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Bond Additive Molecular Descriptors of Cove Edged Graphene Nanoribbon

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Abstract: -In computational and theoretical chemistry, numbers that map some structural appearance of chemical molecules and derivatives from the graph isomorphic to the molecular structure are commonly called topological indices. Topological indices are numerical quantities that are derived through mathematical equations from a molecular graph. Topological indices are used in the study of QSAR and QSPR to predict the bioactivity of the structure. In this article, we calculate some bond additive molecular descriptors of cove-edged graphene nanoribbons.

Keywords*: Bond Additive, QSAR and QSPR, graphene nanoribbons.*

1. Introduction

A topological descriptor is a mathematical value related to chemical structure that describes the relationship of chemical structure with a variety of chemical reactivity, physical properties, and biological activity. Molecular compounds are frequently modeled by molecular graphs. The detailed information on this topic can be found in [1-10]. Topological property expressions are necessary for the QSAR and QSPR of chemical compounds. To describe organic chemical networks as hydrogen-depleted graphs, where points represent atoms and edges represent bonds, mathematical chemistry plays a crucial role in QSAR/QSPR education. When applied to the numerical modeling of chemical events, the chemical graph hypothesis forms the topological partition of numerical chemistry. Those who believe in the hypothesis hold that a particle's hypothetical demonstration on a graph provides invaluable insight into the phenomena of substances, as these graphs keep the properties of a chemical graph.

Mathematical chemistry is a subfield of computational chemistry in which mathematical models are used to discuss and predict molecule structure without directly referencing quantum mechanics. Mathematical modeling of chemical events using graph theory is known as chemical graph theory [11-14]. The advancement of chemistry was greatly aided by this notion.

Let $G = (V(G), E(G))$ be the molecular graph. The cardinality of the sets $V(G)$ and $E(G)$ reflects the respective number of vertices (atoms) and edges (bonds). An edge with the ending vertices u and v in $E(G)$ is denoted by $e = uv$. If an edge exists between them, two vertices, $u$and v, are considered to be adjacent.

2. Bond Additive Descriptors

Many molecular descriptors are defined based on their bond additiveness. Firstly, we categorize the edges of a molecular graph, and we proceed with the descriptor *Des* calculation based on the general expression as given in [15]

$$Des(G) = \sum_{uv \in E(G)} f\left(d_G(u), d_G(v)\right).$$

here, the set $E(G)$ is the collection of edges, and f is a function that mapps a real value to an ordered pair that defines and edge. If the ordered pair does not contribute an edge, then we count null for that case. Since there are several ways of determining f, it is clear that this definition is fairly broad.

Table 1: Adriatic Indices and its Relavance

Index	$f(d_G(u), d_G(v))$	Relavance
Randić type lordeg index (RLI)	$\ln(d_u)\ln(d_v)$	Heat capacity at constant T
lnverse sum lordeg index (ISLI)	$\frac{1}{\sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}}$	-do-
Sum lordeg index (SLI)	$\sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}$	Octanol-water partition coefficients
lnverse sum indeg index (ISI)	$\frac{d_u d_v}{d_u + d_v}$	Total surface area
Misbalance irdeg index (MIRI)	$\lvert \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \rvert$	Enthalpy of vaporisation and of standard enthalpy of vaporisation
Misbalance lordeg index (MLI)	$\lvert \ln d_u - \ln d_v \rvert$	-do-
Misbalance losdeg index (MLSI)	$\lvert \ln^2 d_u - \ln^2 d_v \rvert$	-do-
Misbalance indeg index (MII)	$\lvert \frac{1}{d_u} - \frac{1}{d_v} \rvert$	-do-
Min-max rodeg index (MMRI)	$\sqrt{\frac{\min(d_u, d_v)}{\max(d_u, d_v)}}$	-do-
Misbalance deg index (MDI)	$\lvert d_u - d_v \rvert$	-do-
Misbalance rodeg index (MRI)	$\lvert \sqrt{d_u} - \sqrt{d_v} \rvert$	-do-
Misbalance hadeg index (MHI)	$\lvert \left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v} \rvert$	-do-
Max-min rodeg index (MMRDI)	$\sqrt{\frac{\max(d_u, d_v)}{\min(d_u, d_v)}}$	Enthalpy of vaporisation
Max-min deg index (MMDI)	$\frac{\max(d_u, d_v)}{\min(d_u, d_v)}$	Log water activity coefficient for polychlorobiphenyls
Max-min sdeg index (MMSDI)	$\left(\frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right)^2$	-do-
Symmetric division deg index (SDDI)	$\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}$	Total surface area for polychlorobiphenyls

