

Invariant Polynomials of n-coronene

Y . Shanthakumari and V. Lokesh

Department of Studies in Mathematics
Vijayanagara Sri Krishnadevaraya University
Vinayaka Nagara, Ballari-583 105, Karnataka, India.
Email: yskphd2019@gmail.com, v.lokesha@gmail.com

M. Manjunath

Department of Mathematics, BITM College, Ballari, Karnataka, India
Email: manju3479@gmail.com

(Received January 10, 2021)

Abstract: Graph invariants are used to characterize the graph of a molecule and are defined by means of the vertices, edges and face numbers of a graph. In this research, we focus on the structure of Coronene Polycyclic Aromatic Hydrocarbons PAH_2 (or $\text{C}_{24} \text{H}_{12}$) and we draft some general expression for some discrete invariant polynomials and their topological indices.

Keywords: Topological indices, invariant polynomials, Coronene Polycyclic Aromatic Hydrocarbons, n-coronene, subdivision graph, semi-total point graph.

AMS Subject Classification: 2000: 05C90, 05C12

1. Introduction

A graph invariant is a graph theoretical property that has the same value for isomorphic graphs. A graph invariant may be a polynomial, a sequence of numbers or a single number. A single real number characterizing a molecular graph is usually called a topological index (TI). Topological indices are the numbers reflecting certain structural features of any molecule collected from the respective molecular graph. Structural information described in a molecular graph, quantified in terms of topological indices. The purpose of defining a topological index is to represent each chemical structure with a numerical value. Such indices not

only classify the structure but also predict chemical and biological properties.

The significant advantage of TI over other descriptors is in characterizing in a simple way the structure of flexible compounds that can exist in many conformations. For the purpose of reflecting molecular topology and correlating structure and properties quantitatively, graphs are converted into a mathematical expression, which may be a matrix, a polynomial, a sequence of numbers or a numerical index. For more attention on the topological indices may refer¹⁻⁵.

In chemical graph theory, we have invariant polynomials and topological indices for any molecular graphs. Such that topological indices of molecular graphs and nanostructures are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of molecular graphs and their physicochemical properties.

Coronene is a Polycyclic Aromatic Hydrocarbon (PAH) comprising six peri-fused benzene rings. Its molecular formula is $C_{24}H_{12}$. It is a yellow material that dissolves in such solvents such as benzene, toluene, and dichloromethane. A structural formula of a chemical compound can be represented by a molecular graph, its vertices being atoms and edges corresponding to covalent bonds. Usually hydrogen atoms are not depicted and in such a case, we speak of hydrogen depleted molecular graphs. The following figure is the hydrogen depleted molecular graph of Coronene.



Figure 1. Molecular graph of coronene

Dicoronylene is the trivial name for a very large polycyclic aromatic hydrocarbon. Its formal name is benzo phenanthro chryseno coronene or benzo dicoronene. It has 15 rings and is a brick-red solid. Its formula is $C_{48}H_{20}$.

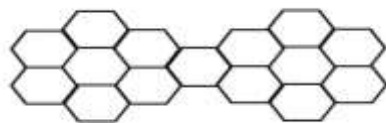


Figure 2. Molecular graph of Dicoronylene

This article, dealt with three sections. In section 1 surrounds introduction, followed by essential prerequisite results in section 2 and final section concentrated with main results.

2. Essential Prerequisite

Let G be a graph and d_u is a degree of vertex $u \in V(G)$ where $uv \in E(G)$ in this section, we recall some essential definitions and discuss prerequisites useful to development of the article.

Definition 2.1: *The subdivision graph $S(G)$ is the graph obtained by replacing each of its edge by a path of length 2 or equivalently, by inserting an additional vertex into each edge of G .*

Definition^{6,7} 2.2: *Let G be graph and $ST(G)$ is the semi-total point graph of G obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.*

Lemma⁶ 2.1: *Let G be graph with n vertices and m edges, then graph $R[G]$ has $(n+m)$ vertices and $3m$ edges.*

D. Vukicevic^{8,9} notified the 148 discrete adriatic indices. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good presaging properties in many cases. We discuss some of them in this paper.

