Applicable Analysis and Discrete Mathematics
available online at http://pefmath.etf.rs

Appl. Anal. Discrete Math. **18** (2024), 173–192.
https://doi.org/10.2298/AADM230901002C

VERTEX-DEGREE-BASED TOPOLOGICAL INDICES OF ARBITRARY SETS OF HEXAGONS IN THE REGULAR HEXAGONAL GRID

Lidija Čomić and Nebojša M. Ralević*

Vertex-degree-based indices have been widely used for describing and predicting physical, chemical and biological properties of molecules. They are expressed through the numbers $m_{i,j}$ of the edges connecting the vertices of degrees i and j. We generalize some known formulae for $m_{i,j}$ from graphs defined by simply connected sets of hexagons to those defined by sets of arbitrary topology in the regular hexagonal grid. We compute the most commonly used indices for three families of graphs in this grid.

1. INTRODUCTION

Let S be a set of h hexagons in the hexagonal grid, which may or may not be (simply) connected, with β_0 connected components, β_1 holes and the Euler characteristic $\chi = \beta_0 - \beta_1$, and let $G = (V, E)$ be the simple plane graph with n vertices and m edges, induced by S: the vertices and edges of G correspond to the vertices and edges of the hexagons in S, respectively, in the obvious manner. In chemical graph theory, simply connected sets S are called benzenoid systems [**23**], and connected sets with one hole (the hole containing at least two hexagons) are coronoid systems [**10**].

The degree d_v of a vertex v is equal to the number of the edges incident to v. The number of the vertices in V of degree i is denoted by n_i, $i \in \{2, 3\}$. The

*Corresponding author. Lidija Čomić
2020 Mathematics Subject Classification. 05C09 Graphical indices (Wiener index, Zagreb index, Randić index, etc., 05C92 Chemical graph theory).
Keywords and Phrases. Regular hexagonal grid, Benzenoid systems, Coronoid systems, Graph indices, Vertex-degree-based topological indices.

number of the edges connecting a vertex of degree i to a vertex of degree j (type i,j edges) is denoted by $m_{i,j}$, $i,j \in \{2,3\}$, $i \leq j$.

Boundary edges are incident to exactly one hexagon in S. Boundary vertices are incident to boundary edges. The boundary of S is composed of cycles surrounding components and holes of S. The number of boundary vertices and edges is denoted by n^* and $m^* = n^*$, respectively. Similarly, n_3^* and $m_{3,3}^*$ denote the number of boundary vertices of degree 3, and the number of edges connecting them, respectively. Each edge of type $2,2$ or $2,3$ is a boundary edge. Non-boundary vertices and edges are called interior. Their number is denoted by n_i and m_i, respectively. Each interior vertex is of degree 3 and each vertex of degree 2 is a boundary vertex. The quantities h and n_i determine the basic properties of benzenoid systems [**24**].

A topological index of a graph G is a real number associated with G. It is a graph invariant describing and predicting chemical, physical and biological properties of chemical graphs (modeling molecules). A wide class of topological indexes is based on vertex degrees. The general form of a vertex-degree-based topological index $I(G)$ of a graph G is given by

$$I(G) = \sum_{uv \in E(G)} f(d_u, d_v),$$

where f is a real function such that $f(x,y) = f(y,x)$. Well-known indices are obtained for different choices of f:

1. $f(x,y) = x + y$ for the first Zagreb index M_1 [**28, 15**]
2. $f(x,y) = xy$ for the second Zagreb index M_2 [**26**]
3. $f(x,y) = \frac{x+y}{xy}$ for the first redefined Zagreb index $ReZG_1$ [**39**]
4. $f(x,y) = \frac{xy}{x+y}$ for the second redefined Zagreb index $ReZG_2$ [**39**] (inverse sum indeg index ISI [**43**])
5. $f(x,y) = xy(x+y)$ for the third redefined Zagreb index $ReZG_3$ [**39**] (generalized Zagreb index $M_{\{1,2\}}$ [**4**])
6. $f(x,y) = \frac{1}{\sqrt{xy}}$ for the Randić index R [**38**]
7. $f(xy) = \sqrt{xy}$ for the reciprocal Randić index RR [**25**]
8. $f(x,y) = (xy)^\alpha$ for the general Randić index R_α [**5, 6, 30, 31**] (variable second Zagreb index ${}^vM_2$ [**34**])
9. $f(x,y) = (x-1)(y-1)$ for the reduced second Zagreb index $RM_2 = M_2 - M_1 + m$ [**21**]
10. $f(x,y) = x^\alpha y^\beta + y^\alpha x^\beta$ for the generalized Zagreb index $M_{\{\alpha,\beta\}}$[**4**]
11. $f(x,y) = \sqrt{(x-1)(y-1)}$ for the reduced reciprocal Randić index RRR [**33**]

12. $f(x,y) = \frac{1}{\max\{x,y\}}$ for the variation of the Randić index R' [**16**]

13. $f(x,y) = \frac{1}{\sqrt{x+y}}$ for the sum-connectivity index χ [**44**]

14. $f(x,y) = (x+y)^\alpha$, for the general sum-connectivity index χ_α [**45**]

15. $f(x,y) = \frac{2\sqrt{xy}}{x+y}$ for the geometric-arithmetic index GA [**42**]

16. $f(x,y) = \frac{x^2+y^2}{xy} = \frac{x}{y} + \frac{y}{x}$ for the symmetric division deg index SDD [**43**]

17. $f(x,y) = \sqrt{\frac{2(x+y-2)}{xy}}$ for the atom-bond connectivity index ABC [**17**]

18. $f(x,y) = \frac{2}{x+y}$ for the harmonic index H [**18**]

19. $f(x,y) = \left(\frac{xy}{x+y-2}\right)^3$ for the augmented Zagreb index AZI [**20**]

20. $f(x,y) = x^2 + y^2$ for the forgotten topological index F [**28**]

21. $f(x,y) = \sqrt{x^2+y^2}$ for the Sombor index SO [**22**]

22. $f(x,y) = \sqrt{(x-1)^2+(y-1)^2}$ for the reduced Sombor index RSO [**22**]

