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MOLECULAR TOPOLOGICAL CHARACTERIZATION OF TESSELLATIONS OF RECTANGULAR KEKULENE STRUCTURES

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Abstract This study presents a comprehensive molecular topological characterization of tessellations derived from rectangular Kekulene structures, focusing on degree-based topological indices. By employing advanced graph-theoretical approaches, we systematically analyze the intricate connectivity patterns inherent in Kekulene structures, which are significant in various chemical applications. We derive and calculate key topological indices, including the Randić, First Zagreb indices, . . . to elucidate their relationships with molecular properties such as stability and reactivity. Our findings reveal distinct patterns in the topological indices as they relate to the geometric configurations of the tessellated structures. This research enhances the understanding of molecular architecture and provides a valuable framework for predicting the behavior of complex molecular systems such as Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) Studies predicting biological activity, chemical reactivity, and physicochemical properties of compounds, aid in understanding the stability, boiling points, and reactivity of chemical compounds, studying surface interactions and conductivity, predict biodegradability and toxicity of pollutants. The implications of our results extend to fields such as material science and organic chemistry, offering insights into the design of novel molecular structures with tailored properties.

1 Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds composed of multiple fused aromatic rings. They are ubiquitous in nature and play significant roles in various fields, including environmental science, materials science, and organic chemistry. Due to their unique electronic and optical properties, PAHs have garnered substantial interest for applications in organic electronics, photonics, and nanotechnology. Among these structures, Kekulene—a specific type of PAH characterized by its alternating single and double bonds—exhibits remarkable stability and intriguing geometric properties. The study of Kekulene and its derivatives, particularly in the context of their molecular topology, has revealed critical insights into the relationship between molecular structure and chemical behavior. One approach to exploring this relationship is through the application of degree-based topological indices, which serve as quantitative descriptors of molecular connectivity. These indices provide valuable information on properties such as stability, reactivity, and the potential for functionalization. In this paper, we focus on the molecular topological characterization of tessellations based on rectangular Kekulene structures. By systematically analyzing the degree-based topological indices associated with these tessellations, we aim to deepen our understanding of the influence of molecular architecture on the properties of PAHs. Our findings will contribute to the broader field of molecular design, highlighting the potential for tailoring properties through strategic manipulation of molecular topology. Through this research, we aspire to bridge theoretical insights with practical applications, paving the way for innovative advancements in the synthesis and application of PAHs and their derivatives.

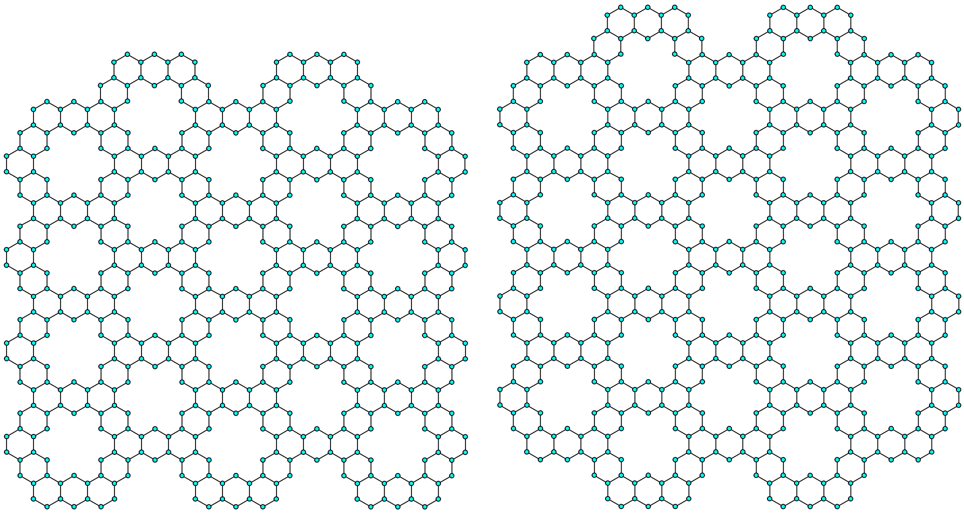
Benzenoid structures, characterized by their fused aromatic rings, exhibit unique stability and reactivity due to their extensive π -electron delocalization, making them fundamental to the chemistry of polycyclic aromatic hydrocarbons. Kekulene is a unique polycyclic aromatic hydrocarbon (PAH) consisting of a series of interconnected benzene rings arranged in a specific alternating pattern of single and double bonds. Named after the chemist August Kekulé, who contributed significantly to the understanding of aromatic compounds, Kekulene exhibits remarkable stability and unique electronic properties due to its highly conjugated structure. Its planar geometry allows for efficient π -electron delocalization, contributing to its notable chemical reactivity and potential applications in materials science. Rectangular Kekulenes, a variant of the traditional Kekulene structure, maintain the same fundamental characteristics but feature a rectangular arrangement of the fused rings. This distinct geometry results in a different set of electronic and topological properties, which can influence the compound's reactivity and stability. The rectangular configuration allows for interesting interactions and variations in molecular behavior, making it a subject of interest in the study of molecular topology and the design of new materials. By exploring these structures, researchers aim to uncover new insights into the relationships between molecular shape, electronic properties, and potential applications in various fields.