The Sum-connectivity index $SC(G)$ is a invention by Bo Zhou and Nenad Trinajstić¹⁰ and is defined as

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

The first genuine degree-based topological index was put forward in⁴ named it as Randic or connectivity topological index and is defined as

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

Three new vertex-degree based topological indices are introduced in 2014 by I.Gutman et.al¹¹. The reciprocal Randic index (RR) and the reduced second Zagreb index $RM_2(G)$ are respectively given by

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d_u(G)d_v(G)},$$

$$RM_2(G) = (d_u(G) - 1)(d_v(G) - 1),$$

and reduced reciprocal Randic index is defined as

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

The first and second Gourava indices of a graph G are introduced by V. R. kulli¹² and they are defined as follows

$$GO_1(G) = \sum_{uv \in E(G)} (d_u(G) + d_v(G)) + (d_u(G)d_v(G)),$$

$$GO_2(G) = \sum_{uv \in E(G)} (d_u(G) + d_v(G))(d_u(G)d_v(G)).$$

The aim of this paper is to compute the zagreb indices, generalized randic index, inverse randic index and SDD index, M -polynomials of carbon nanocones using $Q(G)$ operator, hexagonal networks and probabilistic neural network.

Definition 2.3: M -polynomial of graph G is defined as

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

where $m_{i,j}(G)$, $(i, j \geq 1)$ be the number of edges $e=uv$ of G such that $(d_u, d_v)=(i, j)$. The following Table 1 relates some well-known degree-based topological indices with M -polynomials.

The derivation of the invariant polynomial is formed whose derivatives or integrals or composition of both are evaluated at some particular point. Then, its reduced form gives the molecular descriptor. The M -polynomial will open up new results of chemical graphs and insights in the study of molecular descriptors based on degrees. The main importance of this polynomial is that it can give exact forms of more than ten degree-based molecular descriptors.

Table 1. Derivation of some degree-based topological indices from M-polynomials.

Topological index	$f(x, y)$	Derivation from $M(G; x, y)$
Sum connectivity	$\frac{2}{\sqrt{x+y}}$	$\frac{2}{\sqrt{D_x + D_y}}(M(G; x, y))/x=y=1$
Randic	$\frac{1}{\sqrt{xy}}$	$\sqrt{S_x S_y}(M(G; x, y))/x=y=1$
The reciprocal Randic	$\sqrt{xy}$	$\sqrt{S_x S_y}(M(G; x, y))/x=y=1$
Reduced second Zagreb	$(x-1)(y-1)$	$(D_x - 1) + (D_y - 1)(M(G; x, y))/x=y=1$
Reduced reciprocal Randic	$\sqrt{(x-1)(y-1)}$	$\sqrt{(D_x - 1) + (D_y - 1)}(M(G; x, y))/x=y=1$

The graphical structure of n -coronene is obtained by linking n number of coronene as chain. The graph of n -coronene, $p, q=1, 2, 3, \dots$ has $nq + 2(n-1)$ edges and np vertices and is shown in Figure 1.

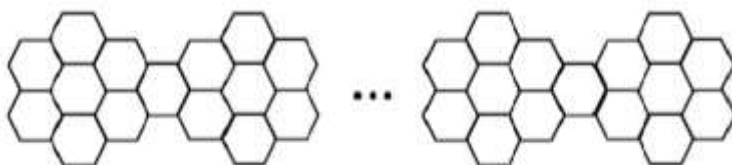


Figure 3. Molecular graph of n-coronene

Table 2. The edge partition of n – coronene $C_{24}H_{12}$ based on degrees of end vertices of each edge.

(d_u, d_v)	Number of edges
$(2, 2)$	$2n+4$
$(2, 3)$	$12n$
$(3, 3)$	$18n-6$

Table 3. The edge partition of subdivision graph of n – coronene $(n(p+q+2)-2, 2nq+4(n-1))$ based on degrees of end vertices of each edge.

(d_u, d_v)	Number of edges
$(2, 2)$	$16n+8$
$(2, 3)$	$48n-12$

Table 4. The edge partition of semi-total point graph of carbon nanocone $R[n\text{-coronene}]$ based on degrees of end vertices of each edge.

