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FULL PAPER

Some new degree based topological indices of h-naphtalenic graph *via* M-polynomial approach

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In this object, we present some new formulas of the reduced reciprocal Randić index, the arithmetic geometric $_1$ index, the SK, SK_1, SK_2 indices, first Zagreb index, the general sum-connectivity index, the SCI index and the forgotten index. They were utilized for new degree-based topological indices *via* M-polynomial. We retrieved these topological indices for H-Naphtalenic nanotubes.

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KEYWORDS

Topological indices; H-Naphtalenic nanotube; chemical molecule; graph polynomial; M-polynomial.

Introduction

Chemical graph theory is a branch of mathematics, which combines chemistry and graph theory. Graph theory is a mathematical imitation of molecules to construct insight into the properties of those chemical mixtures. Each carbon atom forms four bonds in a stable organic compound, such as ethane, ethene (ethylene), and ethyne (acetylene). The carbon atom in ethene forms four single bonds, each of the three hydrogen atoms and one to the neighboring carbon atoms of each hydrogen atom has one chemical bond.

The topological indices assist in the physical features, chemical and bio-logical reactivity. The topological index is surveying the principal part that shows each molecular structure of the real number, implemented as a descriptor of the molecule under checking. This graphical representation of topological indices shows the dependency of a confirmed index on the structure.

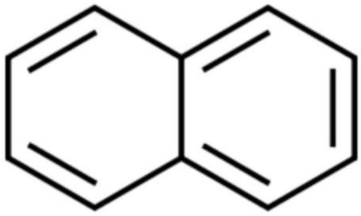


FIGURE 1 H-Naphtalenic nanotube

A nanotube is chiefly sheets build up into a tube. Nanotubes concern different graph-theoretic frameworks in graph theory, like polynomials and topological indices. H-Naphtalenic is rising in the same way by a sheet cover with squares, hexagons and octagons. The topological indices are also computed via M-polynomial. Several works have already been done in this area [1,2,3-6,22,23].

The M-polynomial introduced by Emeric Deutsch and Sandi Klavžar [7] is defined for a graph G as the first topological index invented by wiener [8]. Topological indices are used in the development, quantitative activity and also other properties of molecules correlate in chemical structure. The connection between atoms is shown as topological indices of different chemical compound such as boiling point, the heat of formation, heat of evaporation, surface tension, vapor pressure and etc. Now we define some topological indices.

The reduced reciprocal Randić index

$$RRR(G)=\sum_{jk\in E(G)}\sqrt{(d_j-1)(d_k-1)}.$$

In 2015 [9], I. Gutman ed ul., invented a reduced reciprocal index. The reduced reciprocal Randić (RRR) index is a molecular structure descriptor (more precisely, a topological index), which is helpful for the divine level of enthalpy creation and the usual boiling point of isomeric octanes.

The arithmetic geometric index

$$AG_1(G)=\sum_{jk\in E(G)}\frac{d_j+d_k}{2\sqrt{d_j.d_k}}.$$

In 2016 [10]. V. Shegehalli and R. Kanabur are used arithmetic geometric index.
The SK, SK_1, SK_2 indices are defined as:

$$SK(G)=\sum_{jk\in E(G)}\frac{d_j+d_k}{2},$$

$$SK_1(G)=\sum_{jk\in E(G)}\frac{d_j.d_k}{2},$$

$$SK_2(G)=\sum_{jk\in E(G)}(\frac{d_j.d_k}{2})^2.$$

In 2016 [10] Shegehalli and Kanabur used SK, SK_1, SK_2 indices.

The first Zagreb index

First Zagreb index was used in 2014 [11].

$$EM_1(G)=\sum_{jk\in E(G)}(d_{jk})^2.$$

The general sum-connectivity index

It was first used by Zhibin Du ed al., in 2011 [12].

$$SCI(G)=\sum_{jk\in E(G)}\frac{1}{\sqrt{d_j+d_k}}.$$

The SCI index

It was also first used by Zhibin Du ed al., in 2011 [11].

$$SCI_\lambda=\sum_{jk\in E(G)}(d_j+d_k)^\lambda.$$

The forgotten index

Gutman and Furtula (2105) introduced it the first time [9].

$$F(G)=\sum_{jk\in E(G)}(d_j^2+d_k^2).$$

Definition: The M-polynomial was first used in 2015 [7], determined as:

$$M(G,x,y)=\sum_{\rho\le j\le k\le\phi}m_{ij}(G)x^jy^k,$$

Where $\rho=\max\{d_v : v\in V(G)\}$, $\phi=\min\{d_v : v\in V(G)\}$ and $m_{jk}(G)$ is the total number of edges vu∈E(G) where $\{d_v; d_u\}=\{j; k\}$. Recently, M-polynomial of several graphs was invented [13-20]