23. $f(x,y) = |x-y|$ for the third Zagreb (or Albertson [**3**]) index M_3 [**19**] (misbalance deg index [**43**])

24. $f(x,y) = x+y-2$ for the Platt index Pl [**36**]

25. $f(x,y) = \frac{1}{x^3} + \frac{1}{y^3}$ for the first modified Zagreb index ${}^mM_1$ [**35**]

26. $f(x,y) = \frac{1}{xy}$ for the second modified Zagreb index ${}^mM_2$ [**35**] (first order overall index [**7**])

27. $f(x,y) = (x+y)^2$ for the hyper-Zagreb index $HM = F + 2M_2$ [**40**]

28. $f(x,y) = x^{\alpha-1} + y^{\alpha-1}$, $\alpha \neq 0, 1$ for the first general Zagreb index M_α [**32**]

29. $f(x,y) = \begin{cases} \frac{1}{|x-y|} & x \neq y \\ 0 & x = y \end{cases}$ for the inverse misbalance deg index IM_3 [**43**]

30. $f(x,y) = (x-y)^2$ for the sigma index $\sigma = F - 2M_2$ [**27**]

For the graph G of S, $I(G)$ can be expressed as [**24, 41**]

$$I(G) = m_{2,2}f(2,2) + m_{2,3}f(2,3) + m_{3,3}f(3,3).$$

For simply connected sets S, Gutman [**23**] and Gutman and Furtula [**24**] proposed a general formula expressing $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ through the (easier to determine and chemically significant) numbers h of hexagons, n_i of interior vertices and $m^*_{3,3}$ of boundary edges connecting two vertices of degree 3 (also known as the number b of bay regions, as illustrated in Figure 1):

$$\begin{aligned} m_{2,2} &= 6 + m^*_{3,3} \\ m_{2,3} &= 4h - 4 - 2m^*_{3,3} - 2n_i \\ m_{3,3} &= h - 1 + m^*_{3,3} + n_i. \end{aligned} \tag{1}$$

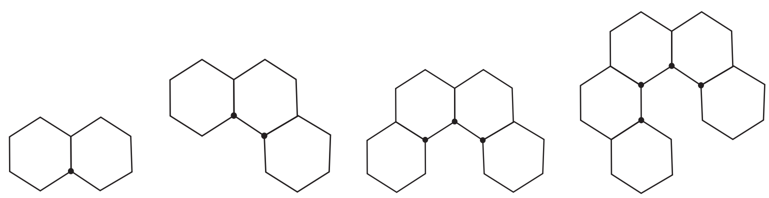


Figure 1: Inlets defined by one, two, three and four consecutive boundary vertices of degree three (marked by dots), respectively, and bays defined by the edges connecting them.

Alternative expressions for simply connected sets S have been proposed by Rada et al. [**37**], involving the number n of vertices, h of hexagons and r of inlets (maximal contiguous sequences of degree 3 vertices along the boundary of S of length at most 4, as illustrated in Figure 1):

$$\begin{aligned} m_{2,2} &= n - 2h - r + 2 \\ m_{2,3} &= 2r \\ m_{3,3} &= 3h - r - 3. \end{aligned} \tag{2}$$

Interestingly, despite the long history and large body of research on vertex-degree-based topological indices for simply connected sets S, no analogous expressions have been proposed for sets S of arbitrary topology, not even for connected sets with only one hole [**10**]. We fill this gap in Propositions 3 and 4, by extending Equalities (1) and (2) to arbitrary sets S of hexagons, by taking the topology of S into account, i.e., by expressing $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ not only through h, n_i and $m^*_{3,3}$ or n, h and r, but also through the Euler characteristic χ of S, thus enabling easier determination of $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ not only for simply connected, but for sets S of arbitrary topology, (simply) connected or not.

For plane graphs G with vertices of degree 2 or 3, Deutsch and Klavžar [**12**] proposed a formula expressing $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ through the number n_2 of vertices of degree 2, $m_{2,2}$ of the edges connecting such vertices, and f of the faces in G:

$$\begin{aligned} m_{2,2} &= m_{2,2} \\ m_{2,3} &= 2n_2 - 2m_{2,2} \\ m_{3,3} &= 3f - n_2 + m_{2,2} - 6, \end{aligned} \tag{3}$$

Recently, Deutsch et al. [**13**] extended this result to graphs with degree 2 or p, $p \geq 3$. These results are valid in a more general setting (finite plane graphs) then the one we consider (graphs induced by finite sets of hexagons in the hexagonal grid). This generality, however, prohibits the distinction both between (inner) faces and holes, significant for chemical graphs, and between interior and boundary graph entities (edges and vertices). Our more restricted setting, on the other hand, allows considerations of sets S with holes consisting of one hexagon only. In Proposition 5, we adapt Equalities 3 to graphs G induced by finite sets of hexagons in the hexagonal grid of arbitrary topology.

We also obtain several other expressions for $m_{3,3}$ by using the Euler-Poincaré formula [**2, 8**]

$$\chi = \beta_0 - \beta_1 = n - m + h,$$

and equalities

$$\begin{aligned} n_2 + n_3 &= n \\ 2m_{2,2} + m_{2,3} &= 2n_2 \\ m_{2,3} + 2m_{3,3} &= 3n_3 \\ 2n_2 + 3n_3 &= 2m. \end{aligned}$$

To demonstrate the versatility of the proposed formulas, we determine the numbers $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ and a general expression for an arbitrary vertex-degree-based index for three families of graphs, zigzag-edge coronoid fused by starphene $ZCS(l, m, n)$ [**1**] and $K_1(k, p, q, r)$ and $K_2(k, p, q, r)$ [**29**]. For the benefit of interested practitioners, for these families we compute all of the most common vertex-degree-based indices listed above, not only those [**1, 29**] that can be obtained from their M-polynomial [**11**]

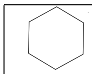
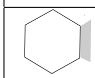
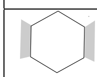
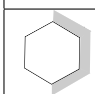
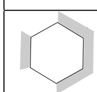
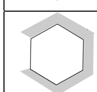
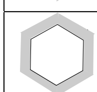
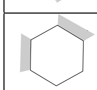
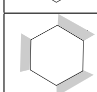
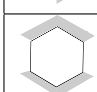
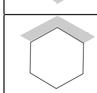
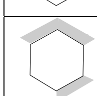
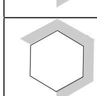
$$M(G; x, y) = m_{2,2}x^2y^2 + m_{2,3}x^2y^3 + m_{3,3}x^3y^3$$

through differentiation or integration. We also correct an error from the literature for the last two families.