Topological descriptors are quantitative measures derived from the molecular graph of a compound, providing insights into its structural characteristics and chemical properties. These descriptors are essential tools in cheminformatics and computational chemistry, allowing researchers to analyze and predict molecular behavior based on connectivity patterns rather than explicit atomic coordinates. Commonly used topological indices include the Wiener index, which reflects the molecular size and branching, the Randić index, which correlates with molecular stability and reactivity, and the Zagreb indices, which provide information about the distribution of bonds within the structure. By encapsulating essential features of molecular connectivity, topological descriptors facilitate the understanding of complex relationships between structure and properties, aiding in the design of new compounds with tailored functionalities in materials science, drug design, and other fields.

The study of degree-based topological indices in rectangular Kekulene structures holds significant implications beyond theoretical graph analysis. In material science, these indices are instrumental in predicting the electronic, optical, and mechanical properties of novel materials, particularly in the development of organic semiconductors and conductive polymers. The unique tessellation patterns of Kekulene structures influence charge transport and stability, making them promising candidates for applications in flexible electronics, organic light-emitting diodes (OLEDs), and photovoltaic devices. Furthermore, in organic chemistry, understanding the molecular topology of such structures aids in elucidating aromaticity, reactivity patterns, and stability of large polycyclic aromatic hydrocarbons. The calculated indices can also assist in modeling molecular interactions in supramolecular chemistry, contributing to the design of new catalysts and functionalized materials. By establishing clear correlations between molecular topology and chemical properties, our study provides a foundation for targeted molecular design in advanced materials and chemical synthesis.

QSPR and QSAR are predictive modeling techniques that leverage molecular structure data to correlate chemical features with specific properties or biological activities, facilitating the design and optimization of new compounds in drug development and materials science [1, 2, 3, 4, 5]. The development and refinement of topological indices, reflect the growing complexity of scientific problems and the need for precise tools to bridge molecular structure with properties in fields like chemistry, materials science, and biochemistry [6, 7]. Refer [8, 9, 10, 11, 12, 13, 14, 15] for similar works.

Given the complex tessellation and aromatic nature of rectangular Kekulene structures, understanding their molecular topology requires robust mathematical descriptors. Degree-based topological indices are particularly useful in this context because they capture essential structural features such as vertex connectivity, edge distribution, and the degree of branching, which are critical for predicting the chemical and physical properties of these systems. In the following section, we present the theoretical background necessary for the computation and interpretation of these indices within the framework of rectangular Kekulene structures.



(a) (b)

Figure 1: Rectangular Kekulene (a) $RK(4,3)$ Type I; (b) $RK(4,3)$ Type II.

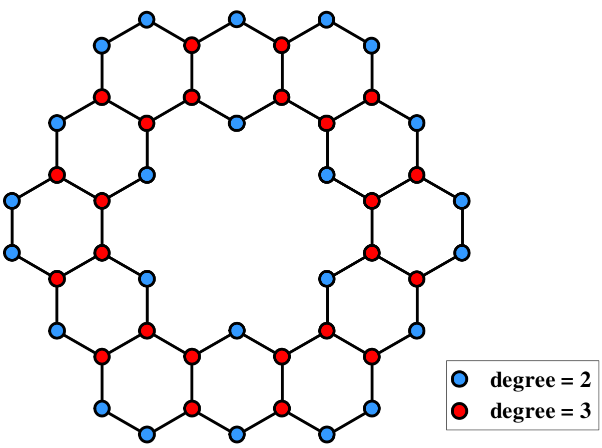


Figure 2: Kekulene: degree of the vertex

2 Graph-theortical Terminologies

Throughout this paper, the graphs are assumed to be undirected, and finite. V and edge set E are the vertex set and edge set of molecular graph $G = (V, E)$. The degree of a vertex v is the number of edges incident with a vertex $v \in V(G)$, denoted by $d_G(v)$. Equations for various degree-based topological indices are provided in Table 1, while the structures of Type I and II rectangular kekulene are illustrated in Figure 1, and the vertex partition of the basic kekulene structure is shown in Figure 2. For further details or definitions regarding this, we can refer [9, 11]. Denote $RK(m,n) - I$ and $RK(m,n) - II$ for type I and II rectangular kekulene.