TABLE 1 Degree dependent topological indices via M-polynomial [21]

Topological index	Derivation from M(G;x;y)
The reduced reciprocal Randić index	$RRR[G]=D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}Q_{y(-1)}Q_{x(-1)}[g(x,y)]_{x=y=1}$
The arithmetic geometric $_1$ index	$AG_1[G]=\frac{1}{2}D_xJS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[g(x,y)]_{x=1}$
The SK index	$SK[G]=\frac{1}{2}(D_x+D_y)g(x,y)]_{x=y=1}$

The SK_1 index	$SK_1[G]=\frac{1}{2}(D_xD_y)[g(x,y)]_{x=y=1}$
The SK_2 index	$SK_2[G]=\frac{1}{4}D_x^2J[g(x,y)]_{x=y=1}$
The first Zagreb index	$EM_1[G]=D_x^2Q_{x(-2)}J[g(x,y)]_{x=1}$
The general sum-connectivity index	$SCI[G]=S_x^{\frac{1}{2}}J[g(x,y)]_{x=1}$
The SCI index	$SCI_\lambda[G]=D_x^\lambda J[g(x,y)]_{x=1}$
The forgotten index	$F[G]=(D_x^2+D_y^2)[g(x,y)]_{x=1}$

Where

$$D_xg(x,y)=x\frac{\partial(g(x,y))}{\partial x},$$
$$D_yg(x,y)=y\frac{\partial(g(x,y))}{\partial y},$$
$$Jg(x,y)=g(x,x),$$
$$Q_{x(\alpha)}g(x,y)=x^\alpha g(x,y),$$
$$D_x^{\frac{1}{2}}(g(x,y)=\sqrt{x\frac{\partial(g(x,y))}{\partial x}}\cdot\sqrt{g(x,y)},$$
$$D_y^{\frac{1}{2}}(g(x,y)=\sqrt{y\frac{\partial(g(x,y))}{\partial y}}\cdot\sqrt{g(x,y)},$$
$$S_x^{\frac{1}{2}}(g(x,y)=\sqrt{\int_0^x\frac{g(t,y)}{t}dt}\cdot\sqrt{g(x,y)},$$
$$S_y^{\frac{1}{2}}(g(x,y)=\sqrt{\int_0^y\frac{g(x,t)}{t}dt}\cdot\sqrt{g(x,y)}.$$

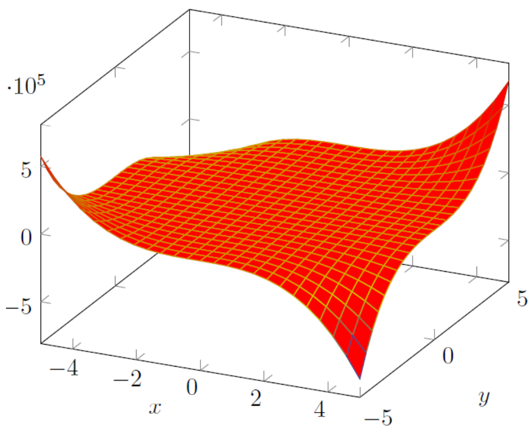


FIGURE 2 3D plot of M-polynomial of some new degree based topological indices via M-polynomial m=n=2.

H-naphtalenic nanotube

Carbon nanotubes were initially used in 1991, and one-dimensional material appeared. Nanotubes are created by rolling up sheets into a tube. The nanotubes are largely studied in graph theory such as polynomials and topological indices. H-Naphtalenic nanotubes are formed in same way with sheets covered by squares, hexagons and octagons.

Let $HNnt_{mn}$ be a H-Naphtalenic nanotube then for m; n≥1, M-polynomial of $HNnt_{mn}$ is given as:

$M(HNnt_{mn};x;y)=8nx^2y^3+5n(3m-2)x^3y^3$

Topological indices of H-Naphtalenic nanotube via M-polynomial

Theorem 3.1. Let *HNnt* be a H-Naphtalenic nanotube then for m; n≤ 1, M-polynomial is given as:

$M(HNnt_{mn};x;y)=8nx^2y^3+5n(3m-2)x^3y^3$:

$$(1)RRR[HNnt_{mn}]=30mn+8\sqrt{2}n-20n$$
$$(2)AG_1[HNnt_{mn}]=15mn-10n+\frac{20}{\sqrt{6}}n$$
$$(3)SK[HNnt_{mn}]=45mn-10n$$
$$(4)SK_1[HNnt_{mn}]=\frac{135mn-42n}{2}$$
$$(5)SK_2[HNnt_{mn}]=135mn-40n$$
$$(6)EM_1HNnt_{mn}=240mn-88n$$
$$(7)SCI[HNnt_{mn}]=\frac{15\sqrt{5}mn+8\sqrt{6}n-10\sqrt{5}n}{\sqrt{30}}$$
$$(8)SCI_\lambda[HNnt_{mn}]=90^\lambda mn-20^\lambda n$$
$$(9)F[HNnt_{mn}]=270mn-76n.$$