2. MAIN RESULTS

In Propositions 3, 4 and 5, we present generalizations of Equalities (1) and (2) and an adaptation of Equalities (3) to arbitrary sets of hexagons in the hexagonal grid, respectively. We begin with a technical lemma.

Table 1: The different configurations around the added hexagon H (shaded parts belong to S'), and the induced changes in n, m, n_2, n_i, χ, $\tilde{n} = 4h - n_i + 2\chi$, $\tilde{m} = 5h - n_i + \chi$ and $\tilde{n}_2 = 2h - n_i + 4\chi$.

Conf.	Δn	Δm	Δn_2	Δn_i	$\Delta\chi$	$\Delta\tilde{n}$	$\Delta\tilde{m}$	$\Delta\tilde{n}_2$
	6	6	6	0	1	6	6	6
	4	5	2	0	0	4	5	2
	2	4	−2	0	−1	2	4	−2
	2	3	0	2	0	2	3	0
	0	2	−4	2	−1	0	2	−4
	0	1	−2	4	0	0	1	−2
	0	0	0	6	1	0	0	0
	2	4	−2	0	−1	2	4	−2
	0	3	−6	0	−2	0	3	−6
	0	2	−4	2	−1	0	2	−4
	3	4	1	1	0	3	4	1
	1	3	−3	1	−1	1	3	−3
	1	2	−1	3	0	1	2	−1

Lemma 1. *For a finite set S of h hexagons in the hexagonal grid*

$$\begin{array}{rcl} n & = & 4h - n_i + 2\chi \\ m & = & 5h - n_i + \chi \\ n_2 & = & 2h - n_i + 4\chi \end{array} \tag{4}$$

Proof. We proceed by induction on h. For $h = 0$, Equalities (4) trivially hold. Let (4) be true for all sets of $h-1$ hexagons, $h \in \mathbb{N}$, and let S be a set of h hexagons. Let H be a hexagon in S, and $S' = S - H$ be the set of $h' = h - 1$ hexagons satisfying Equalities (4). We denote by q' each quantity of S' corresponding to the quantity q of S, $q \in \{h, n, m, n_i, n_2, \chi\}$ and by Δq we denote $q - q'$. If Δq satisfy Equalities (4), then these equalities are true also for q, i.e., for S.

The hexagon H can be in one of the thirteen modes (up to rotation and symmetry) with respect to its neighbors in S' and their position [**23**], as illustrated in the first column of Table 1. In the next five columns, we show by how much n, m, n_2, n_i and χ change as H is added to S' ($\Delta h = 1$ for all configurations), and in the last three columns we show the change in the right hand sides of (4). For the configuration in the e.g. third row, two vertices (of degree 2) and four edges are added. Four boundary vertices that were of degree 2 and transformed to boundary vertices of degree 3, and either two connected components are merged (decreasing β_0 by 1) or a hole is created (increasing β_1 by 1), thus decreasing χ by 1. Thus, for this configuration, $\Delta n = 2 = \Delta(4h - n_i + 2\chi)$, and similarly for Δm and Δn_2, as well as for each of the remaining twelve configurations.

□

Corollary 2.

$$\begin{array}{rcl} m & = & n + h - \chi \\ n^* & = & 4h - 2n_i + 2\chi \\ n_3 & = & 2h - 2\chi \\ n_3^* & = & 2h - n_i - 2\chi \\ m_i & = & h + n_i - \chi \end{array}$$

Proposition 3. *For a finite set S of h hexagons in the hexagonal grid*

$$\begin{array}{rcl} m_{2,2} & = & m_{3,3}^* + 6\chi \\ m_{2,3} & = & 4h - 2n_i - 4\chi - 2m_{3,3}^* \\ m_{3,3} & = & h + n_i - \chi + m_{3,3}^* \end{array} \tag{5}$$

Proof. For the first equality, we consider separately each of the cycles C bounding components and holes of S, and we denote by $m_{2,2}^C$ and $m_{3,3}^{*C}$ the number of the edges of type $2,2$ and $3,3$ in C (relative to S).

- For each cycle bounding a component of S, by the first equality in (1), we have that $m_{2,2}^C = 6 + m_{3,3}^{*C}$.
- For each cycle bounding a hole, noting that each edge of type $2,2$ in C relative to S is a boundary edge of type $3,3$ relative to the set of hexagons in the hole and vice versa, we have that $m_{3,3}^{*C} = 6 + m_{2,2}^C$, i.e., $m_{2,2}^C = m_{3,3}^{*C} - 6$.

Summing over all cycles, we obtain

$$\begin{aligned} m_{2,2} &= m^*_{3,3} + 6\beta_0 - 6\beta_1 \\ &= m^*_{3,3} + 6\chi \end{aligned}$$

The remaining two equalities follow directly from Proposition 3 and Corollary 2.

□

Proposition 4. *For a finite set S of h hexagons in the hexagonal grid, without holes consisting of a single hexagon,*

$$\begin{aligned} m_{2,2} &= n - 2h - r + 2\chi \\ m_{2,3} &= 2r \\ m_{3,3} &= 3h - r - 3\chi \end{aligned} \tag{6}$$

Proof. The second equality is a direct consequence of the definition of inlets: each maximal contiguous sequence of degree 3 boundary vertices is preceded and followed by a degree 2 vertex, i.e., each inlet uniquely determines a pair of type $2,3$ edges. The first equality follows from $n_3 = 2h - 2\chi$ (third equality in Corollary 2) and $m_{2,3} + 2m_{3,3} = 3n_3$, i.e., $2r + 2m_{3,3} = 6h - 6\chi$. The first equality follows from the Euler-Poincaré formula $n - m + h = \chi$ and $m = m_{2,2} + m_{2,3} + m_{3,3}$.