Table 1: Degree based topological indices

Topological Indices	**Mathematical Expressions**
Harmonic [16]	$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$
Sum-connectivity [17]	$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$
First Zagreb [18]	$M_1(G) = \sum_{u \in V(G)} d(u)^2$
Second Zagreb [18]	$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$
Reduced Second Zagreb [19]	$RM_2(G) = \sum_{uv \in E(G)} (d(u)-1)(d(v)-1)$
Randić [20]	$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$
Reciprocal Randić [21]	$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}$
Reduced reciprocal Randić [22]	$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)(d(v)-1)}$
Augmented Zagerb [23]	$AZ(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$
Hyper Zagerb [24]	$HM(G) = \sum_{uv \in E(G)} [d(u)+d(v)]^2$
Atom bond connectivity [25]	$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$
Geometric arithmetic [26]	$GA(G) = \sum_{uv \in E(G)} 2\left(\frac{\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)$
Inverse sum indeg [27]	$ISI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)}\right)$

3 Rectangular Kekulene type I

For a $RK(m, n) - I$ structure, number of vertices are $36mn - 2m + 32n - 18$ and number of edges are $48mn + 40n - 4m - 24$. The edge partition were presented in Table 2 and vertex partition presented in Table 3. Corresponding figures were Figure 3 and 4.

Table 2: Edge partition frequency of $RK(m, n) - I$ structure

S. No	Edge Type	$(d(u), d(v))$	Frequency
1	E_1	(2,2)	$f_1 = 2m + 6n - 2$
2	E_2	(2,3)	$f_2 = 24mn + 28n - 16$
3	E_3	(3,3)	$f_3 = 24mn - 6m + 6n - 6$

Table 3: Vertex partition frequency of $RK(m,n) - I$

S. No	Vertex Type	$d(u)$	Frequency
1	V_1	2	$f_4 = 12mn + 2m + 16n - 6$
2	V_2	3	$f_5 = 24mn - 4m + 16n - 12$

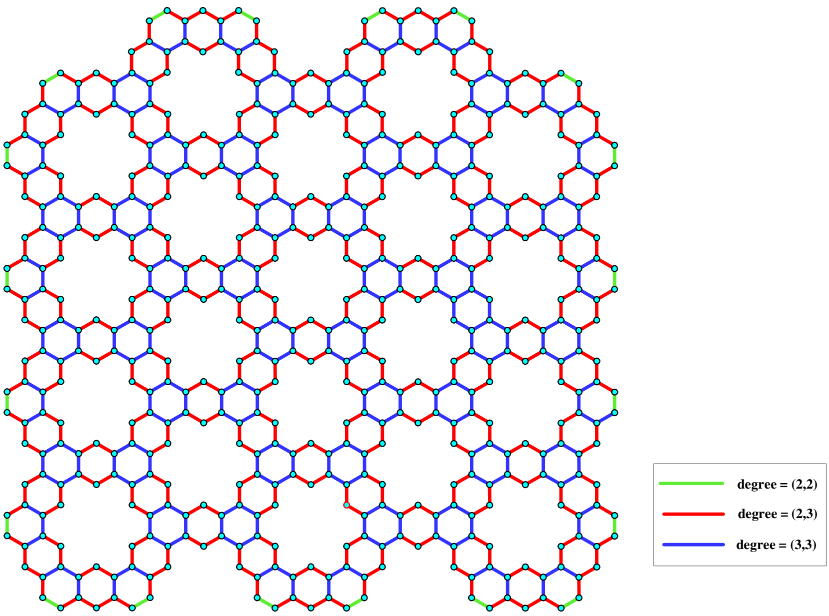


Figure 3: Edge partition of $RK(4,3) - I$ structure.