Proof. Let *HNnt* be a H-Naphtalenic nanotube. The M-polynomial is given as:

$M(HNnt_{mn};x;y)=8nx^2y^3+5n(3m-2)x^3y^3$

1. The reduced reciprocal Randić index

$$Q_{x(-1)}g(x,y)=8nxy^3+5n(3m-2)x^2y^3$$
$$Q_{y(-1)}Q_{x(-1)}g(x,y)=8nxy^2+5n(3m-2)x^2y^2$$
$$D_y^{\frac{1}{2}}Q_{y(-1)}Q_{x(-1)}g(x,y)=8n\sqrt{2}xy^2+5\sqrt{2}n(3m-2)x^2y^2$$
$$D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}Q_{y(-1)}Q_{x(-1)}g(x,y)=8n\sqrt{2}xy^2+10n(3m-2)x^2y^2$$
$$RRR[HNnt_{mn}]=D_x^{\frac{1}{2}}D_y^{\frac{1}{2}}Q_{y(-1)}Q_{x(-1)}[g(x,y)]_{x=1}$$
$$=30mn+8\sqrt{2}n-20n.$$

2. The arithmetic geometric 1 index

$$S_y^{\frac{1}{2}}g(x,y)=\frac{8}{\sqrt{3}}nx^2y^3+\frac{5}{\sqrt{3}}n(3m-2)x^3y^3$$
$$S_x^{\frac{1}{2}}S_y^{\frac{1}{2}}g(x,y)=\frac{8}{\sqrt{6}}nx^2y^3+\frac{5}{3}n(3m-2)x^3y^3$$
$$JS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}g(x,y)=\frac{8}{\sqrt{6}}nx^5+\frac{5}{3}n(3m-2)x^6$$
$$D_xJS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}g(x,y)=\frac{40}{\sqrt{6}}nx^5+10n(3m-2)x^6$$
$$\frac{1}{2}D_xJS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}g(x,y)=\frac{20}{\sqrt{6}}nx^5+5n(3m-2)x^6$$
$$AG_1[HNnt_{mn}]=\frac{1}{2}D_xJS_x^{\frac{1}{2}}S_y^{\frac{1}{2}}[g(x,y)]_{x=y=1}$$
$$=15mn-10n+\frac{20}{\sqrt{6}}n.$$

3. The SK index

$$D_yg(x,y)=24nx^2y^3+15n(3m-2)x^3y^3$$
$$D_xg(x,y)=16nx^2y^3+15n(3m-2)x^3y^3$$
$$(D_x+D_y)g(x,y)=40nx^2y^3+30n(3m-2)x^3y^3$$
$$\frac{1}{2}(D_x+D_y)g(x,y)=20nx^2y^3+15n(3m-2)x^3y^3$$
$$SK[HNnt_{mn}]=\frac{1}{2}(D_x+D_y)g(x,y)]_{x=y=1}=45mn-10n.$$

The SK_1 index

$$D_yg(x,y)=24nx^2y^3+15n(3m-2)x^3y^3$$
$$(D_xD_y)g(x,y)=48nx^2y^3+45n(3m-2)x^3y^3$$
$$\frac{1}{2}(D_xD_y)g(x,y)=24nx^2y^3+\frac{45}{2}n(3m-2)x^3y^3$$
$$SK_1[HNnt_{mn}]=\frac{1}{2}(D_xD_y)[g(x,y)]_{x=y=1}$$
$$=\frac{135mn-42n}{2}.$$

4. The SK_2 index

$$Jg(x,y)=8nx^5+5n(3m-2)x^6$$
$$D_x^2Jg(x,y)=200nx^5+180n(3m-2)x^6$$
$$\frac{1}{4}D_x^2Jg(x,y)=50nx^5+45n(3m-2)x^6$$
$$SK_2[HNnt_{mn}]=\frac{1}{4}D_x^2J[g(x,y)]_{x=y=1}$$
$$=135mn-40n..$$

5. The first Zagreb index

$$Jg(x,y)=8nx^5+5n(3m-2)x^6$$
$$Q_{x(-2)}Jg(x,y)=8nx^3+5n(3m-2)x^4$$
$$D_x^2Q_{x(-2)}Jg(x,y)=72nx^3+80n(3m-2)x^4$$
$$EM_1[HNnt_{mn}]=D_x^2Q_{x(-2)}J[g(x,y)]_{x=1}$$
$$=240mn-88n.$$