□

For some graphs, it might be easier to determine the quantities n_2 and $m_{2,2}$, pertaining to the vertices of degree 2 [**12**].

Proposition 5. *For a finite set S of h hexagons in the hexagonal grid*

$$\begin{aligned} m_{2,2} &= m_{2,2} \\ m_{2,3} &= 2n_2 - 2m_{2,2} \\ m_{3,3} &= 3h - n_2 + m_{2,2} - 3\chi \end{aligned} \tag{7}$$

Proof. Direct substitution of $n_2 = 2h - n_i + 4\chi$ from (4) and $m_{2,2} = m^*_{3,3} + 6\chi$ from (5). □

The second equality above (for $m_{2,3}$) is the same as the one in [**13**]. If we apply the last equality (for $m_{3,3}$) to a connected graph induced by S, and we treat both hexagons and holes of S as faces in this graph, we get the expression $m_{3,3} = 3f - n_2 + m_{2,2} - 6$ from [**13**]: the number f of faces is equal to the number h of hexagons plus the number β_1 of holes plus 1 for the outer face, and for connected graphs β_0 is equal to 1 so $\chi = 1 - \beta_1$.

Alternatively, the number $m_{3,3}$ can also be expressed only through the number of vertices and edges of various types as

$$\begin{aligned} m_{3,3} = &= -n_2 + m_{2,2} + 3m - 3n \\ &= -n_2 + m_{2,2} + \tfrac{3}{2}n_3 \\ &= -n_2 + m - \tfrac{1}{2}m_{2,3}. \end{aligned}$$

3. APPLICATION

We obtain general expressions for an arbitrary vertex-degree-based topological index of three families of multiply connected graphs: zigzag-edge coronoid fused by starphene $ZCS(l, m, n)$ (see Figure 2) [**1**] and for $K_1(k, p, q, r)$ (see Figure 3) and $K_2(k, p, q, r)$ (see Figure 4) [**29**], using Propositions (3) and (5), respectively. To ease the work of researchers interested in practical applications, we compute the most commonly used such indices for these graph families. Other multiply connected families have also been investigated in the literature, such as monolayered cyclofusenes with given parameters [**14**], and fenestrene [**9**].

3.1 Vertex-Degree-Based Topological Indices of $ZCS(p, q, s)$

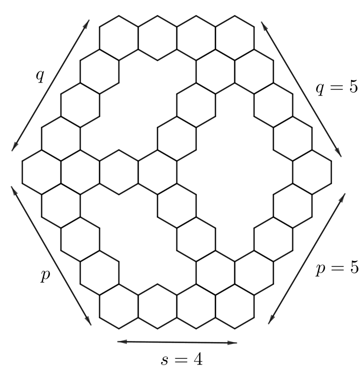


Figure 2: The graph of $ZCS(5, 5, 4)$.

Proposition 6. *If G is the graph of $ZCS(p, q, s)$, then*

$$I(G) = (12f(2,3) + 3f(3,3))(p + q + s) + 6f(2,2) - 84f(2,3) + 15f(3,3)$$

for any vertex-degree-based topological index $I(G)$ induced by f.

Proof. Using Proposition 3, we have that

$$\begin{aligned} h &= 3(p+q+s) - 11 \\ n_i &= 6 \\ \chi &= 1 - 3 = -2 \\ m^*_{3,3} &= 18 \end{aligned}$$

and

$$\begin{aligned} m_{2,2} &= m^*_{3,3} + 6\chi = 18 - 12 = 6 \\ m_{2,3} &= 4h - 2n_i - 4\chi - 2m^*_{3,3} \\ &= 12(p+q+s) - 84 \\ m_{3,3} &= h + n_i - \chi + m^*_{3,3} \\ &= 3(p+q+s) + 15. \end{aligned}$$

Thus,

$$\begin{aligned} I(G) &= m_{2,2}f(2,2) + m_{2,3}f(2,3) + m_{3,3}f(3,3) \\ &= 6f(2,2) + (12(p+q+s) - 84)f(2,3) + (3(p+q+s)+15)f(3,3) \\ &= (12f(2,3) + 3f(3,3))(p+q+s) + 6f(2,2) - 84f(2,3) + 15f(3,3). \end{aligned}$$

□

Corollary 7. *For $ZCS(p,q,s)$,*

1. $M_1(G) = -306 + 78(p+q+s)$;
2. $M_2(G) = -345 + 99(p+q+s)$;
3. $ReZG_1(G) = -54 + 12(p+q+s)$;
4. $ReZG_2(G) = ISI(G) = -\frac{723}{10} + \frac{189}{10}(p+q+s)$;
5. $ReZG_3(G) = -1614 + 522(p+q+s)$;
6. $R(G) = 8 - 14\sqrt{6} + (1+2\sqrt{6})(p+q+s)$;
7. $RR(G) = 57 - 84\sqrt{6} + (9+12\sqrt{6})(p+q+s)$;
8. $R_\alpha(G) = 6 \cdot 4^\alpha + 12(p+q+s-7)6^\alpha + 3(p+q+s+5)9^\alpha$;
9. $RM_2(G) = -102 + 36(p+q+s)$;
10. $M_{\{\alpha,\beta\}} = 12 \cdot 2^{\alpha+\beta} + 12(p+q+s-7)(2^\alpha 3^\beta + 3^\alpha 2^\beta) + 6(p+q+s+5)3^{\alpha+\beta}$;
11. $RRR(G) = 36 - 84\sqrt{2} + (6+12\sqrt{2})(p+q+s)$;
12. $R'(G) = -20 + 5(p+q+s)$;
13. $\chi(G) = 3 + \frac{5\sqrt{6}}{2} - \frac{84\sqrt{5}}{5} + (\frac{\sqrt{6}}{2} + \frac{12\sqrt{5}}{5})(p+q+s)$;
14. $\chi_\alpha(G) = 6 \cdot 4^\alpha + 12(p+q+s-7)5^\alpha + 3(p+q+s+5)6^\alpha$;
15. $GA(G) = 21 - \frac{168\sqrt{6}}{5} + (3 + \frac{24\sqrt{6}}{5})(p+q+s)$;
16. $SDD(G) = -140 + 32(p+q+s)$;
17. $ABC(G) = -78 + 10\sqrt{2} + (12+2\sqrt{2})(p+q+s)$;
18. $H(G) = -\frac{128}{5} + \frac{29}{5}(p+q+s)$;