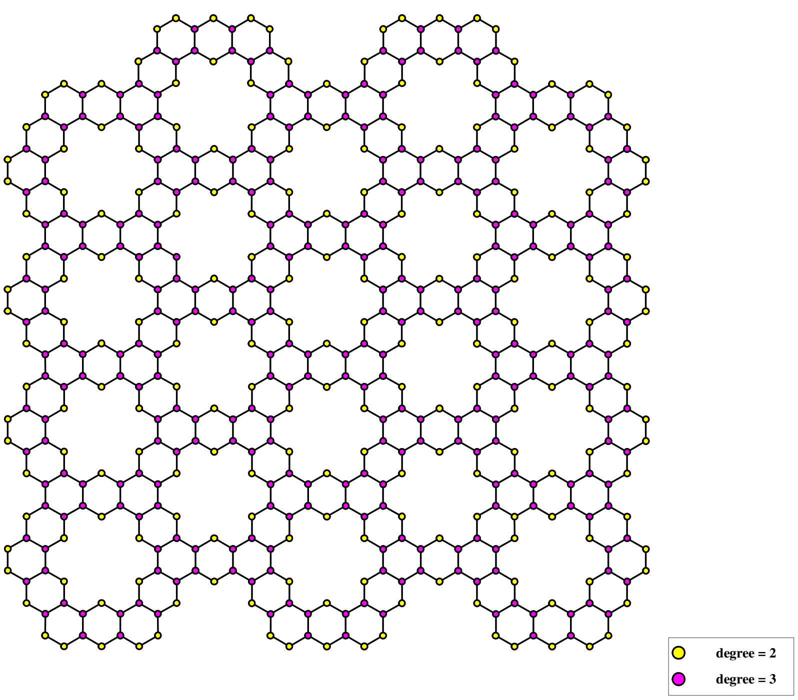


Figure 4: Edge partition of $RK(4,3) - I$ structure.

Theorem 3.1. *Let G be a rectangular kekulene, $RK(m,n) - I$ strecture. Then*

(i) $R(G) = (30n - 6m + \sqrt{6}(28n + 24mn - 16) + 48mn - 18)/6$.

(ii) $RR(G) = 30n - 14m + \sqrt{6}(28n + 24mn - 16) + 72mn - 22$

(iii) $RRR(G) = 18n - 10m + \sqrt{2}(28n + 24mn - 16) + 48mn - 14$.

(iv) $M_1(G) = 264mn - 28m + 208n - 132$.

(v) $M_2(G) = 246n - 46m + 360mn - 158$.

(vi) $RM_2(G) = 86n - 22m + 144mn - 58$.

(vii) $HM(G) = 1012n - 184m + 1464mn - 648$.

(viii) $AZ(G) = (10891n - 1675m + 14892mn - 6795)/32$.

(ix) $ABC(G) = (8n - 8m + 2\sqrt{2}m + 34\sqrt{2}n + 32mn - 18\sqrt{2} + 24\sqrt{2}mn - 8)/2$.

(x) $H(G) = (81n - 5m + 88mn - 47)/5$.

(xi) $SC(G) = (30m + 90n + 6\sqrt{5}(28n + 24mn - 16) - 5\sqrt{6}(6m - 6n - 24mn + 6) - 30)/30$.

(xii) $GA(G) = (60n - 20m + 2\sqrt{6}(28n + 24mn - 16) + 120mn - 40)/5$.

(xiii) $ISI(G) = (243n - 35m + 324mn - 151)/5$.

Proof. Use the definition of topological indices in Table 1 and compute for each topological indices. □

The visual illustration of our topological descriptors of type I rectangular kekulene are depicted in Figure 5 and Figure 6. Corresponding table values were presented in Table 4 and 5.

Table 4: Value of topological indices for $RK(m, n) - I$

(m, n)	$R(G)$	$RR(G)$	$RRR(G)$	$M_1(G)$	$M_2(G)$	$RM(G)$
$(1, 1)$	23.697	154.18	92.912	312	402	150
$(2, 2)$	92.522	631.13	386.33	1284	1682	646
$(3, 3)$	196.94	1369.7	843.64	2784	3682	1430
$(4, 4)$	336.96	2369.8	1464.8	4812	6402	2502
$(5, 5)$	512.57	3631.4	2249.9	7368	9842	3862
$(6, 6)$	723.78	5154.7	3198.8	10452	14002	5510
$(7, 7)$	970.58	6939.5	4311.7	14064	18882	7446
$(8, 8)$	1253	8985.9	5588.4	18204	24482	9670
$(9, 9)$	1571	11294	7029	22872	30802	12182
$(10, 10)$	1924.6	13863	8633.5	28068	37842	14982

Table 5: Value of topological indices for $RK(m,n) - I$

(m,n)	$HM(G)$	$AZ(G)$	$ABC(G)$	$H(G)$	$SC(G)$	$GA(G)$	$ISI(G)$
$(1,1)$	1644	541.03	41.698	23.4	26.448	59.273	76.2
$(2,2)$	6864	2225.2	166.07	91.4	104.56	237.25	312.2
$(3,3)$	15012	4840	356.37	194.6	223.74	510.26	677.8
$(4,4)$	26088	8385.7	612.62	333	383.98	878.3	1173
$(5,5)$	40092	12862	934.82	506.6	585.28	1341.4	1797.8
$(6,6)$	57024	18269	1322.9	715.4	827.65	1899.5	2552.2
$(7,7)$	76884	24607	1777	959.4	1111.1	2552.6	3436.2
$(8,8)$	99672	31876	2297	1238.6	1435.6	3300.8	4449.8
$(9,9)$	125388	40075	2883	1553	1801.1	4144	5593
$(10,10)$	154032	49205	3534.9	1902.6	2207.7	5082.2	6865.8

From the table values above, we can visualize the growth of each topological indices with respect to increase in m and n values.