6. The general sum-connectivity index

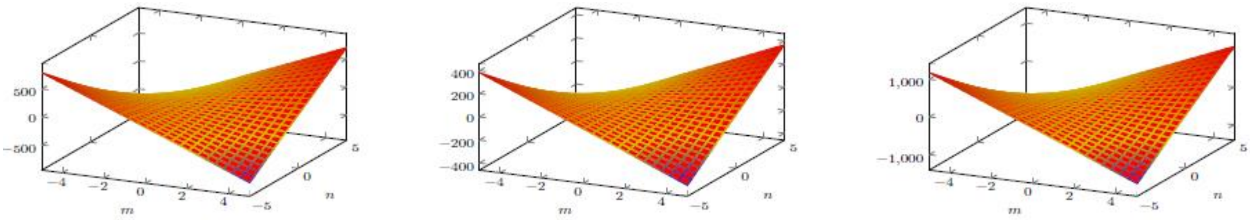
$$Jg(x,y)=8nx^5+5n(3m-2)x^6$$
$$S_x^{\frac{1}{2}}Jg(x,y)=\frac{8}{\sqrt{5}}nx^5+\frac{5}{\sqrt{6}}n(3m-2)x^6$$
$$SCI[HNnt_{mn}]=S_x^{\frac{1}{2}}J[g(x,y)]_{x=1}$$
$$=\frac{8\sqrt{6}n+15\sqrt{5}mn-10\sqrt{5}n}{\sqrt{30}}.$$

7. The SCI index

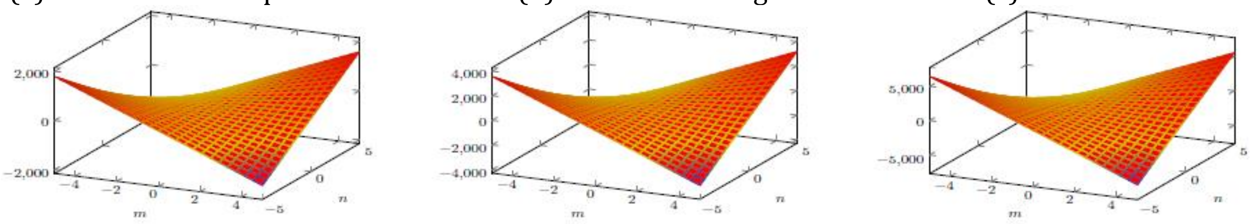
$$Jg(x,y)=8nx^5+5n(3m-2)x^6$$
$$D_x^{\lambda}Jg(x,y)=40^{\lambda}nx^5+30^{\lambda}n(3m-2)x^6$$
$$SCI_{\lambda}[HNnt_{mn}]=D_x^{\lambda}J[g(x,y)]_{x=1}$$
$$=90^{\lambda}mn-20^{\lambda}n.$$

8. The forgotten index

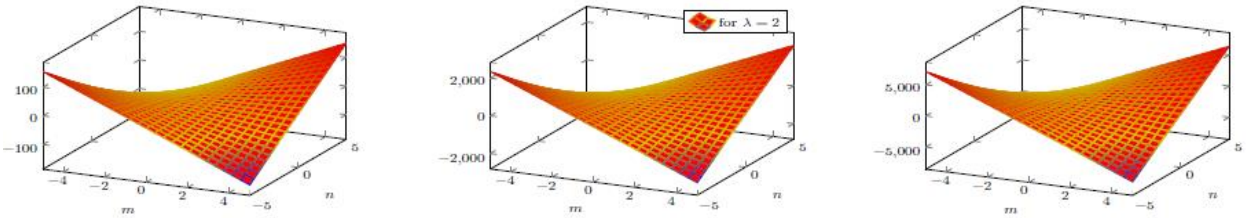
$$D_y^2g(x,y)=72nx^2y^3+45n(3m-2)x^3y^3$$
$$D_x^2g(x,y)=32nx^2y^3+45n(3m-2)x^3y^3$$
$$(D_x^2+D_y^2)g(x,y)=104nx^2y^3+90n(3m-2)x^3y^3$$
$$F[HNnt_{mn}]=(D_x^2+D_y^2)[g(x,y)]_{x=1}$$
$$=270mn-76n.$$



(a) The reduced reciprocal Randić index (b) The arithmetic geometric 1 index (c) The SK index



(d) The SK1 index (e) The SK2 index (f) The first Zagreb index



(g) The general sum-connectivity index (h) The SCI_{λ} index (i) The forgotten index

FIGURE 3 The plot of topological indices of H-Naphtalenic nanotube 1

Conclusion

The induction of new closed formulas was to count the topological indices via M-polynomial. In this study, we determined M-polynomials of H-Naphtalenic ($HNnt_{mn}$). These topological indices are useful for the augury plan of physical features, biological activities, and chemical reactivates of the substance.

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