19. $AZI(G) = -\frac{29001}{64} + \frac{8331}{64}(p+q+s)$;

20. $F(G) = -774 + 210(p+q+s)$;

21. $SO(G) = 57\sqrt{2} - 84\sqrt{13} + (9\sqrt{2} + 12\sqrt{13})(p+q+s)$;

22. $RSO(G) = 36\sqrt{2} - 84\sqrt{5} + (6\sqrt{2} + 12\sqrt{5})(p+q+s)$;

23. $M_3(G) = -84 + 12(p+q+s)$;

24. $Pl(G) = -180 + 48(p+q+s)$;

25. ${}^{m}M_1(G) = -11 + \frac{13}{6}(p+q+s)$;

26. ${}^{m}M_2(G) = -\frac{65}{6} + \frac{7}{3}(p+q+s)$;

27. $HM(G) = -1464 + 408(p+q+s)$;

28. $M_\alpha(G) = 12 \cdot 2^{\alpha-1} + 12(p+q+s-7)(2^{\alpha-1} + 3^{\alpha-1}) + 6(p+q+s+5)3^{\alpha-1}$;

29. $IM_3(G) = -84 + 12(p+q+s)$;

30. $\sigma(G) = -84 + 12(p+q+s)$.

Proof. Direct computation. □

3.2 Vertex-Degree-Based Topological Indices of $K_1(k, p, q, r)$

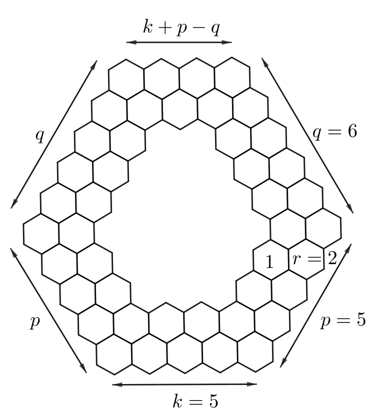


Figure 3: The graph of $K_1(5, 5, 6, 2)$.

Proposition 8. *If G is the graph of $K_1(k,p,q,r)$, then*

$$\begin{array}{rcl} I(G) & = & 6f(2,2) - 24f(2,3) + 12f(3,3) + \\ & & (12f(2,3) - 6f(3,3))p + (4f(2,3) - 2f(3,3))q + \\ & & (8f(2,3) - 4f(3,3))k - (12f(2,3) + 3f(3,3))r + \\ & & 6f(3,3)kr + 9f(3,3)pr + 3f(3,3)qr - 9f(3,3)r^2 \end{array}$$

for any vertex-degree-based topological index $I(G)$ induced by f.

Proof. Using Proposition 5, we have that

$$\begin{array}{rcl} n_2 & = & 2p + 2q + k + (k + p - q) + \\ & & 2(p - r - 1) + 2(q - r - 1) + (k - r - 1) + (k + p - q - r - 1) \\ & = & 2(3p + q + 2k) - 6r - 6 \\ h & = & 2p + 2q + k + k + p - q - 6 + \\ & & 2(p - 1) + 2(q - 1) + k - 1 + k + p - q - 1 - 6 + \\ & & \ldots \\ & & 2(p - r + 1) + 2(q - r + 1) + (k - r + 1) + (k + p - q - r - 1) - 6 \\ & = & 3p + 2k + q - 6 + \\ & & 3p + 2k + q - 12 + \\ & & \ldots \\ & & 3p + 2k + q - 6r \\ & = & r(3p + 2k + q) - 6(1 + 2 + \ldots + r) \\ & = & r(3p + 2k + q) - 3r(r + 1) \\ \chi & = & 1 - 1 = 0 \end{array}$$

and

$$\begin{array}{rcl} m_{2,2} & = & 6 \\ m_{2,3} & = & 2n_2 - 2m_{2,2} \\ & = & 4(3p + 2k + q) - 12r - 24 \\ m_{3,3} & = & 3h - n_2 + m_{2,2} - 3\chi \\ & = & (3p + 2k + q)(3r - 2) - 9r^2 - 3r + 12 \end{array}$$

Thus,

$$\begin{array}{rcl} I(G) & = & m_{2,2}f(2,2) + m_{2,3}f(2,3) + m_{3,3}f(3,3) \\ & = & 6f(2,2) + (4(3p + 2k + q) - 12r - 24)f(2,3) + \\ & & ((3p + 2k + q)(3r - 2) - 9r^2 - 3r + 12)f(3,3) \\ & = & 6f(2,2) - 24f(2,3) + 12f(3,3) + \\ & & (12f(2,3) - 6f(3,3))p + (4f(2,3) - 2f(3,3))q + \\ & & (8f(2,3) - 4f(3,3))k - (12f(2,3) + 3f(3,3))r + \\ & & 6f(3,3)kr + 9f(3,3)pr + 3f(3,3)qr - 9f(3,3)r^2. \end{array}$$

□

Corollary 9. *For $K_1(k,p,q,r)$,*

1. $M_1(G) = -24 + 16k + 24p + 8q - 78r + 36kr + 54pr + 18qr - 54r^2$;
2. $M_2(G) = -12 + 12k + 18p + 6q - 99r + 54kr + 81pr + 27qr - 81r^2$;

3. $ReZG_1(G) = -6 + 4k + 6p + 2q - 12r + 4kr + 6pr + 2qr - 6r^2$;

4. $ReZG_2(G) = ISI(G) = -\frac{24}{5} + \frac{18}{5}k + \frac{27}{5}p + \frac{9}{5}q - \frac{189}{10}r + 9kr + \frac{27}{2}pr + \frac{9}{2}qr - \frac{27}{2}r^2$;