3. Cove Edged Graphene Nanoribbon $CGNR(m, n)$

Graphene nanoribbons appear as a cutting-edge transporter for improving nano-dimensional symptomatic gadgets and medication delivery frameworks because of the exciting and forefront electronic, warm, mechanical and optical properties related to graphene [16]. They have exceptionally evolved graphenes with broad significance because of their peculiar properties, such as enormous surface territory, upgraded mechanical quality, and improved electro-conductivity. These nanoribbons are the best transporter for anticancer medications and other exceptionally aromatic medications [17]. The semi-one-dimensional extended monolayer

segments of graphenes have a high length-to-width proportion. The length and breadth estimations can be used to communicate the dimensions of the GNRs [18]. They are synthetical sp^2 hybridised carbon structures with a honeycomb grid geometry. The edge structure is the important component in GNR characteristics, with armchair-edge GNRs (AGNRs) semiconducting along width-subordinate bandgaps and zigzag-edge GNRs (ZGNRs) probably appealing owing to their edge-restricted states, which can be turned polarised. Furthermore, armchair and zigzag edge configurations, alternative geometries such as cove edges [19, 20] that result in non-planarity owing to the aversion amid nearby hydrogen molecules [21] can also be considered. The cove-edged graphene nanoribbon $CGNR(6,5)$ is depicted in Figure 1.

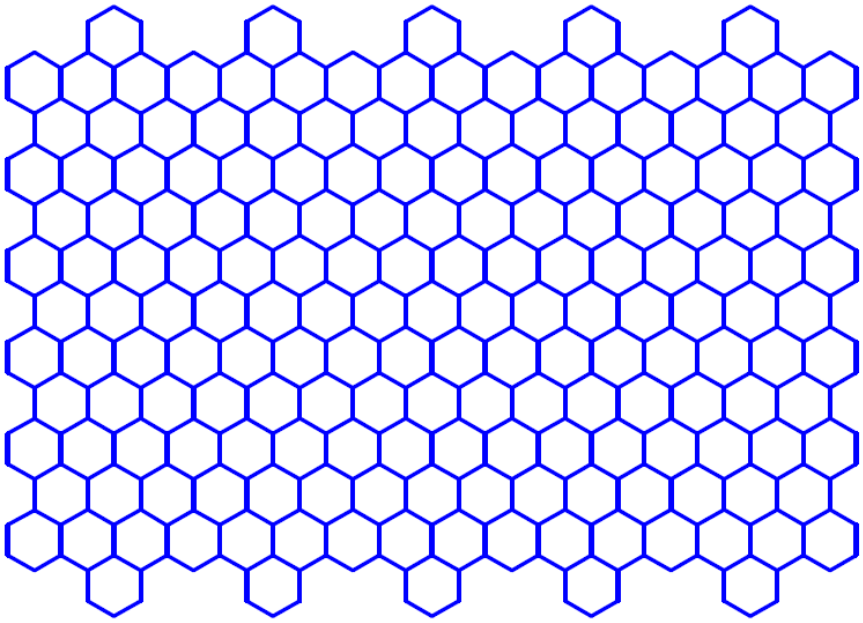


Figure 1: Cove edged graphene nanoribbon $\boldsymbol{CGNR(6,5)}$

Recently [22-25], bottom-up synthesis of graphene permitted a cove-edged graphene nanoribbons (CGNRs) as shown in Figure 1, which is the combination of an armchair and zigzag peripheries. This construction was described as structurally explicit and remarkably long ($> 200nm$). Exchanging electron-rich and electron-poor subunits tunes the frontier orbitals of CGNRs, which are molecularly defined and soluble. In solution-made cove-edged nanoribbons have the added benefit of a strangely shaped, distorted π surface, which is highly dissolvable and processable [26]. These structures have been used in various fascinating classes containing electronic [27], chemical [28], and mechanical applications [29].

