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INVESTIGATION ON SOME TOPOLOGICAL INDICES OF CARBON NANOBUD THROUGH M-POLYNOMIAL

DEEPASREE S KUMAR, P.S.RANJINI AND V. LOKESHA

Abstract. Topological indices are popular descriptors used in chemical graph theory. These are basically numerical values that correlate the topology of chemical compounds to its different physical properties and synthetic reactivities. Among different classes of topological indices, degree based topological indices have prominent role in characterising the topology of molecular graph and are widely used in quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies. Carbon Nanobud exhibits superior properties compared to both Nanotubes and Fullerene. Structure of Carbon nanobud is achieved by fusion of fullerene and Nanotubes with carbon-carbon covalent bond connections between them. Some of the popular degree based topological indices of a typical Nanobud molecular structure is estimated in this article. Here we considered a single fullerene (C_{60}), attached on the surface of a zigzag Single Walled Carbon Nanotube (SWNT) by a [2 x 2] cyclo-addition.

Keywords: Zagreb indices, Link graphs,Carbon Nanobuds

Mathematics Subject Classification: $05C35$; $05C07$; $05C40$

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1. Introduction

In mathematical chemistry, topological indices have become a very valuable tool for predicting properties of a compound from its molecular structure. It is possible to correlate the physical, chemical or biological properties of a compound to its molecular structure through numerical values called topological indices, which are derived from the Molecular graph of the compound. Topological indices can be easily used for chemical modeling with the help of software packages. Graph theory has growing applications in different Science and Engineering fields. The QSAR and QSPR studies, which relate biological or chemical features, are the most common uses of Topological index[2,3,17,18,19]. Topological Index was introduced by Wiener in 1947, called Wiener index [13], which correlates the topology of alkanes with its boiling points. A subclass of these descriptors called Adriatic indices [20] are widely used by researchers in chemical characterisation. In the upcoming sections, some of the popular topological indices are discussed and they are computed for a simple Carbon nanobud structure. M-Polynomial of the structure is derived first and then the indices are estimated using M Polynomial.

1.1. **Definition.** Among different types of topological indices, degree based topological indices are very popular because of its applications in chemical graph theory.

Some of the important degree based topological indices are considered in this paper and its definitions are given in this section. Molecular graph $G(V,E)$,where the vertex set is represented by V and edge set is represented by E of a molecular structure. The molecular structure is formed by atoms serve as vertices and chemical bonds between atoms serve as edges. The degree refers to the total number of vertices attached to each vertex. The degree of a vertex v is represented by dv. We followed the book [9] for definitions and notations in the graph theory.

Gutman and Trinajstić [8] established the Zagreb index , which was verified in a research of total π-electron energy structure -dependence. Kulli [11] studied Zagreb index for Carbon nanotubes in detail.

The terms denoted by M_1 and M_2 commonly known as Zagreb indices of the first and second kind and defined as follows[15] :

$$M_1(G) = \sum_{v \in V} (d_v)^2 = \sum_{uv \in E(G)} (d_u + d_v).$$

Second Modified Zagreb index [13] is defined as

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u d_v}.$$

The Randic index, which is widely utilised in the realm in the field of drug design, is another popular index. This was introduced by Milan Randic [14] in 1974.

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Ernesto Estrada[5] later adjusted the Randic index to relate with the thermodynamic features of alkanes, specifically formation of heats. Atom-bomb connectivity index(ABC-index) is a new version of the Randic index that is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_u - 2}{d_u d_v}}.$$

ABC index was further elaborated by Kulli [12, 20] and applied in certain nanostructures compounds. The Augmented Zagreb index, which is derived from the ABC index, was introduced by Furtula et al[7]. The enhanced Zagreb index is defined as

$$A(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

The Harmonic index, proposed by Fajtlowicz [6] is a version of Randic index that is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

The Symmetric Division Index [3] is a well-known degree-based topological index that can be used to characterise the chemical and physical properties of molecules.

$$SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{min(d_u, d_v)}{max(d_u, d_v)} + \frac{max(d_u, d_v)}{min(d_u, d_v)} \right\}$$

.