5. $ReZG_3(G) = 24 + 24k + 36p + 12q - 522r + 324kr + 486pr + 162qr - 486r^2$;

6. $R(G) = 7 - 4\sqrt{6} + (-\frac{4}{3} + \frac{4\sqrt{6}}{3})k + (-2 + 2\sqrt{6})p + (-\frac{2}{3} + \frac{2\sqrt{6}}{3})q + (-1 - 2\sqrt{6})r + 2kr + 3pr + qr - 3r^2$;

7. $RR(G) = 48 - 24\sqrt{6} + (-12 + 8\sqrt{6})k + (-18 + 12\sqrt{6})p + (-6 + 4\sqrt{6})q + (-9 - 12\sqrt{6})r + 18kr + 27pr + 9qr - 27r^2$;

8. $R_\alpha(G) = ((3p+2n+q)(3r-2) - 9r^2 - 3r + 12)9^\alpha + 4(3p+2n+q-3r-6)6^\alpha + 6 \cdot 4^\alpha$;

9. $RM_2(G) = 6 - 36r + 24kr + 36pr + 12qr - 36r^2$;

10. $M_{\{\alpha,\beta\}} = 2((3p+2n+q)(3r-2) - 9r^2 - 3r + 12)3^{\alpha+\beta} + 4(3p + 2n + q - 3r - 6)(2^\alpha 3^\beta + 3^\alpha 2^\beta) + 12 \cdot 2^{\alpha+\beta}$;

11. $RRR(G) = 30 - 24\sqrt{2} + (-8 + 8\sqrt{2})k + (-12 + 12\sqrt{2})p + (-4 + 4\sqrt{2})q + (-6 - 12\sqrt{2})r + 12kr + 18pr + 6qr - 18r^2$;

12. $R'(G) = -1 + \frac{4}{3}k + 2p + \frac{2}{3}q - 5r + 2kr + 3pr + qr - 3r^2$;

13. $\chi(G) = 3 - \frac{24\sqrt{5}}{5} + 2\sqrt{6} + (-\frac{2\sqrt{6}}{3} + \frac{8\sqrt{5}}{5})k + (\frac{12\sqrt{5}}{5} - \sqrt{6})p + (-\frac{\sqrt{6}}{3} + \frac{4\sqrt{5}}{5})q + (-\frac{\sqrt{6}}{2} - \frac{12\sqrt{5}}{5})r + \sqrt{6}kr + \frac{3\sqrt{6}}{2}pr + \frac{\sqrt{6}}{2}qr - \frac{3\sqrt{6}}{2}r^2$;

14. $\chi_\alpha(G) = ((3p+2n+q)(3r-2) - 9r^2 - 3r + 12)6^\alpha + 4(3p+2n+q-3r-6)5^\alpha + 6 \cdot 4^\alpha$;

15. $GA(G) = 18 - \frac{48\sqrt{6}}{5} + (-4 + \frac{16\sqrt{6}}{5})k + (-6 + \frac{24\sqrt{6}}{5})p + (-2 + \frac{8\sqrt{6}}{5})q + (-3 - \frac{24\sqrt{6}}{5})r + 6kr + 9pr + 3qr - 9r^2$;

16. $SDD(G) = -16 + \frac{28}{3}k + 14p + \frac{14}{3}q - 32r + 12kr + 18pr + 6qr - 18r^2$;

17. $ABC(G) = -18 + 8\sqrt{2} + (8 - \frac{8\sqrt{2}}{3})k + (12 - 4\sqrt{2})p + (4 - \frac{4\sqrt{2}}{3})q + (-12 - 2\sqrt{2})r + 4\sqrt{2}kr + 6\sqrt{2}pr + 2\sqrt{2}qr - 6\sqrt{2}r^2$;

18. $H(G) = -\frac{13}{5} + \frac{28}{15}k + \frac{14}{5}p + \frac{14}{15}q - \frac{29}{5}r + 2kr + 3pr + qr - 3r^2$;

19. $AZI(G) = -\frac{117}{16} + \frac{295}{16}k + \frac{885}{32}p + \frac{295}{32}q - \frac{8331}{64}r + \frac{2187}{32}kr + \frac{6561}{64}pr + \frac{2187}{64}qr - \frac{6561}{64}r^2$;

20. $F(G) = -48 + 32k + 48p + 16q - 210r + 108kr + 162pr + 54qr - 162r^2$;

21. $SO(G) = 48\sqrt{2} - 24\sqrt{13} + (-12\sqrt{2} + 8\sqrt{13})k + (-18\sqrt{2} + 12\sqrt{13})p + (-6\sqrt{2} + 4\sqrt{13})q + (-9\sqrt{2} - 12\sqrt{13})r + 18\sqrt{2}kr + 27\sqrt{2}pr + 9\sqrt{2}qr - 27\sqrt{2}r^2$;

22. $RSO(G) = 30\sqrt{2} - 24\sqrt{5} + (-8\sqrt{2} + 8\sqrt{5})k + (-12\sqrt{2} + 12\sqrt{5})p + (-4\sqrt{2} + 4\sqrt{5})q + (-6\sqrt{2} - 12\sqrt{5})r + 12\sqrt{2}kr + 18\sqrt{2}pr + 6\sqrt{2}qr - 18\sqrt{2}r^2$;

23. $M_3(G) = -24 + 8k + 12p + 4q - 12r$;

24. $Pl(G) = -12 + 8k + 12p + 4q - 48r + 24kr + 36pr + 12qr - 36r^2$;

25. ${}^{m}M_1(G) = -\frac{3}{2} + k + \frac{3}{2}p + \frac{1}{2}q - \frac{13}{6}r + \frac{4}{9}kr + \frac{2}{3}pr + \frac{2}{9}qr - \frac{2}{3}r^2$;

26. ${}^{m}M_2(G) = -\frac{7}{6} + \frac{8}{9}k + \frac{4}{3}p + \frac{4}{9}q - \frac{7}{3}r + \frac{2}{3}kr + pr + \frac{1}{3}qr - r^2$;

27. $HM(G) = -72 + 56k + 84p + 28q - 408r + 216kr + 324pr + 108qr - 324r^2$;

28. $M_\alpha(G) = 2((3p+2n+q)(3r-2) - 9r^2 - 3r + 12)3^{\alpha-1} + 4(3p+2n+q-3r-6)(2^{\alpha-1} + 3^{\alpha-1}) + 12 \cdot 2^{\alpha-1}$;

29. $IM_3(G) = -24 + 8k + 12p + 4q - 12r$;

30. $\sigma(G) = -24 + 8k + 12p + 4q - 12r$.

