : d_u = 2\} \rightarrow |V_2| = 4h,$$

$$V_3 = \{u \in TUC_4(hk) : d_u = 3\} \rightarrow |V_3| = (4hk - 2h).$$

From Figure 1, the edge partition of TUHRC₄ nanotube is

$$E_{2,4}(TUC_4(hk)) = \{e = uv \in TUC_4(hk) : d_u = 2; d_v = 4\}$$

$$\rightarrow |E_{2,4}TUC_4(hk)| = 4h,$$

$$E_{4,4}(TUC_4(hk)) = \{e = uv \in TUC_4(hk) : d_u = 4; d_v = 4\}$$

$$\rightarrow |E_{4,4}TUC_4(hk)| = (4hk - 2h).$$

We get the following result by applying the definition of M-polynomial

$$M(TUC_4(hk); x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(TUC_4(hk)) x^i y^j$$

$$M(TUC_4(hk); x, y) = \sum_{2 \leq i \leq j \leq 4} m_{ij}(TUC_4(hk)) x^i y^j$$

$$M(TUC_4(hk); x, y) = \sum_{2 \leq 4} m_{24}(TUC_4(hk)) x^2 y^4 + \sum_{4 \leq 4} m_{44}(TUC_4(hk)) x^4 y^4$$

$$M(TUC_4(hk); x, y) = |E_{2,4}| x^2 y^4 + |E_{4,4}| x^4 y^4$$

$$M(TUC_4(hk); x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4.$$

The plot of M-polynomial of TUC₄(hk) is shown in Figure 2.

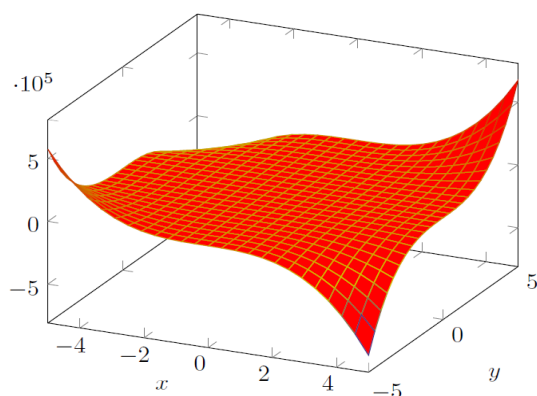


FIGURE 2 3D plot of M-polynomial of TUHRC₄ nanotube(TUC₄(hk)) for g=s=t=4.

Topological indices of TUHRC₄ nanotube

Theorem 6.1. Let TUC₄(hk) be a TUHRC₄ nanotube and $M[TUC_4(hk); x, y] = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$, then:

- 1) $M_1[TUC_4(hk)] = 32hk + 8h$
- 2) $M_2[TUC_4(hk)] = 64hk$
- 3) ${}^m M_2[TUC_4(hk)] = 0.25hk + 0.375h$
- 4) $R_\alpha[TUC_4(hk)] = 16^\alpha 4hk + 8^\alpha 4h - 16^\alpha 2h$
- 5) $RR_\alpha[TUC_4(hk)] = \frac{4}{16^\alpha} hk + \left(\frac{4}{8^\alpha} - \frac{2}{16^\alpha}\right) h$
- 6) $SDD[TUC_4(hk)] = 8hk + 6h$
- 7) $H[TUC_4(hk)] = hk + \frac{5}{8} h$
- 8) $I[TUC_4(hk)] = 8hk + \frac{4}{3} h$

$$9) \quad A[TUC_4(hk)] = \frac{2048}{27} hk - \frac{160}{27} h$$

Proof. Let $M[TUC_4(hk); x, y] = f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$

1. The first Zagreb index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$D_x f(x, y) = 8hx^2 y^4 + 4(4hk - 2h)x^3 y^4$$

$$D_y f(x, y) = 16hx^2 y^3 + 4(4hk - 2h)x^4 y^3$$

$$(D_x + D_y)f(x, y) = 24hx^2 y^4 + 8(4hk - 2h)x^4 y^4$$

$$M_1[TUC_4(hk)] = (D_x + D_y)f(x, y)_{x=y=1} = 32hk + 8h$$

2. The second Zagreb index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$D_y f(x, y) = 16hx^2 y^3 + 4(4hk - 2h)x^4 y^3$$