(d_u, d_v)	Number of edges
$(2, 4)$	$16n+8$
$(2, 6)$	$48n-12$
$(4, 4)$	$2n+4$
$(4, 6)$	$12n$
$(6, 6)$	$18n-6$

3. M-Polynomials of n – Coronene using $S(G)$ and $R(G)$ Operator

In this section closed forms of M – polynomials of n – coronene using $R(G)$ and $S(G)$ operator is calculated and closed forms of various degree-based topological indices of these structures is also computed.

Theorem 3.1: Let G be a graph of n – coronene and $n=1,2,3,.....$ then the M – polynomial is

$$M(G, x, y) = (2n + 4)x^2y^2 + 12nx^2y^3 + (18n - 6)x^3y^3.$$

Proof: Consider n -coronene graph which consists of np vertices and $nq+2(n-1)$ edges as shown in fig 1. There are three edge partitions corresponding to the degree of end vertices which are presented as

$$E_{2,2} = \{uv \in E_S \mid d_u = 2, d_v = 2\},$$

$$E_{2,3} = \{uv \in E_S \mid d_u = 2, d_v = 3\},$$

$$E_{3,3} = \{uv \in E_S \mid d_u = 3, d_v = 3\}.$$

By according to table 1 we have,

$$\left|E_{(2,2)}\right|=2n+4, \left|E_{(2,3)}\right|=12n \text{ and } \left|E_{(3,3)}\right|=18n-16.$$

Thus, the M-polynomial of n-coronene is

$$\begin{aligned} M(G, x, y) &= \sum_{i \leq j} m_{ij}(G) x^i y^j \\ &= \sum_{i=j=2} m_{22}(G) x^2 y^2 + \sum_{2 \leq 3} m_{23}(G) x^2 y^3 + \sum_{i=j=3} m_{33}(G) x^3 y^3 \\ &= \left|E_{(2,2)}\right| x^2 y^2 + \left|E_{(2,3)}\right| x^2 y^3 + \left|E_{(3,3)}\right| x^3 y^3, \end{aligned}$$

$$M(G, x, y) = (2n+4)x^2y^2 + 12x^2y^3 + (18n-6)x^3y^3.$$

Theorem 3.2: Let G be a graph of n -coronene and $n=1,2,3,\dots$. Then

$$SC[G] = (2n+4) + \frac{24n}{\sqrt{5}} + 2\sqrt{6}(3n-1)$$

$$R[G] = 7n + 2n\sqrt{6}, \quad RR[G] = 58n + 12n\sqrt{6} - 10$$

$$RM_2[G] = 98n - 20, \quad RRR[G] = 38n + 12\sqrt{2}n - 8$$

$$GO_1[G] = 418n - 58, \quad GO_2[G] = 1364n - 260.$$

Proof: In order to prove seven results, we use the following:

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

and

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

For the above polynomial equation by applying the table 1 value, we obtained the required results.

Theorem 3.3: *Let H be the graph of hexagonal network HX_n . Then the M -polynomial is*

$$M(H, x, y) = (6n + 8)x^2y^2 + (48n - 12)x^2y^3.$$

Proof: Consider the subdivision graph of n -coronene graph which consists of $n(p+q+2)-2$ vertices and $2nq+4(n-1)$ edges as shown in fig 1. There are two edge partitions corresponding to the degree of end vertices which are presented as

$$E_{2,2} = \{uv \in E_S \mid d_u = 2, d_v = 2\} \text{ and } E_{2,3} = \{uv \in E_S \mid d_u = 2, d_v = 3\},$$

by according to table 1 we have,

$$|E_{(2,2)}| = 16n + 8 \text{ and } |E_{(2,3)}| = 48n - 12.$$

Thus, the M -polynomial of n -coronene is

$$\begin{aligned} M(H, x, y) &= \sum_{i \leq j} m_{ij}(H) x^i y^j \\ &= \sum_{i=j=2} m_{22}(G) x^2 y^2 + \sum_{2 \leq 3} m_{23}(G) x^2 y^3 \\ &= |E_{(2,2)}| x^2 y^2 + |E_{(2,3)}| x^2 y^3 \end{aligned}$$