Cheminformatics plays a vital part in keeping up and accessing the gigantic measure of chemical data created by chemists utilizing a legitimate database. Furthermore, research requires a creative approach for extracting information from data to demonstrate complicated interconnections amid the structure of a chemical and biological activity, as well as the impact of reaction conditions on chemical reactivity [30]. Structure portrayal manages reaction characterization, structure descriptors and searching molecular modelling, and computer-assisted structure elucidation. The interactions between countless chemical and, in particular, biological facts of substances and their structure are far too complicated to be reliably anticipated using fundamental principles. Structure descriptors (Topological indices) must be determined for the structures of a dataset [31]. At that stage, data analysis or a model-building method must be used to create a model for the connection between the structure descriptors and the explored property. For the two stages, a lot of strategies have been created. A large group of techniques, including in large numbers, for computing structure descriptors is accessible [32]. Increasingly, more consideration presently moves to the utilization of molecular descriptors that can be deciphered and consequently give a model that builds experiences into the connection between a compound's structure and properties. The atomic descriptors are helpful in portraying the 1D, 2D, and 3D structures or the

sub-atomic surface properties [33]. Furthermore, the representation of chemical molecules is given more attention than just a subatomic characterization [34].

4. Main Results

In this section, we find bond additive molecular descriptors of $CGNR(m,n)$. There are $12mn+6m+6n$, vertices and $18mn+7m+5n-1$ edges of $CGNR(m,n)$, respectively. The edges of $CGNR(m,n)$ are partitioned based on their end vertex degrees as given in Table 2.

Table 2: The edge partition of cove edged graphene nanoribbon

(d_u, d_v)	Number of edges in $CGNR(m,n)$
(2,2)	$2m+4n+4$
(2,3)	$4m+8n-4$
(3,3)	$18mn+m-7n-1$

Theorem 1 *Let G be a $CGNR(m,n)$, then*

1. $RLI(CGNR(m,n)) = 21.7251mn + 5.2138m - 0.4348n - 2.3311.$
2. $SLI(CGNR(m,n)) = 37.7333mn + 12.9493m + 7.0319n - 2.9587.$
3. $ISLI(CGNR(m,n)) = 8.5866mn + 3.8050m + 3.3168n - 0.2017.$
4. $ISI(CGNR(m,n)) = 27mn + 8.3m + 3.1n - 2.3.$
5. $MLI(CGNR(m,n)) = 1.6219m + 3.2437n - 1.6219.$
6. $MLSI(CGNR(m,n)) = 2.906m + 5.812n - 2.906.$
7. $MII(CGNR(m,n)) = 0.6667m + 1.3333n - 0.6667.$
8. $MIRI(CGNR(m,n)) = 0.519m + 1.0381n - 0.519.$
9. $MRI(CGNR(m,n)) = 1.2713m + 2.5427n - 1.2713.$
10. $MDI(CGNR(m,n)) = 4m + 8n - 4.$
11. $MHI(CGNR(m,n)) = 0.5m + n - 0.5.$
12. $MMRI(CGNR(m,n)) = 18mn + 6.266m + 3.532n - 0.266.$
13. $MMRDI(CGNR(m,n)) = 18mn + 7.8988m + 6.7976n - 1.8988.$
14. $MMDI(CGNR(m,n)) = 18mn + 9m + 9n - 3.$
15. $MMSDI(CGNR(m,n)) = 18mn + 12m + 15n - 6.$
16. $SDDI(CGNR(m,n)) = 36mn + 14.6667m + 11.3333n - 2.6667.$

Proof.