$$x^4 y^4 D_x D_y f(x, y) = 32hx^2 y^4 + 16(4hk - 2h)$$

$$x^4 y^4 M_2[TUC_4(hk)] = (D_x D_y)f(x, y)_{x=y=1} = 64hk$$

3. The modified second Zagreb index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$S_y f(x, y) = hx^2 y^4 + \frac{1}{4}(4hk - 2h)$$

$$x^4 y^4 S_x S_y f(x, y) = \frac{1}{2} hx^2 y^4 + \frac{1}{16}(4hk - 2h)$$

$$x^4 y^4 M_2[TUC_4(hk)] = (S_x S_y)f(x, y)_{x=y=1} = \frac{1}{4} hk + \frac{3}{8} h$$

4. The general Randić index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$D_y^\alpha f(x, y) = 4 \cdot 4^\alpha hx^2 y^4 + 4^\alpha (4hk - 2h)x^4 y^4$$

$$D_x^\alpha D_y^\alpha f(x, y) = 4 \cdot 8^\alpha hx^2 y^4 + 16^\alpha (4hk - 2h)x^4 y^4$$

$$R_\alpha[TUC_4(hk)] = (D_x^\alpha D_y^\alpha)f(x, y)_{x=y=1} = 4 \cdot 16^\alpha hk + [2 \cdot 8^\alpha - 16^\alpha] 2h$$

5. The inverse Randić index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$S_y^\alpha f(x, y) = \frac{4}{4^\alpha} hx^2 y^4 + \frac{1}{4^\alpha} (4hk - 2h)x^4 y^4$$

$$S_x^\alpha S_y^\alpha f(x, y) = \frac{4}{8^\alpha} hx^2 y^4 + \frac{1}{16^\alpha} (4hk - 2h)x^4 y^4$$

$$RR_\alpha[TUC_4(hk)] = (S_x^\alpha S_y^\alpha)[f(x, y)]_{x=y=1} = \frac{4}{16^\alpha} hk + \left[\frac{4}{8^\alpha} - \frac{2}{16^\alpha}\right] h$$

6. The symmetric division index

$$f(x, y) = 4hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$S_y f(x, y) = hx^2 y^4 + \frac{1}{4}(4hk - 2h)x^4 y^4$$