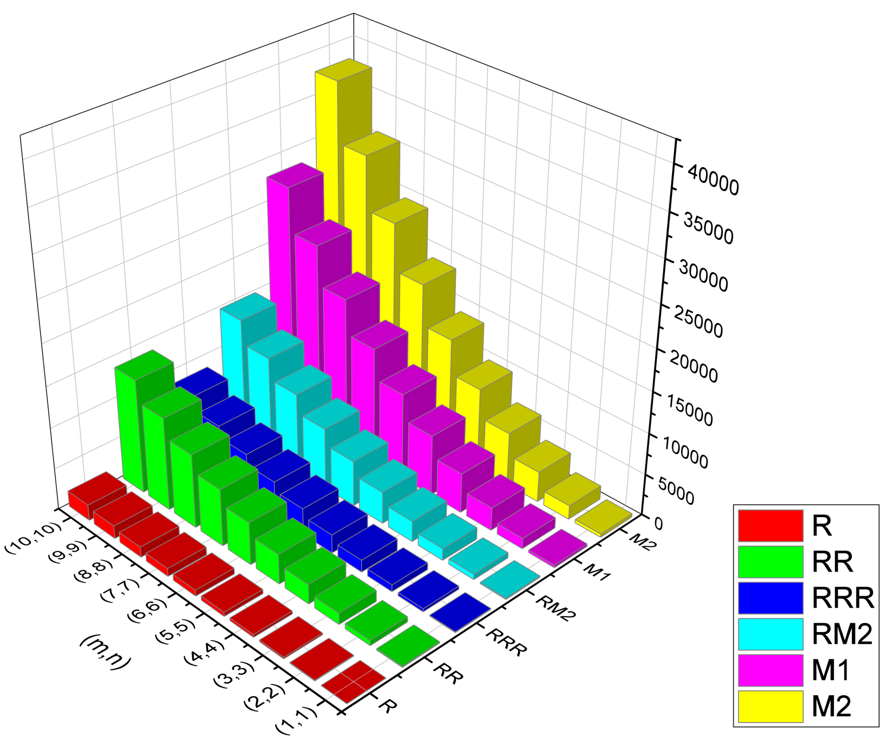


Figure 5: The growth of specific indices with increasing m and n for $RK(m,n) - I$

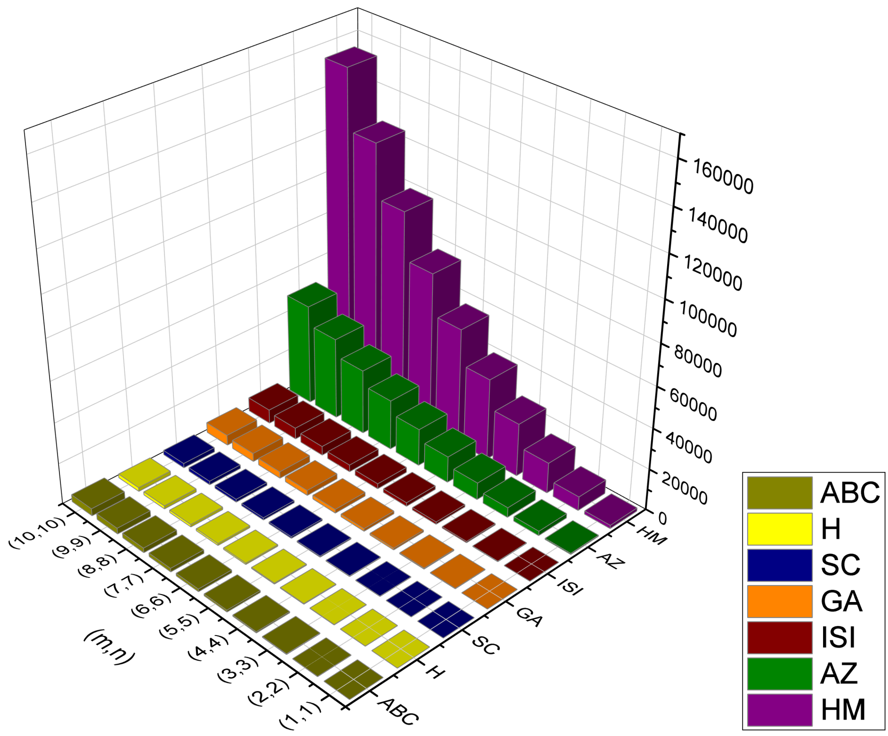


Figure 6: The growth of specific indices with increasing m and n for $RK(m,n) - I$