Proof. Direct computation. □

3.3 Vertex-Degree-Based Topological Indices of $K_2(k, p, q, r)$

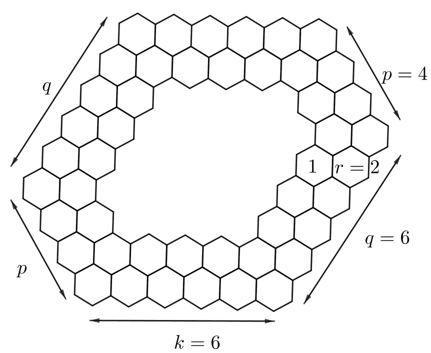


Figure 4: The graph of $K_2(6, 4, 6, 2)$

Proposition 10. *If G is the graph of $K_2(k, p, q, r)$, then*

$$\begin{array}{rcl} I(G) & = & 6f(2,2) - 24f(2,3) + 12f(3,3)+ \\ & & (8f(2,3) - 4f(3,3))(p+q+k) + 6f(3,3)(pr+qr+kr)- \\ & & (12f(2,3) + 3f(3,3))r - 9f(3,3)r^2. \end{array}$$

for any vertex-degree-based topological index $I(G)$ induced by f.

Proof. Using Proposition 5. we have that

$$\begin{array}{rcl} n_2 & = & 2p+2q+2k \\ & & 2(p-r-1)+2(q-r-1)+2(k-r-1) \\ & = & 4(p+q+k)-6r-6 \\ h & = & 2p+2q+2k-6+ \\ & & 2(p-1)+2(q-1)+2(k-1)-6+ \\ & & ... \\ & & 2(p-r+1)+2(q-r+1)+2(k-r+1)-6 \\ & = & 2p+2q+2k-6+ \\ & & 2p+2q+2k-12+ \\ & & ... \\ & & 2p+2q+2k-6r \\ & = & r(2p+2q+2k)-6(1+2+...+r) \\ & = & 2r(p+q+k)-3r^2-3r \\ \chi & = & 1-1=0 \end{array}$$

and

$$\begin{array}{rcl} m_{2,2} & = & 6 \\ m_{2,3} & = & 2n_2-2m_{2,2} \\ & = & 8(p+q+k)-12r-24 \\ m_{3,3} & = & 3h-n_2+m_{2,2}-3\chi \\ & = & 2(p+q+k)(3r-2)-9r^2-3r+12. \end{array}$$

Thus,

$$\begin{array}{rcl} I(G) & = & m_{2,2}f(2,2)+m_{2,3}f(2,3)+m_{3,3}f(3,3) \\ & = & 6f(2,2)+(8(p+q+k)-12r-24)f(2,3)+ \\ & & (2(p+q+k)(3r-2)-9r^2-3r+12)f(3,3) \\ & = & 6f(2,2)-24f(2,3)+12f(3,3)+ \\ & & (8f(2,3)-4f(3,3))(p+q+k)+6f(3,3)(pr+qr+kr)- \\ & & (12f(2,3)+3f(3,3))r-9f(3,3)r^2. \end{array}$$

□

Corollary 11. *For* $K_2(k,p,q,r)$,

1. $M_1(G) = -24+16k+16p+16q-78r+36kr+36pr+36qr-54r^2$;
2. $M_2(G) = -12+12k+12p+12q-99r+54kr+54pr+54qr-81r^2$;
3. $ReZG_1(G) = -6+4k+4p+4q-12r+4kr+4pr+4qr-6r^2$;
4. $ReZG_2(G) = ISI(G) = -\frac{24}{5}+\frac{18}{5}k+\frac{18}{5}p+\frac{18}{5}q-\frac{189}{10}r+9kr+9pr+9qr-\frac{27}{2}r^2$;
5. $ReZG_3(G) = 24+24k+24p+24q-522r+324kr+324pr+324qr-486r^2$;
6. $R(G) = 7-4\sqrt{6}+(-\frac{4}{3}+\frac{4\sqrt{6}}{3})k+(-\frac{4}{3}+\frac{4\sqrt{6}}{3})p+(-\frac{4}{3}+\frac{4\sqrt{6}}{3})q+(-1-2\sqrt{6})r+2kr+2pr+2qr-3r^2$;

7. $RR(G) = 48 - 24\sqrt{6} + (-12 + 8\sqrt{6})k + (-12 + 8\sqrt{6})p + (-12 + 8\sqrt{6})q + (-9 - 12\sqrt{6})r + 18kr + 18pr + 18qr - 27r^2$;

8. $R_\alpha(G) = 6 \cdot 4^\alpha + (8(p+q+k) - 12r - 24)6^\alpha + (2(p+q+k)(3r-2) - 9r^2 - 3r + 12)9^\alpha$;

9. $RM_2(G) = 6 - 36r + 24kr + 24pr + 24qr - 36r^2$;

10. $M_{\{\alpha,\beta\}} = 12 \cdot 2^{\alpha+\beta} + (8(p+q+k) - 12r - 24)(2^\alpha 3^\beta + 3^\alpha 2^\beta) + 2(2(p+q+k)(3 * r - 2) - 9r^2 - 3r + 12)3^{\alpha+\beta}$;

11. $RRR(G) = 30 - 24\sqrt{2} + (-8 + 8\sqrt{2})k + (-8 + 8\sqrt{2})p + (-8 + 8\sqrt{2})q + (-6 - 12\sqrt{2})r + 12kr + 12pr + 12qr - 18r^2$;