The Inverse Sum Index [1] is a well-established method for predicting the total surface area of octane isomers.

$$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

Definition 1.[4] Let G be a graph. Then M-Polynomial of G is defined as

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

where $m_{ij}(G)$, $i, j \geq 1$ be the number of edges uv of G such that d_u, d_v=$\{i, j\}$.

Table 1[4]: Topological indices and expression with M-Polynomial.

Topological Index	$f(x,y)$	Expression with M-Polynomial
First Zagreb	$x+y$	$(D_x + D_y)M(G : x, y)_{x=y=1}$
Second Zagreb	xy	$(D_x D_y)M(G : x, y)_{x=y=1}$
Second Modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)M(G : x, y)_{x=y=1}$
Symmetric division dug Index(SDD)	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)M(G : x, y)_{x=y=1}$
Augmented Index	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (M(G; x, y))_{x=y=1}$
General Randic Index($\alpha \in N$)	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)M(G; x, y)_{x=y=1}$
ABC Index	$\sqrt{\frac{x+y-2}{xy}}$	$S_x^{-\frac{1}{2}} \left[Q_{-2} (J D_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}}) \right]_{x=y=1}$
Harmonic Index	$\frac{2}{x+y}$	$2 S_x J M(G; x, y)_{x=y=1}$
Inverse sum Index	$\frac{2}{x+y}$	$S_x J D_x D_y M(G; x, y)_{x=y=1}$

1.2. **Preliminaries of Carbon nanobuds(NB).** In general Carbon Nanobud structure has fullerenes attached to the sidewalls of a Carbon nanotube. There exist a covalent bond between Carbon-Carbon atoms of fullerene and Carbon nanotube. This additional fullerene modifies some of the properties of Carbon nanotube. Carbon nanotube possesses good mechanical properties and electrical conductivity whereas the fullerene attached to the Carbon nanotubes restricts movement of Carbon nanotubes in the matrix materials. As a result, the properties of final composites could be improved. Degree-based topological indices listed in the previous sections are estimated for a Carbon nanobud structure using M-polynomial method. These degree based topological indices will help us to understand dependency of molecular structure on different properties of the compound[10].

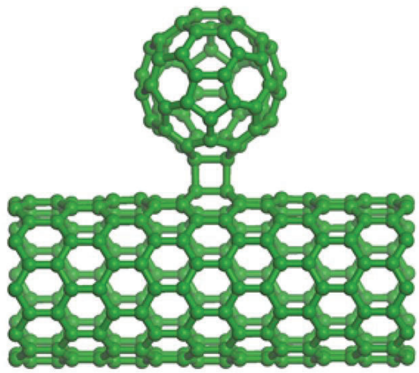

Figure 1[21]: A SWCNT based Carbon Nanobud : [2x2]-hp zigzag (10,0).

1.3. **Remarks.** The molecular graph of Nanobud considered here has a fullerene with 60 numbers of carbon atoms (also called Bucky ball,C_{60}) [16] covalently connected to the (k,0) zigzag nanotube [21], where k is the number of benzenes along the circumference. Number of benzene rows along the length of nanotube is denoted as 'n'. Fullerene has a spherical shaped structure made of 60 number of Carbon atoms. Chemical bonds between the Carbon atoms are covalent bonds and there are 90 number of such bonds exists in a single fullerene compound. [20] gives the studies on chemical bond between fullerene and nanotube, and stable configurations of Nanobuds. In this paper we consider two covalent bonds between fullerene and nanotube which makes a stable compound. Hence the molecular graph of Fullerene has 90 edges and 60 vertices. All vertices are of degree 3. Similarly, structure of Nanotube has its entire vertices with degree 3, except for those vertices which are situated on the free ends. These end vertices are of degree 2. A single fullerene (C_{60}), attached on the surface of a zigzag Single Walled Carbon Nano tube (SWNT) by a [2 x 2] cyclo-addition gives a stable Nanobud compound [21]. Addition of two covalent bonds between Carbon nanotube and fullerene modify the degrees of Carbon nanotube and C_{60} and estimate of these quantities from the final topology is given in the coming sections.