$$M(H, x, y) = (6n + 8)x^2y^2 + (48n - 12)x^2y^3.$$

Theorem 3.4: *Let G be a subdivision graph of n -coronene for $m \geq 3$ and $n=1,2,3,\dots$. Then*

$$SC[G] = (16n + 8) + \frac{2(48n - 12)}{\sqrt{5}}, \quad R[G] = (8n + 4) + \frac{1}{\sqrt{6}}(48n - 12)$$

$$RR[G] = (32n + 16) + \sqrt{6}(48n - 12), \quad RM_2[G] = 112n - 16$$

$$RRR[G] = 16n + 8 + \sqrt{2}(48n - 12), \quad GO_1[G] = 656n - 68$$

$$GO_2[G] = 1696n - 412$$

Proof: For polynomial equation applying the table 1 values, we obtain the required results.

Theorem 3.5: Let G be a graph of n -coronene and $n = 1, 2, 3, \dots$ then the M -polynomial is

$$M(G, x, y) = (16n + 8)x^2y^4 + (48n - 12)x^2y^6 \\ + (2n + 4)x^4y^4 + 12nx^4y^6 + (18n - 6)x^6y^6.$$

Proof: Consider semi total graph of n -coronene graph which consists of $n(p+q+2)-2$ vertices and $3nq+6(n-1)$ edges as shown in fig 1. There are three edge partitions corresponding to the degree of end vertices which are presented as

$$E_{2,4} = \{uv \in E_S \mid d_u = 2, d_v = 4\}, \quad E_{2,6} = \{uv \in E_S \mid d_u = 2, d_v = 6\}, \\ E_{4,4} = \{uv \in E_S \mid d_u = 4, d_v = 4\}, \quad E_{4,6} = \{uv \in E_S \mid d_u = 4, d_v = 6\}, \\ E_{6,6} = \{uv \in E_S \mid d_u = 6, d_v = 6\}.$$

By according to table 1 we have,

$$\left| E_{(2,4)} \right| = 16n + 8, \left| E_{(2,6)} \right| = 48n - 12, \left| E_{(4,4)} \right| = 2n + 4, \\ \left| E_{(4,6)} \right| = 12n, \left| E_{(6,6)} \right| = 18n - 6.$$

Thus, the M -polynomial of n -coronene is

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

$$\begin{aligned}
&= \sum_{2 \leq 4} m_{24}(G)x^2y^4 + \sum_{2 \leq 6} m_{26}(G)x^2y^6 + \sum_{i=j=4} m_{44}(G)x^4y^4 \\
&+ \sum_{4 \leq 6} m_{46}(G)x^4y^6 + \sum_{i=j=6} m_{66}(G)x^6y^6 \\
&= |E_{(2,4)}| x^2y^4 + |E_{(2,6)}| x^2y^6 + |E_{(4,4)}| x^4y^4 + |E_{(4,6)}| x^4y^6 + |E_{(6,6)}| x^6y^6 \\
M(G, x, y) &= (16n+8)x^2y^4 + (48n-12)x^2y^6 \\
&+ (2n+4)x^4y^4 + 12nx^4y^6 + (18n-6)x^6y^6.
\end{aligned}$$

Theorem 3.6: Let G be a semi-total point graph of n -coronene for $n=1, 2, 3, \dots$ then

$$\begin{aligned}
SC[G] &= \frac{32n+6}{\sqrt{6}} + \frac{48n-12}{\sqrt{2}} + \frac{2n+4}{\sqrt{2}} + \frac{32n}{\sqrt{10}} + \frac{18n-6}{\sqrt{3}} \\
R[G] &= \frac{8n+4}{\sqrt{2}} + \frac{24n-6}{\sqrt{3}} + \frac{n+2}{2} + \frac{3n}{\sqrt{6}} + (3n-1) \\
RR[G] &= (16n+8)\sqrt{8} + n\sqrt{12}(48n-12) - 10 + 24n\sqrt{6} + 116n - 20 \\
RM_2[G] &= 936n - 150 \\
RRR[G] &= \sqrt{3}(16n+8) + \sqrt{5}(48n-12) + 12n\sqrt{15} - (96n-18) \\
GO_1[G] &= 2504n - 320 \\
GO_2[G] &= 16288n - 2848.
\end{aligned}$$

Proof: For polynomial equation applying the table 1 values, we obtain the required results.