$$RLI\big(CGNR(m,n)\big) = \sum_{uv\in E(G)} \ln d_G(u) \ln d_G(v)$$

$$= (\ln 2 \times \ln 2)(2m+4n+4) + (\ln 2 \times \ln 3)(4m+8n-4)$$

$$+(\ln 3 \times \ln 3)(18mn+m-7n-1)$$

$$= 21.7251mn + 5.2138m - 0.4348n - 2.3311.$$

$$SLI(CGNR(m,n)) = \sum_{uv\in E(G)} \sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}$$

$$= \left[\sqrt{\ln(2)} + \sqrt{\ln(2)}\right](2m + 4n + 4) + \left[\sqrt{\ln(2)} + \sqrt{\ln(3)}\right](4m + 8n - 4)$$
$$+\left[\sqrt{\ln(3)} + \sqrt{\ln(3)}\right](18mn + m - 7n - 1)$$
$$= 37.7333mn + 12.9493m + 7.0319n - 2.9587.$$

$$ISLI(CGNR(m,n)) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}}$$
$$= \left[\frac{1}{\sqrt{\ln(2)}+\sqrt{\ln(2)}}\right](2m + 4n + 4) + \left[\frac{1}{\sqrt{\ln(2)}+\sqrt{\ln(3)}}\right](4m + 8n - 4)$$
$$+\left[\frac{1}{\sqrt{\ln(3)}+\sqrt{\ln(3)}}\right](18mn + m - 7n - 1)$$
$$= 8.5866mn + 3.8050m + 3.3168n - 0.2017.$$

$$ISI(CGNR(m,n)) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}$$
$$= \left[\frac{2\times2}{2+2}\right](2m + 4n + 4) + \left[\frac{2\times3}{2+3}\right](4m + 8n - 4)$$
$$+\left[\frac{3\times3}{3+3}\right](18mn + m - 7n - 1)$$
$$= 27mn + 8.3m + 3.1n - 2.3.$$

$$MLI(CGNR(m,n)) = \sum_{uv \in E(G)} |\ln d_u - \ln d_v|$$
$$= |\ln 2 - \ln 2|(2m + 4n + 4) + |\ln 2 - \ln 3|(4m + 8n - 4)$$
$$+|\ln 3 - \ln 3|(18mn + m - 7n - 1)$$
$$= 1.6219m + 3.2437n - 1.6219.$$

$$MLSI(CGNR(m,n)) = \sum_{uv \in E(G)} |\ln^2 d_u - \ln^2 d_v|$$
$$= |\ln^2 2 - \ln^2 2|(2m + 4n + 4) + |\ln^2 2 - \ln^2 3|(4m + 8n - 4)$$
$$+|\ln^2 3 - \ln^2 3|(18mn + m - 7n - 1)$$
$$= 2.906m + 5.812n - 2.906.$$

$$MII(CGNR(m,n)) = \sum_{uv \in E(G)} \left|\frac{1}{d_u} - \frac{1}{d_v}\right|$$
$$= \left|\tfrac{1}{2} - \tfrac{1}{2}\right|(2m + 4n + 4) + \left|\tfrac{1}{2} - \tfrac{1}{3}\right|(4m + 8n - 4)$$
$$+\left|\tfrac{1}{3} - \tfrac{1}{3}\right|(18mn + m - 7n - 1)$$
$$= 0.6667m + 1.3333n - 0.6667.$$

$$MIRI(CGNR(m,n)) = \sum_{uv \in E(G)} \left|\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}}\right|$$
$$= \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{2}}\right|(2m + 4n + 4) + \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{3}}\right|(4m + 8n - 4)$$
$$+\left|\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{3}}\right|(18mn + m - 7n - 1)$$

$$= 0.519m + 1.0381n - 0.519.$$

$$MRI(CGNR(m,n)) = \sum_{uv\in E(G)} |\sqrt{d_u} - \sqrt{d_v}|$$

$$= |\sqrt{2} - \sqrt{2}|(2m + 4n + 4) + |\sqrt{2} - \sqrt{3}|(4m + 8n - 4)$$
$$+|\sqrt{3} - \sqrt{3}|(18mn + m - 7n - 1)$$
$$= 1.2713m + 2.5427n - 1.2713.$$

$$MDI(CGNR(m,n)) = \sum_{uv\in E(G)} |d_u - d_v|$$

$$= |2 - 2|(2m + 4n + 4) + |2 - 3|(4m + 8n - 4)$$
$$+|3 - 3|(18mn + m - 7n - 1)$$
$$= 4m + 8n - 4.$$

$$MHI(CGNR(m,n)) = \sum_{uv\in E(G)} \left|\left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v}\right|$$