It is computed that the Carbon Nanobud configuration described here (Refer Figure 1) has total number of vertices $=2(30 + k(n + 1))$ and total number of edges $=92 + k(3n + 2)$.

2. Results and Discussions

In this section, an expression for M-Polynomial is derived for the given molecular structure and numerical values of different indices are computed using this expression.

Theorem 2.1. *Let G represents the molecular graph of Nanobud, then M-Polynomial of the Nanobud is given by*

$M(G;x,y) = 4kx^2y^3 + (80 + k(3n-2))x^3y^3 + 8x^3y^4 + 4x^4y^4.$

Proof. Carbon Nanobud considered here has a Bucky ball attached to a Carbon nanotube (k,0) through two covalent bonds. Number of edges of the compound are derived as given below: Let G be the graph with vertices of degree 2, 3 and 4. Hence, all the edges can be categorised under following 4 partitions.

$$E_{33} = \{uv \in E(G)/du = 3, dv = 3\} \implies |E_{33}| = [(90-5)] + [k(3n-2) - 5].$$

$$E_{23} = \{uv \in E(G)/du = 2, dv = 3\} \implies |E_{23}| = 4k.$$

$$E_{44} = \{uv \in E(G)/du = 4, dv = 4\} \implies |E_{44}| = 4.$$

$$E_{34} = \{uv \in E(G)/du = 3, dv = 4\} \implies |E_{34}| = 8.$$

M-Polynomial is derived as:

$$M(G;x,y) = m_{23}x^2y^3 + m_{33}x^3y^3 + m_{34}x^3y^4 + m_{44}x^4y^4.$$

$$= 4kx^2y^3 + [80 + k(3n-2)]x^3y^3 + 8x^3y^4 + 4x^4y^4$$

□

Theorem 2.2. *Let the Nanobud has bucky ball (C_60) attached to a (k,0) zigzag Nanotube with even number of benzene rows ;*
Then,

(1) $M_1(NB) = 2k(9n+4) + 568,$

(2) $M_2(NB) = 3k(9n+2) + 880,$

(3) ${}^mM_2(NB) = \frac{2}{3}k + \frac{k(3n-2)}{9} + \frac{353}{36},$

(4) $SDD(NB) = 6k + k(3n-2) + 100.$

Proof. (1) First Zagreb index, $M_1(NB) = (D_x + D_y)M(G;x,y)_{x=y=1}$

$$D_x = x\,\frac{\partial M(G;x,y)}{\partial x} = 8ky^3x^2 + 3k(3n-2)y^3x^3 + 24y^4x^3 + 16y^4x^4 + 240y^3x^3,$$

$$D_y = y\,\frac{\partial M(G;x,y)}{\partial y} = 12ky^3x^2 + 3k(3n-2)y^3x^3 + 32y^4x^3 + 16y^4x^4 + 240y^3x^3,$$

On Simpilification we get, $M_1(NB) = 2k(9n+4) + 568$.

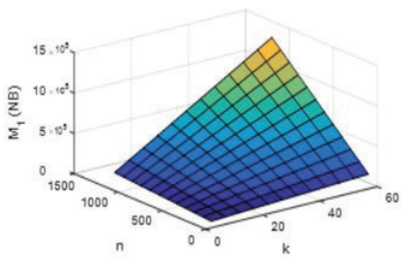

Figure 2: Firtst Zagreb Index of Nanobud.

(2) Second Zagreb Index $M_2(NB) = D_x D_y(M(x,y))|_{x=y=1}$

$D_x D_y = x\frac{\partial Dy}{\partial x}$=$24ky^3x^2 + 9k(3n-2)y^3x^3 + 96y^4x^3 + 64y^4x^4 + 720y^3x^3$

On simplification, we get Second Zagreb index

$M_2(NB) = 3k(9n+2) + 880$.