4 Rectangular Kekulene type II

For a rectangular Kekulene type II structure, there are $36mn + 50n - 2m - 36$ number of vertices and $48mn + 64n - 4m - 48$ number of edges. The edge partition were presented in Table 6 and vertex partition presented in 7. Corresponding figures we can seen in Figure 7 and 8.

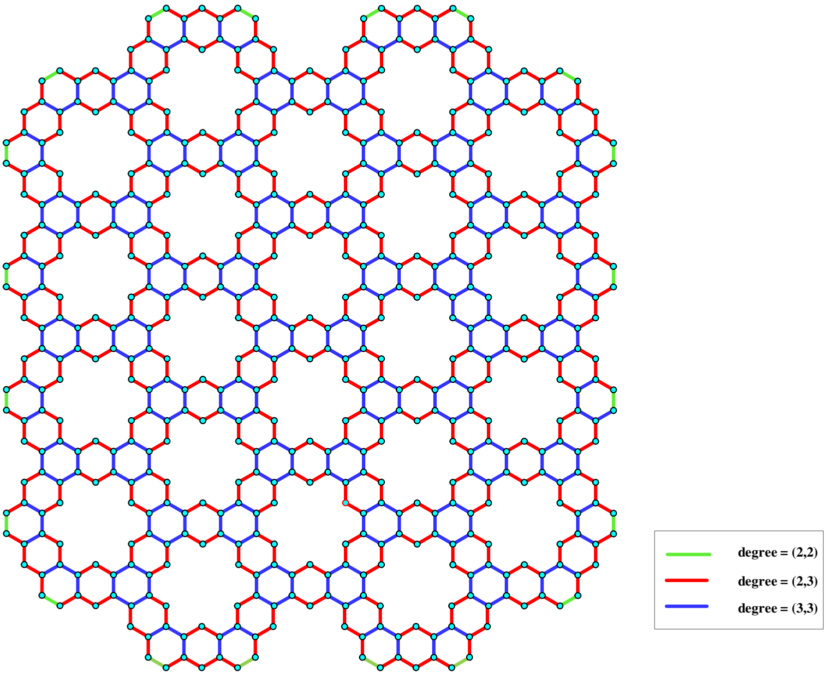


Figure 7: Edge partition of $RK(4,3) - II$ structure.

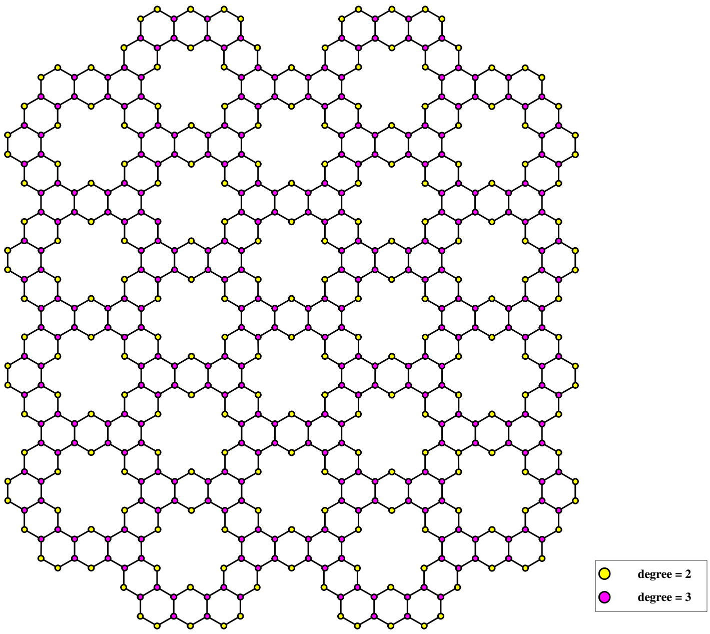


Figure 8: Edge partition of $RK(4,3)-II$ structure.

Table 6: Edge partition frequency of $RK(m,n)-II$ structure.