12. $R'(G) = -1 + \frac{4}{3}k + \frac{4}{3}p + \frac{4}{3}q - 5r + 2kr + 2pr + 2qr - 3r^2$;

13. $\chi(G) = 3 - \frac{24\sqrt{5}}{5} + 2\sqrt{6} + (-\frac{2\sqrt{6}}{3} + \frac{8\sqrt{5}}{5})k + (-\frac{2\sqrt{6}}{3} + \frac{8\sqrt{5}}{5})p + (-\frac{2\sqrt{6}}{3} + \frac{8\sqrt{5}}{5})q + (-\frac{\sqrt{6}}{2} - \frac{12\sqrt{5}}{5})r + \sqrt{6}kr + \sqrt{6}pr + \sqrt{6}qr - \frac{3\sqrt{6}}{2}r^2$;

14. $\chi_\alpha(G) = 6 \cdot 4^\alpha + (8(p+q+k) - 12r - 24)5^\alpha + (2(p+q+k)(3r-2) - 9r^2 - 3r + 12)6^\alpha$;

15. $GA(G) = 18 - \frac{48\sqrt{6}}{5} + (-4 + \frac{16\sqrt{6}}{5})k + (-4 + \frac{16\sqrt{6}}{5})p + (-4 + \frac{16\sqrt{6}}{5})q + (-3 - \frac{24\sqrt{6}}{5})r + 6kr + 6pr + 6qr - 9r^2$;

16. $SDD(G) = -16 + \frac{28}{3}k + \frac{28}{3}p + \frac{28}{3}q - 32r + 12kr + 12pr + 12qr - 18r^2$;

17. $ABC(G) = -18 + 8\sqrt{2} + (8 - \frac{8\sqrt{2}}{3})k + (8 - \frac{8\sqrt{2}}{3})p + (8 - \frac{8\sqrt{2}}{3})q + (-12 - 2\sqrt{2})r + 4\sqrt{2}kr + 4\sqrt{2}pr + 4\sqrt{2}qr - 6\sqrt{2}r^2$;

18. $H(G) = -\frac{13}{5} + \frac{28}{15}k + \frac{28}{15}p + \frac{28}{15}q - \frac{29}{5}r + 2kr + 2pr + 2qr - 3r^2$;

19. $AZI(G) = -\frac{117}{16} + \frac{295}{16}k + \frac{295}{16}p + \frac{295}{16}q - \frac{8331}{64}r + \frac{2187}{32}kr + \frac{2187}{32}pr + \frac{2187}{32}qr - \frac{6561}{64}r^2$;

20. $F(G) = -48 + 32k + 32p + 32q - 210r + 108kr + 108pr + 108qr - 162r^2$;

21. $SO(G) = 48\sqrt{2} - 24\sqrt{13} + (-12\sqrt{2} + 8\sqrt{13})k + (-12\sqrt{2} + 8\sqrt{13})p + (-12\sqrt{2} + 8\sqrt{13})q + (-9\sqrt{2} - 12\sqrt{13})r + 18\sqrt{2}kr + 18\sqrt{2}pr + 18\sqrt{2}qr - 27\sqrt{2}r^2$;

22. $RSO(G) = 30\sqrt{2} - 24\sqrt{5} + (-8\sqrt{2} + 8\sqrt{5})k + (-8\sqrt{2} + 8\sqrt{5})p + (-8\sqrt{2} + 8\sqrt{5})q + (-6\sqrt{2} - 12\sqrt{5})r + 12\sqrt{2}kr + 12\sqrt{2}pr + 12\sqrt{2}qr - 18\sqrt{2}r^2$;

23. $M_3(G) = -24 + 8k + 8p + 8q - 12r$;

24. $Pl(G) = -12 + 8k + 8p + 8q - 48r + 24kr + 24pr + 24qr - 36r^2$;

25. ${}^mM_1(G) = -\frac{3}{2} + k + p + q - \frac{13}{6}r + \frac{4}{9}kr + \frac{4}{9}pr + \frac{4}{9}qr - \frac{2}{3}r^2$;

26. ${}^mM_2(G) = -\frac{7}{6} + \frac{8}{9}k + \frac{8}{9}p + \frac{8}{9}q - \frac{7}{3}r + \frac{2}{3}kr + \frac{2}{3}pr + \frac{2}{3}qr - r^2$;

27. $HM(G) = -72 + 56k + 56p + 56q - 408r + 216kr + 216pr + 216qr - 324r^2$;

28. $M_\alpha(G) = 12 \cdot 12 \cdot 2^{\alpha-1} + (8(p+q+k) - 12r - 24)(2^{\alpha-1} + 3^{\alpha-1}) + 2(2(p+q+k)(3r-2) - 9r^2 - 3r + 12)3^{\alpha-1}$;

29. $IM_3(G) = -24 + 8k + 8p + 8q - 12r$;

30. $\sigma(G) = -24 + 8k + 8p + 8q - 12r$.

Proof. Direct computation. □

The last two families ($K_1(k,p,q,r)$ and $K_2(k,p,q,r)$) have been investigated in [**29**], however the obtained values for $m_{2,3}$ ($4k+6p+2q+22$ and $4k+4p+4q+24$, respectively) are (incorrectly) independent of the parameter r. We correct this mistake here.

Acknowledgements. This research has been supported by the Science Fund of the Republic of Serbia through PRIZMA program, project "Mathematical Methods in Image Processing under Uncertainty" and the Provincial Secretariat for Higher Education and Scientific Research (AP Vojvodina, Republic of Serbia) through the project no. 142-451-3188/2023-01 "The Application of Aggregation Operators for Face Recognition".

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(Received 01. 09. 2023.)
(Revised 18. 01. 2024.)

Lidija Čomić
Faculty of Technical Sciences,
University of Novi Sad,
Novi Sad, Serbia
E-mail: *comic@uns.ac.rs, lidija.comic@gmail.com*

Nebojša M. Ralević
Faculty of Technical Sciences,
University of Novi Sad,
Novi Sad, Serbia
E-mail: *nralevic@uns.ac.rs*