(3) Second Modified Zagreb index, ${}^mM_2(NB) = (S_xS_y)M(G;x,y)|_{x=y=1}$

$S_x = \int_0^x \frac{M(t,y)}{t}dt = \int_0^x 4ky^3t + [80 + 4(3n-2)y^3t^2 + 8y^4t^2 + 4y^4t^3]dt$

$= 2ky^3x^2 + \left[\frac{80}{3} + \frac{k}{3}(3n-2)\right]y^3x^3 + \frac{8}{3}y^4x^3 + y^4x^4$

$S_y = \int_0^y \frac{M(x,t)}{t}dt = \int_0^y 4kx^2t^2 + [80 + 4(3n-2)x^3t^2 + 8y^3t^3 + 4y^4t^4]dt$

$= \frac{4}{3}kx^2y^3 + \left[\frac{80}{3} + \frac{k}{3}(3n-2)\right]x^3y^3 + 2x^3y^4 + x^4y^4$

$S_xS_y = \int_0^x \frac{S_y(t,y)}{t}dt = \int_0^x [\frac{4}{3}ky^3t + \left[\frac{80}{3} + \frac{k}{3}(3n-2)\right]y^3t^2 + 2y^4t^2 + y^4t^3]dt$

$= \frac{2}{3}ky^3x^2 + \left[\frac{80}{9} + \frac{k}{9}(3n-2)\right]y^3x^3 + \frac{2}{3}y^4x^3 + \frac{1}{4}y^4x^4$

On simplification we get Second modified Zagreb index,

${}^mM_2(NB) = \frac{2}{3}k + \frac{k}{9}(3n-2) + \frac{353}{36}$.

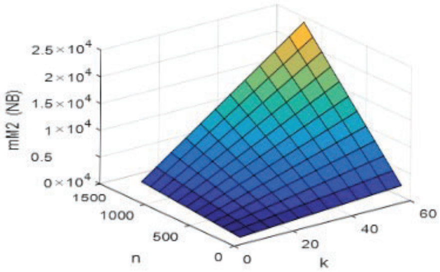

Figure 3: Second modified Zagreb Index of Nanobud.

(4) $SDD = (D_xS_y + S_xD_y)M(G;x,y)_{x=y=1}$

$$D_xS_y = x\left[\tfrac{4}{3}ky^3 2x + \left(\tfrac{80}{3} + \tfrac{k}{3}(3n-2)\right)y^3 3x^2 + 2y^4 3x^2 + y^4 4x^3\right]$$

$$= \tfrac{8}{3}ky^3x^2 + \left(80 + k(3n-2)\right)y^3x^3 + 6y^4x^3 + 4y^4x^4$$

$$S_xD_y = \int_0^x \frac{D_y(t,y)}{t}dt$$

$$= \int_0^x \left[12ky^3t + \left[3k(3n-2)y^3t^2\right] + 32y^4t^2 + 16y^4t^3 + 240y^3t^2\right]dt$$

$$= 6ky^3x^2 + \left[k(3n-2)\right]y^3x^3 + \tfrac{32}{3}y^4x^3 + 4y^4x^4 + 80y^3x^3$$

On Simplification we get, $SDD(NB) = 6k + k(3n-2) + 100$.

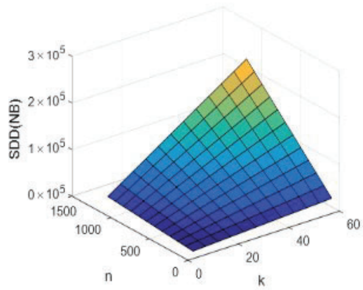

Figure 4: SDD Index of Nanobud.

□

Theorem 2.3. *Let the Nanobud has bucky ball* (C_{60}) *attached to a (k,0) zigzag Nanotube with even number of benzene rows ;*

Then,

(1) $H(NB) = \left(\frac{14}{15} + n\right)k + \frac{629}{21}$,

(2) $I(NB) = \left(\frac{9}{2}n - \frac{9}{5}\right)k + \frac{992}{7}$,

(3) $ABC(NB) = 2\sqrt{2} + \left(\frac{160+k(3n-2)}{3}\right) + \frac{4\sqrt{5}}{\sqrt{3}} + \sqrt{6}$,

(4) $A(NB) = 4\left[2^5 + (3n-2)\frac{3^6}{4^3}\right] + \frac{5}{4}X3^6 + \frac{24^3}{5^3} + \frac{4^7}{6^3}$.