S. No	Edge Type	$(d(u),d(v))$	Frequency
1	E_1	(2,2)	$f_1 = 2m + 8n - 4$
2	E_2	(2,3)	$f_2 = 24mn + 44n - 32$
3	E_3	(3,3)	$f_3 = 24mn - 6m + 12n - 12$

Table 7: Vertex partition frequency of $RK(m,n)-II$ structure

S. No	Vertex Type	$d(u)$	Frequency
1	V_1	2	$f_4 = 12mn + 2m + 22n - 12$
2	V_2	3	$f_5 = 24mn - 4m + 28n - 24$

Theorem 4.1. *Let G be a rectangular kekulene, $RK(m,n)-II$ strecture. Then*

(i) $R(G) = (48n - 6m + \sqrt{6}(44n + 24mn - 32) + 48mn - 36)/6$.

(ii) $RR(G) = 52n - 14m + \sqrt{6}(44n + 24mn - 32) + 72mn - 44$.

(iii) $RRR(G) = 32n - 10m + \sqrt{2}(44n + 24mn - 32) + 48mn - 28$.

(iv) $M_1(G) = 264mn - 28m + 340n - 264$.

(v) $M_2(G) = 404n - 46m + 360mn - 316$.

(vi) $RM_2(G) = 144n - 22m + 144mn - 116$.

(vii) $HM(G) = 1660n - 184m + 1464mn - 1296$.

(viii) $AZ(G) = (17686n - 1675m + 14892mn - 13590)/32$.

(ix) $ABC(G) = (16n - 8m + 2\sqrt{2}m + 52\sqrt{2}n + 32mn - 36\sqrt{2} + 24\sqrt{2}mn - 16)/2$.

(x) $H(G) = (128n - 5m + 88mn - 94)/5.$

(xi) $SC(G) = (30m+120n+6\sqrt{5}(44n+24mn-32)-5\sqrt{6}(6m-12n-24mn+12)-60)/30.$

(xii) $GA(G) = (100n - 20m + 2\sqrt{6}(44n + 24mn - 32) + 120mn - 80)/5.$

(xiii) $ISI(G) = (394n - 35m + 324mn - 302)/5.$

Proof. Use the definition of topological indices in Table 1 and compute for each topological indices. □

The numerical values of topological indices of $RK(m, n) - II$ are depicted in Table 8 and 9. The visual illustrations are depicted in Figure 9 and Figure 10.

Table 8: Value of various topological indices for $RK(m, n) - II$

(m, n)	$R(G)$	$RR(G)$	$RRR(G)$	$M_1(G)$	$M_2(G)$	$RM(G)$
$(1, 1)$	23.697	154.18	92.912	312	402	150
$(2, 2)$	102.05	692.32	422.96	1416	1840	704
$(3, 3)$	216.01	1492	916.89	3048	3998	1546
$(4, 4)$	365.56	2553.3	1574.7	5208	6876	2676
$(5, 5)$	550.7	3876.2	2396.4	7896	10474	4094
$(6, 6)$	771.44	5460.6	3382	11112	14792	5800
$(7, 7)$	1027.8	7306.7	4531.4	14856	19830	7794
$(8, 8)$	1319.7	9414.3	5844.8	19128	25588	10076
$(9, 9)$	1647.2	11783	7322	23928	32066	12646
$(10, 10)$	2010.4	14414	8963.1	29256	39264	15504

Table 9: Value of various topological indices for $RK(m, n) - II$

(m, n)	$HM(G)$	$AZ(G)$	$ABC(G)$	$H(G)$	$SC(G)$	$GA(G)$	$ISI(G)$
$(1, 1)$	1644	541.03	41.698	23.4	26.448	59.273	76.2
$(2, 2)$	7512	2437.5	182.79	100.8	115.17	260.93	342.4
$(3, 3)$	16308	5264.7	389.83	213.4	244.95	557.62	738.2
$(4, 4)$	28032	9022.7	662.81	361.2	415.8	949.33	1263.6
$(5, 5)$	42684	13711	1001.7	544.2	627.7	1436.1	1918.6
$(6, 6)$	60264	19331	1406.6	762.4	880.67	2017.9	2703.2
$(7, 7)$	80772	25881	1877.4	1015.8	1174.7	2694.7	3617.4
$(8, 8)$	104208	33362	2414.1	1304.4	1509.8	3466.5	4661.2
$(9, 9)$	130572	41774	3016.8	1628.2	1886	4333.4	5834.6
$(10, 10)$	159864	51116	3685.4	1987.2	2303.2	5295.3	7137.6

From the table values above, we can visualize the growth of each topological indices with respect to increase in m and n values, that is depicted below.