$$= \left|\left(\frac{1}{2}\right)^{2} - \left(\frac{1}{2}\right)^{2}\right|(2m + 4n + 4) + \left|\left(\frac{1}{2}\right)^{2} - \left(\frac{1}{2}\right)^{3}\right|(4m + 8n - 4)$$
$$+\left|\left(\frac{1}{2}\right)^{3} - \left(\frac{1}{2}\right)^{3}\right|(18mn + m - 7n - 1)$$
$$= 0.5m + n - 0.5.$$

$$MMRI(CGNR(m,n)) = \sum_{uv\in E(G)} \sqrt{\frac{\min(d_u, d_v)}{\max(d_u, d_v)}}$$

$$= \sqrt{\frac{\min(2,2)}{\max(2,2)}}(2m + 4n + 4) + \sqrt{\frac{\min(2,3)}{\max(2,3)}}(4m + 8n - 4)$$
$$+\sqrt{\frac{\min(3,3)}{\max(3,3)}}(18mn + m - 7n - 1)$$
$$= 18mn + 6.266m + 3.532n - 0.266.$$

$$MMRDI(CGNR(m,n)) = \sum_{uv\in E(G)} \sqrt{\frac{\max(d_u, d_v)}{\min(d_u, d_v)}}$$

$$= \sqrt{\frac{\max(2,2)}{\min(2,2)}}(2m + 4n + 4) + \sqrt{\frac{\max(2,3)}{\min(2,3)}}(4m + 8n - 4)$$
$$+\sqrt{\frac{\max(3,3)}{\min(3,3)}}(18mn + m - 7n - 1)$$
$$= 18mn + 7.8988m + 6.7976n - 1.8988.$$

$$MMDI(CGNR(m,n)) = \sum_{uv\in E(G)} \frac{\max(d_u, d_v)}{\min(d_u, d_v)}$$

$$= \frac{\max(2,2)}{\min(2,2)}(2m + 4n + 4) + \frac{\max(2,3)}{\min(2,3)}(4m + 8n - 4)$$
$$+\frac{\max(3,3)}{\min(3,3)}(18mn + m - 7n - 1)$$

$$= 18mn + 9m + 9n - 3.$$

$$MMSDI(CGNR(m,n)) = \sum_{uv \in E(G)} \left(\frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right)^2$$

$$= \left(\frac{\max(2,2)}{\min(2,2)}\right)^2 (2m + 4n + 4) + \left(\frac{\max(2,3)}{\min(2,3}\right)^2 (4m + 8n - 4)$$