Proof. We have M-polynomial of Nanobud is

$$M(G;x,y) = 4x^2y^3 + \big(80 + k(3n-2)\big)x^3y^4 + 4x^4y^4.$$

(1) $J\left[M(G;x'y)\right] = 4kx^5 + \big[80 + k(3n-2)\big]x^6 + 8x^7 + 4x^8$

$$S_xJ\left[M(G;x'y)\right] = \int_0^x 4kt^4 + \big[80 + k(3n-2)\big]t^5 + 8t^6 + 4t^7 dt$$

$$= \frac{4}{5}kx^5 + \big[80 + k(3n-2)\big]\frac{x^6}{6} + \frac{8}{7}x^7 + \frac{1}{2}x^8$$

$$H(NB) = 2S_xJ(M(G;x,y))_{x=y=1}$$

$$= \left(\frac{14}{15} + n\right)k + \frac{629}{21}.$$

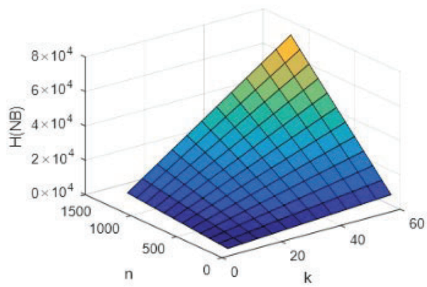

Figure 5: Harmonic Index of Nanobud.

(2) $D_xD_y = x\frac{\partial Dy}{\partial x} = 24ky^3x^2 + 9k(3n-2)y^3x^3 + 96y^4x^3 + 64y^4x^4 + 720y^3x^3$

$$JD_xD_y = 24kx^5 + 9k(3n-2)x^6 + 96x^7 + 64x^8 + 720x^6$$

$$S_xJD_xD_y = \int_0^x \left[24kt^4 + 9k(3n-2)t^5 + 96t^6 + 64t^7 + 720t^5\right]dt$$

$$= \frac{24}{5}kx^5 + \frac{3}{2}k(3n-2)x^6 + \frac{96}{7}x^7 + 8x^8 + 120x^6$$

$$I(NB) = S_xJD_xD_y(M(G;x,y))_{x=y=1} = \left(\frac{9}{2}n - \frac{9}{5}\right)k + \frac{992}{7}$$

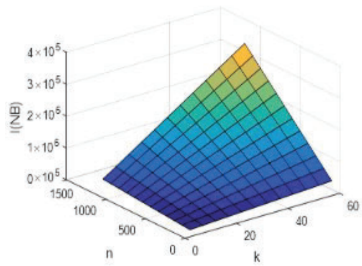

Figure 6: Inverse sum Index of Nanobud.

(3) $D_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}} = 4k\big(\frac{1}{\sqrt{3}}y^3\big)\big(\frac{1}{\sqrt{2}}x^2\big) + 80\big(\frac{1}{\sqrt{3}}y^3\big)\big(\frac{1}{\sqrt{3}}x^3\big) + k(3n-2)\big(\frac{1}{\sqrt{3}}y^3\big)\big(\frac{1}{\sqrt{3}}x^3\big) + 8\big(\frac{1}{\sqrt{4}}y^4\big)\big(\frac{1}{\sqrt{3}}x^3\big) + 4\big(\frac{1}{\sqrt{4}}y^4\big)\big(\frac{1}{\sqrt{4}}x^4\big)$

$$JD_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}} = \tfrac{4k}{\sqrt{6}}x^5 + \big(\tfrac{80+k(3n-2)}{3}\big)x^6 + \tfrac{4}{\sqrt{3}}x^7 + x^8$$

$$Q_{-2}\big[JD_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}}\big] = \tfrac{4k}{\sqrt{6}}x^3 + \big(\tfrac{80+k(3n-2)}{3}\big)x^4 + \tfrac{4}{\sqrt{3}}x^5 + x^6$$