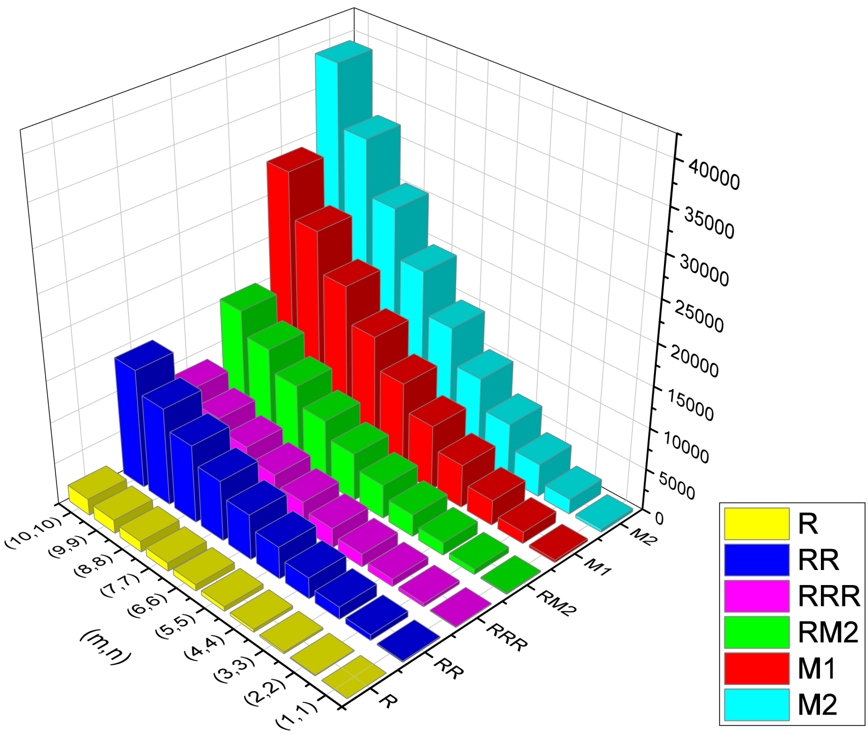


Figure 9: The growth of specific indices with increasing m and n for $RK(m,n) - II$

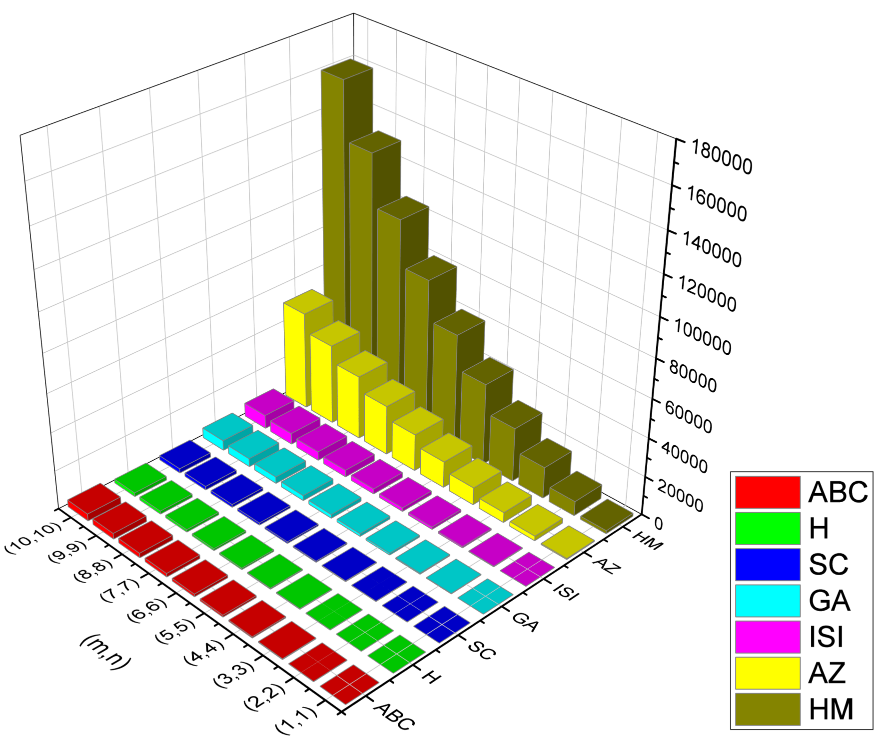


Figure 10: The growth of specific indices with increasing m and n for $RK(m,n) - II$

5 Conclusion

This study on the molecular topological characterization of tessellations of rectangular kekulene successfully identified and analyzed various degree-based topological indices. These indices provide valuable insights into the structural properties of rectangular kekulene, contributing to a deeper understanding of its chemical behavior. The findings demonstrate the utility of these topological indices in a wide range of applications within chemistry, including the prediction of molecular stability, reactivity, and other key properties. This work paves the way for future research exploring topological indices in more complex molecular structures and their potential impact on material science and drug design.

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