4. Conclusions

In this paper, we reclaimed thirteen degree based topological indices of carbon nanocone. We have used the algebraic method i.e., edge partition method for these compounds to compute the general expression. It is clear that, these results have benefits to forecast the physical properties of elemental chemical compounds for example discrete adriatic indices is useful for determining the physio-chemical properties of alkanes as remarked by D. Vukicevic and his co-workers. He noticed that there is

perfect correlation between discrete adriatic indices and polychlorobiphenyls, octane isomers.

References

1. I. Gutman, Degree-Based Topological Indices, *Croatica Chemical Acta*, (2013), 351-361.
2. I. Gutman and A. R. Ashra, The edge version of the Szeged Index, *Croat. Chem. Acta.*, **81** (2008), 263-266.
3. V. Lokesha, A. Usha, P. S. Ranjini and K. M. Devendraiah, Topological indices on model graph structure of Alveoli in human lungs, *Proc. Jang. Mathematical society*, **18(4)** (2015), 435-453.
4. Y. Shanthakumari, P. S. K. Reddy, V. Lokesha and P. S. Hemavathi, Topological aspects of boron triangularnanotubeand boron- α nanotube-II, *South East Asian J. Of Mathematics sciences*, (2020), 145-156.
5. B. S. Shwetha, V. Lokesha, A. Bayad and P. S. Ranjini, A Comparative Study of Topological Indices and Molecular Weight of Some Carbohydrates, *Journal of the Indian Academy of Mathematics*, **34(2)** (2012), 627-636.
6. A. R. Bindusree, V. Lokesha and P. S. Ranjini, ABC index on subdivision graphs and line graphs, *IOSR Journal of Mathematics*, (2016), 01-06.
7. V. Lokesha, R. Shruti, P. S. Ranjini and A. Sinan cevik, On Certain Topological indices of Nanostructures using Q(G) and R(G) operators, *Commun. Fac. Sci. Univ. Ank. Ser. A1 Math. Stat.*, **66(2)** (2018), 178-187.
8. D. Vukicevic and M. Gasperov, Bond Additive Modeling 1. Adriatic Indices, *Croatica chemical acta*, (2010), 243-26.
9. D. Vukicevic, Bond Additive Modeling 2. Mathematical Properties of Max-min Rodeg Index, *Croatica chemical acta*, **83(3)** (2010), 261-273.
10. B. Zhou and N. Trinajstić, on a novel connectivity index, *J. Math. Chem.*, **46** (2009), 1252-1270.
11. Ivan Gutman, Boris Furtula and Clive Elphick, Three New/Old Vertex–Degree–Based Topological Indices, *Match Commun. Math. Comput. Chem.*, **72** (2014), 617-632.
12. V. R. Kulli, The Gourava indices and coindices of graphs, *Annals of Pure and Applied Mathematics*, **14(1)** (2017), 33-38.
13. C. K. Gupta, K. Lokesha, B. S. Shetty and P. S. Ranjini, On the Symmetric Division deg Index of Graph, *Southeast Asian Bulletin of Mathematics*, (2016), 59-80.
14. S. M. Hosamani, Computing Sanskruti Index of certain nanostructures, *J. Appl. Math. Comput.*, (2016), 1-9.
15. S. Iijima, Helical microtubules of graphitic carbon, *Nature*, **354** (1991), 56-58.

16. K. Lokesha, T. Deepika, P. S. Ranjini and I. N. Cangul, Operations of Nanostructures via SDD, ABC4 and GA5 indices, *Applied Mathematics and Nonlinear Sciences*, **2(1)** (2017), 173-180.
17. V. Lokesha and T. Deepika, Symmetric division deg index of tricyclic and tetracyclic graphs, *International Journal of Scientific and Engineering Research*, **7(5)** (2016), 53-55.