$$+ \left(\frac{\max(3,3)}{\min(3,3)}\right)^2 (18mn + m - 7n - 1)$$

$$= 18mn + 12m + 15n - 6.$$

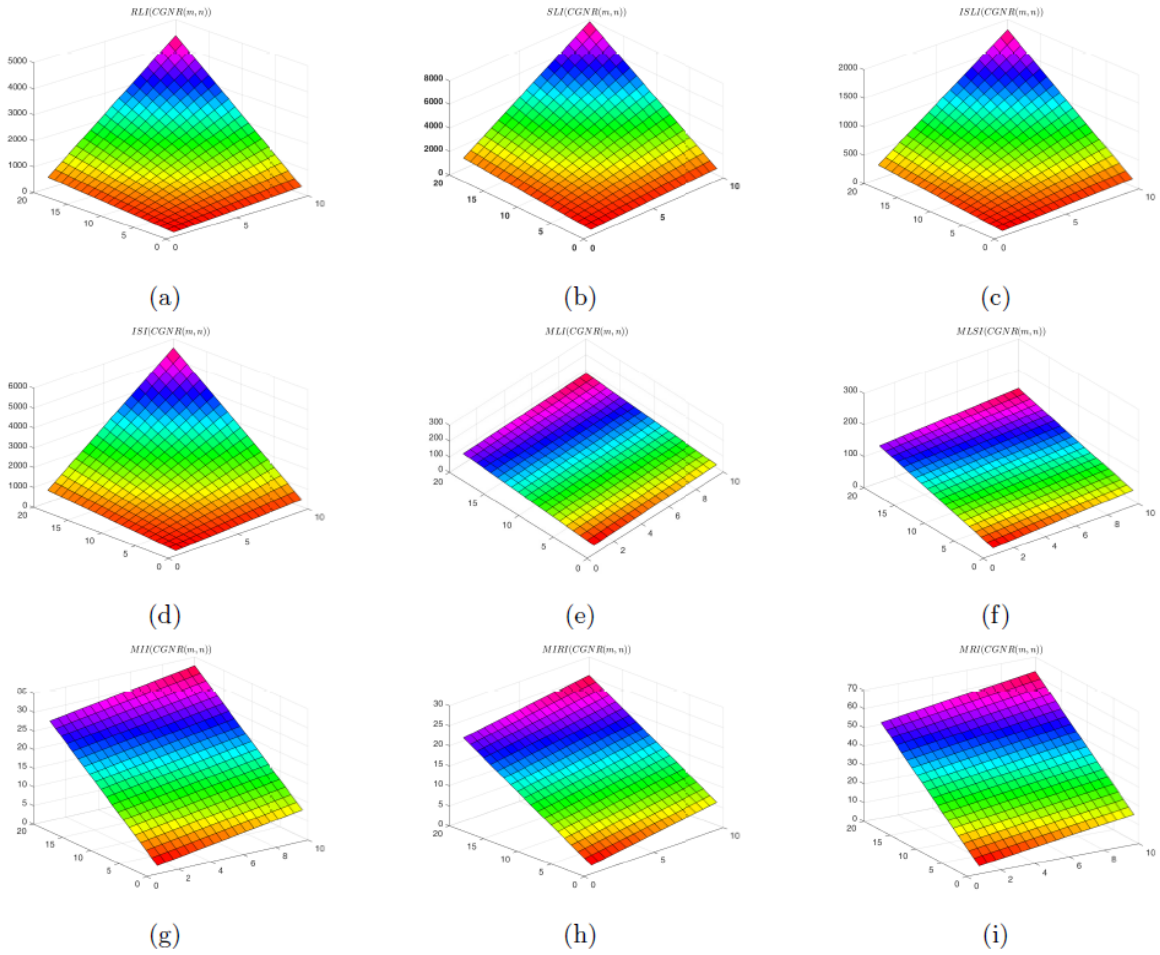
$$SDDI(CGNR(m,n)) = \sum_{uv \in E(G)} \left[\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right]$$

$$= \left[\frac{\min(2,2)}{\max(2,2)} + \frac{\max(2,2)}{\min(2,2)}\right] (2m + 4n + 4)$$

$$+ \left[\frac{\min(2,3)}{\max(2,3)} + \frac{\max(2,3)}{\min(2,3)}\right] (4m + 8n - 4)$$

$$+ \left[\frac{\min(3,3)}{\max(3,3)} + \frac{\max(3,3)}{\min(3,3)}\right] (18mn + m - 7n - 1)$$