$$S_x^{-\frac{1}{2}}\big[Q_{-2}\big(JD_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}}\big)\big] = \big[\tfrac{4k}{\sqrt{6}}\tfrac{t^3}{3^{-\frac{1}{2}}} + \big(\tfrac{80+k(3n-2)}{3}\big)\tfrac{t^4}{4^{-\frac{1}{2}}} + \tfrac{4}{\sqrt{3}}\tfrac{t^5}{5^{-\frac{1}{2}}} + \tfrac{t^6}{6^{-\frac{1}{2}}}\big]_{t=0}^{x}$$
$$= 2\sqrt{2} + \big(\tfrac{160+k(3n-2)}{3}\big)x^4 + \tfrac{4\sqrt{5}}{\sqrt{3}}x^5 + \sqrt{6}x^6$$

$$ABC(NB) = S_x^{-\frac{1}{2}}\big[Q_{-2}\big(JD_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}}\big)\big]_{x=y=1}$$
$$= 2\sqrt{2} + \big(\tfrac{160+k(3n-2)}{3}\big) + \tfrac{4\sqrt{5}}{\sqrt{3}} + \sqrt{6}.$$

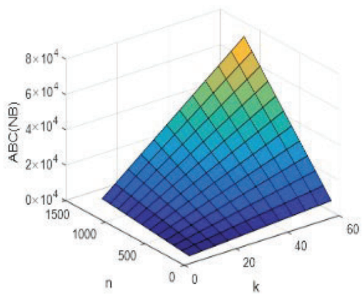

Figure 7: ABC Index of Nanobud.

(4) $D_x^3 D_y^3 = k \times 3^3 \times 2^3 y^3 x^2 + 80 \times 3^3 y^3 x^3 + 4 \times 3^3 \times 3^3(3n-2)y^3x^3 + 8 \times 4^3 \times 3^3 y^4 x^3 + 4 \times 4^3 \times 4^3 y^4 x^4$

$Q_{-2}J(D_x^3 D_y^3) = k \times 3^3 \times 2^5 x^3 + 80 \times 3^6 \times x^4 + k(3n-2) \times 3^6 \times x^4 + 8 \times 4^3 \times 3^3 \times x^5 + 4^7 x^6$

$S_x^3\big(Q_{-2}J(D_x^3 D_y^3)\big) = k \times 3^3 \times \times 2^5 \times \frac{x^3}{3^3} + 80 \times 3^6 \times \frac{x^4}{4^3} + k(3n-2) \times 3^6 \times \frac{x^4}{4^3} + 2 \times 4^4 \times 3^3 \times \frac{x^5}{5^3} + 4^7 \times \frac{x^6}{6^3}$

$$A(NB) = 2^5k + 80 \times \frac{3^6}{4^3} + k(3n-2)\frac{3^6}{4^3} + 2 \times 4^4 \times \frac{3^3}{5^3} + \frac{4^7}{6^3}$$
$$= k\big[2^5 + (3n-2)\frac{3^6}{4^3}\big] + \frac{5}{4} \times 3^6 + \frac{24^3}{5^3} + \frac{4^7}{6^3}$$

□

3. Conclusion

In this study, we used M-Polynomial to calculate various prominent topological indices such as the First Zagreb index, Second Zagreb index, Modified Zagreb index, and SDD index for a stable Carbon Nanobud compound. Through M-Polynomial, we also discovered Harmonic index, Inverse sum index, ABC index, and Augmented index. The topological indices for the carbon nanobud structure generated in this way can be utilised to investigate the compound's physical characteristics, chemical reactivity, and biological activities.

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Deepasree S Kumar
Acharya Institute of Technology, Bangalore-560060, Karnataka, India.
Email address: deepasreebiju84@gmail.com

Ranjini.P.S
Department of Mathematics,Don Boscco Institute Of Technology, Kumbalagudu, Bangaluru-56, Karnataka, India.
Email address: drranjinips@gmail.com

V. Lokesha
DOS in Mathematics, Vijyanagara Sri Krishnadevaraya University, Ballari-583105, India.
Email address: v.lokesha@gmail.com