$$D_x S_y f(x, y) = 2hx^2 y^4 + (4hk - 2h)x^3 y^4$$

$$D_y f(x, y) = 16hx^2 y^3 + 4(4hk - 2h)x^4 y^3$$

$$D_y f(x, y) = 8hx^2 y^4 + (4hk - 2h)x^4 y^4$$

$$(D_x S_y + S_x D_y)f(x, y) = 10hx^2 y^4 + 2(4hk - 2h)x^4 y^4$$

$$SDD[TUC_4(hk)] = (D_x S_y + S_x D_y)f(x, y)_{x=y=1} = 8hk + 6h$$

7. The harmonic index

$$f(x, y) = 4hx^2y^4 + (4hk - 2h)x^4y^4 \quad Jf(x, y) = 4hx^6 + (4hk - 2h)x^8$$

$$S_x Jf(x, y) = \frac{2}{3}hx^6 + \frac{1}{8}(4hk - 2h)x^8$$

$$2S_x Jf(x, y) = \frac{4}{3}hx^6 + \frac{1}{4}(4hk - 2h)x^8$$

$$H[TUC_4(hk)] = 2S_x Jf(x, y)_{x=1} = hk + \frac{5}{6}h$$

8. The inverse sum index

$$f(x, y) = 4hx^2y^4 + (4hk - 2h)x^4y^4$$

$$D_y f(x, y) = 16hx^2y^4 + 4(4hk - 2h)x^4y^4$$

$$D_x D_y f(x, y) = 32hx^2y^4 + 16(4hk - 2h)x^4y^4$$

$$JD_x D_y f(x, y) = 32hx^6 + 16(4hk - 2h)x^8$$

$$S_x JD_x D_y f(x, y) = \frac{16}{3}hx^6 + 2(4hk - 2h)x^8$$

$$I[TUC_4(hk)] = (S_x JD_x D_y) f(x, y)_{x=1} = 8hk + \frac{4}{3}h$$

9. The augmented Zagreb index

$$f(x, y) = 4hx^2y^4 + (4hk - 2h)x^4y^4$$

$$D_y^3 f(x, y) = 256hx^2y^4 + 64(4hk - 2h)x^4y^4$$

$$D_x^3 D_y^3 f(x, y) = 2048hx^2y^4 + 4096(4hk - 2h)x^4y^4$$

$$JD_x^3 D_y^3 f(x, y) = 2048hx^6 + 4096(4hk - 2h)x^8$$

$$Q_{-2} JD_x^3 D_y^3 f(x, y) = 2048hx^4 + 4096(4hk - 2h)x^6$$

$$S_x^3 Q_{-2} JD_x^3 D_y^3 f(x, y) = 32hx^4 + \frac{512}{27}(4hk - 2h)x^6$$

$$A[TUC_4(hk)] = S_x^3 Q_{-2} JD_x^3 D_y^3 f(x, y)_{x=1} = \frac{2048}{27}hk - \frac{160}{27}h$$

Figure 3 is the graphical representation of topological indices of $TUC_4(hk)$. From graphs,

we see the behavior of the topological indices along different parameters. Despite the fact that the graphs are looking to be identical, but have distinct gradients.

Conclusion

In the present article, we calculated the closed-form of M-polynomial for the graph $TUHC_4$ nanotube. Then, we recovered many degree-based topological indices as well. Topological indices help to reduce the number of experiments. These topological indices can support biological, chemical and physical characteristics of a molecule. So, topological indices have a key role and represent the chemical structure of a molecule to a mathematical number and are used to express the molecule structure which is tested. The results calculated in this article are very cooperative in understanding and forecasting the physiochemical behavior of these chemical compounds. The study on distance-related topological indices for much important chemical structure is still open to further research.

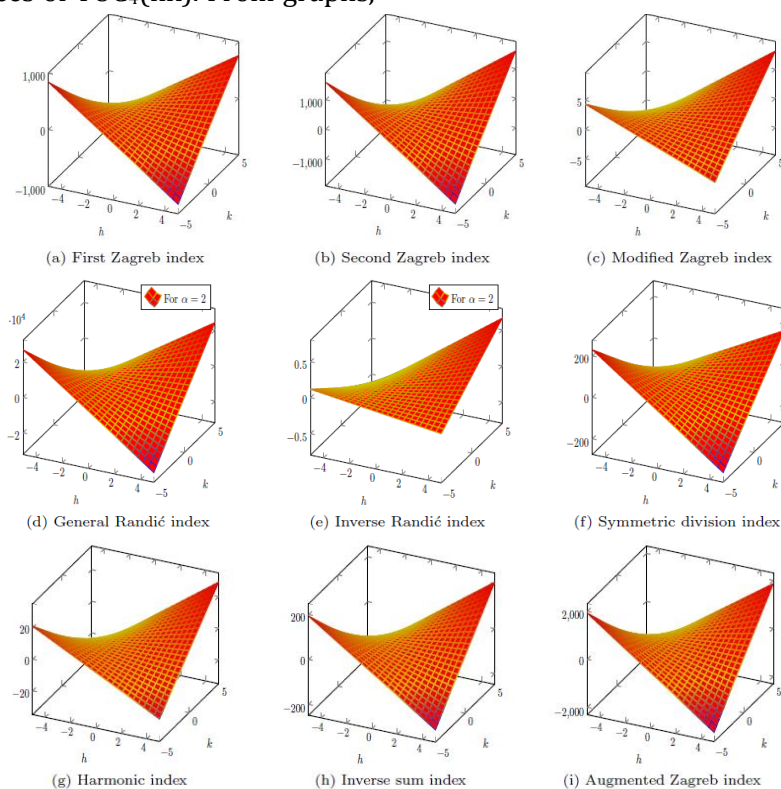


FIGURE 3 The plot of topological indices of $TUHC_4$ nanotube ($TUC_4(hk)$)

Acknowledgments

The authors would like to thank the reviewers for their helpful suggestions and comments.

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How to cite this article: Faryal Chaudhry, Muhammad Ehsan, Farkhanda Afzal*, Mohammad Reza Farahani, Murat Cancan, Idris Çiftçi. Computing M-polynomial and topological indices of TUHRC₄ molecular graph. *Eurasian Chemical Communications*, 2021, 3(2), 103-109. **Link:** http://www.echemcom.com/article_126404.html