$$= 36mn + 14.6667m + 11.3333n - 2.6667.$$



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

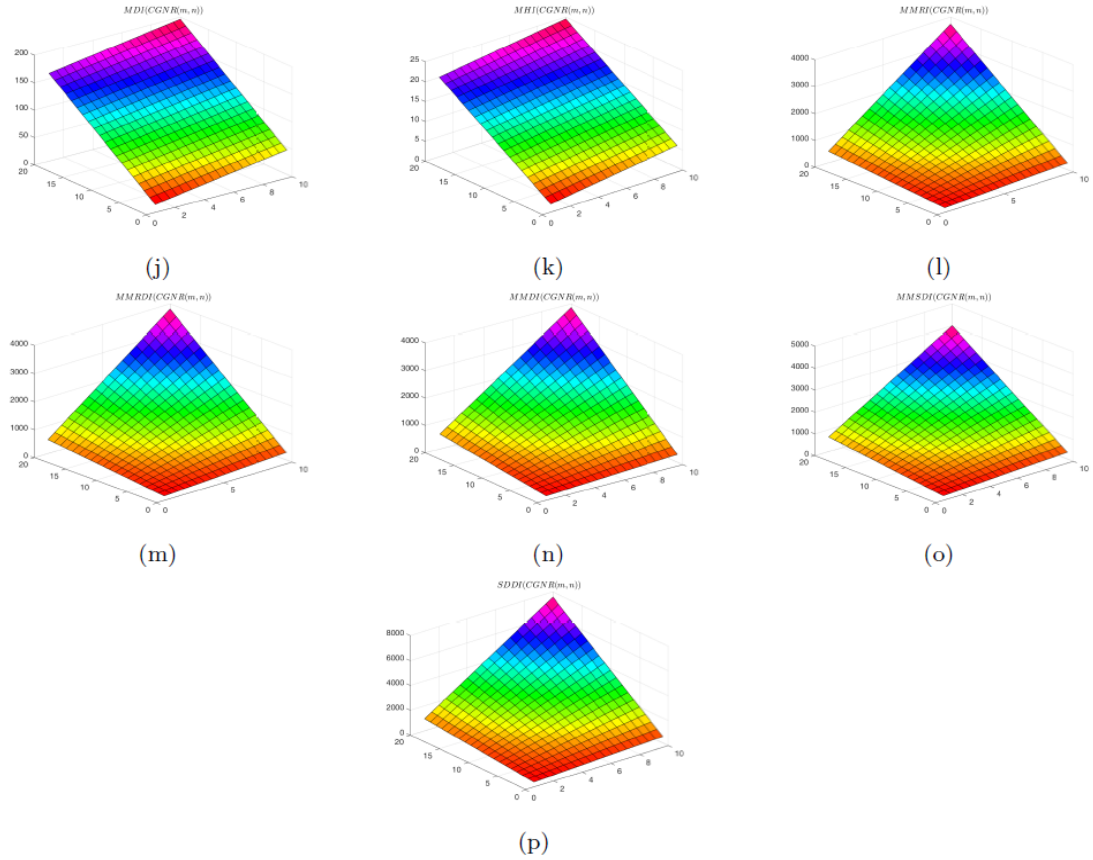


Figure 2: Graphical representation of various indices of cove edged graphene nanoribbon

The numerical values and the graphical representation of various indices were given in Table 3 and Figure 2.

Table 3: Numerical Values of various molecular descriptor of cove edged graphene nanoribbon

TIs	$m=1,n=1$	$m=2,n=2$	$m=3,n=3$	$m=4,n=4$
$RLI(CGNR(m,n))$	24.173	94.1273	207.5318	364.3865
$SLI(CGNR(m,n))$	54.7558	187.9369	396.5846	680.6989
$ISLI(CGNR(m,n))$	15.5067	48.3883	98.4431	165.6711
$ISI(CGNR(m,n))$	36.1	128.5	274.9	475.3
$MLI(CGNR(m,n))$	3.2437	8.1093	12.9749	17.8405
$MLSI(CGNR(m,n))$	5.812	14.53	23.248	31.966
$MII(CGNR(m,n))$	1.3333	3.3333	5.3333	7.3333
$MIRI(CGNR(m,n))$	1.0381	2.5952	4.1523	5.7094
$MRI(CGNR(m,n))$	2.5427	6.3567	10.1707	13.9847
$MDI(CGNR(m,n))$	8	20	32	44
$MHI(CGNR(m,n))$	1	2.5	4	5.5
$MMRI(CGNR(m,n))$	27.532	91.33	191.128	191.128
$MMRDI(CGNR(m,n))$	30.7976	99.494	204.1904	344.8868
$MMDI(CGNR(m,n))$	33	105	213	357
$MMSDI(CGNR(m,n))$	39	120	237	390
$SDDI(CGNR(m,n))$	59.3333	193.3333	399.3333	677.3333

5.Conclusion

This paper computes the closed value of the Randićlodeg index, Invers sum lordeg index, Sum lordeg index of the cove edged graphene nanoribbon for any m and n values. In addition, the Misbalance type indices namely, Misbalance losdeg index, lodeg index, indeg index, irdeg index, deg index, rodeg index, hadeg index, Min-max rodeg index, Max-min rodex index, Max-min deg index, Max-min sdeg index and Symmetric division deg index of cove edged graphene nanoribbon. The graphical representation of these indices was also reported. The techniques used to calculate the numerous vertex degree-based topological indices and entropies provide chemically pertinent data and insights into these structures. It can also be used to calculate bond enthalpies, sequential bond energies, and atomization energies.

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