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

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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  $\beta_0$  connected components,  $\beta_1$  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

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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  $R_{\alpha}$  [5, 6, 30, 31] (variable second Zagreb index  $^{v}M_{2}$  [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  $\chi$  [44]
- 14.  $f(x,y) = (x+y)^{\alpha}$ , for the general sum-connectivity index  $\chi_{\alpha}$  [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  ${}^{m}M_{2}$  [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  $M_{\alpha}$  [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):

(1) 
$$m_{2,2} = 6 + m_{3,3}^* m_{2,3} = 4h - 4 - 2m_{3,3}^* - 2n_i m_{3,3} = h - 1 + m_{3,3}^* + n_i.$$



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):

(2) 
$$m_{2,2} = n - 2h - r + 2 m_{2,3} = 2r m_{3,3} = 3h - r - 3.$$

Interestingly, despite the long history and large body of research on vertexdegree-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 Sinto 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  $\chi$  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:

(3) 
$$m_{2,2} = m_{2,2} m_{2,3} = 2n_2 - 2m_{2,2} m_{3,3} = 3f - n_2 + m_{2,2} - 6,$$

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

$$n_2 + n_3 = n$$
  

$$2m_{2,2} + m_{2,3} = 2n_2$$
  

$$m_{2,3} + 2m_{3,3} = 3n_3$$
  

$$2n_2 + 3n_3 = 2m.$$

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 vertexdegree-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.

Conf.	$\Delta n$	$\Delta m$	$\Delta n_2$	$\Delta n_i$	$\Delta \chi$	$\Delta \tilde{n}$	$\Delta \tilde{m}$	$\Delta \tilde{n}_2$
	6	6	6	0	1	6	6	6
	4	5	2	0	0	4	5	2
	2	4	-2	0	-1	2	4	-2
$\bigcirc$	2	3	0	2	0	2	3	0
$\bigcirc$	0	2	-4	2	-1	0	2	-4
$\bigcirc$	0	1	-2	4	0	0	1	-2
$\bigcirc$	0	0	0	6	1	0	0	0
	2	4	-2	0	-1	2	4	-2
$\bigcirc$	0	3	-6	0	-2	0	3	-6
$\bigcirc$	0	2	-4	2	-1	0	2	-4
	3	4	1	1	0	3	4	1
	1	3	-3	1	-1	1	3	-3
$\bigcirc$	1	2	-1	3	0	1	2	-1

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

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

(4) 
$$n = 4h - n_i + 2\chi$$
$$m = 5h - n_i + \chi$$
$$n_2 = 2h - n_i + 4\chi$$

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  $\Delta q$  we denote q - q'. If  $\Delta q$  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  $\chi$  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  $\beta_0$  by 1) or a hole is created (increasing  $\beta_1$  by 1), thus decreasing  $\chi$  by 1. Thus, for this configuration,  $\Delta n = 2 = \Delta(4h - n_i + 2\chi)$ , and similarly for  $\Delta m$  and  $\Delta n_2$ , as well as for each of the remaining twelve configurations.

Corollary 2.

$$m = n + h - \chi$$

$$n^* = 4h - 2n_i + 2\chi$$

$$n_3 = 2h - 2\chi$$

$$n^*_3 = 2h - n_i - 2\chi$$

$$m_i = h + n_i - \chi$$

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

(5) 
$$m_{2,2} = m_{3,3}^* + 6\chi$$
$$m_{2,3} = 4h - 2n_i - 4\chi - 2m_{3,3}^*$$
$$m_{3,3} = h + n_i - \chi + m_{3,3}^*$$

*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

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

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,

(6) 
$$m_{2,2} = n - 2h - r + 2\chi$$
$$m_{2,3} = 2r$$
$$m_{3,3} = 3h - r - 3\chi$$

*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

(7) 
$$\begin{array}{rcl} m_{2,2} &=& m_{2,2} \\ m_{2,3} &=& 2n_2 - 2m_{2,2} \\ m_{3,3} &=& 3h - n_2 + m_{2,2} - 3\chi \end{array}$$

*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  $\beta_1$  of holes plus 1 for the outer face, and for connected graphs  $\beta_0$  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

$$m_{3,3} = = -n_2 + m_{2,2} + 3m - 3n$$
  
=  $-n_2 + m_{2,2} + \frac{3}{2}n_3$   
=  $-n_2 + m - \frac{1}{2}m_{2,3}.$ 

#### **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

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

and

$$m_{2,2} = m_{3,3}^* + 6\chi = 18 - 12 = 6$$
  

$$m_{2,3} = 4h - 2n_i - 4\chi - 2m_{3,3}^*$$
  

$$= 12(p+q+s) - 84$$
  

$$m_{3,3} = h + n_i - \chi + m_{3,3}^*$$
  

$$= 3(p+q+s) + 15.$$

Thus,

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

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

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



# **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

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

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

Proof. Using Proposition 5, we have that

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

and

$$m_{2,2} = 6$$
  

$$m_{2,3} = 2n_2 - 2m_{2,2}$$
  

$$= 4(3p + 2k + q) - 12r - 24$$
  

$$m_{3,3} = 3h - n_2 + m_{2,2} - 3\chi$$
  

$$= (3p + 2k + q)(3r - 2) - 9r^2 - 3r + 12$$

Thus,

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

**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.  $R(G) = 7 4\sqrt{6} + \left(-\frac{4}{3} + \frac{4\sqrt{6}}{3}\right)k + \left(-2 + 2\sqrt{6}\right)p + \left(-\frac{2}{3} + \frac{2\sqrt{6}}{3}\right)q + \left(-1 2\sqrt{6}\right)r + 2kr + 3pr + qr 3r^2;$
- 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.  $R'(G) = -1 + \frac{4}{3}k + 2p + \frac{2}{3}q 5r + 2kr + 3pr + qr 3r^2;$
- $13. \ \chi(G) = 3 \frac{24\sqrt{5}}{5} + 2\sqrt{6} + \left(-\frac{2\sqrt{6}}{3} + \frac{8\sqrt{5}}{5}\right)k + \left(\frac{12\sqrt{5}}{5} \sqrt{6}\right)p + \left(-\frac{\sqrt{6}}{3} + \frac{4\sqrt{5}}{5}\right)q + \left(-\frac{\sqrt{6}}{2} \frac{12\sqrt{5}}{5}\right)r + \sqrt{6}kr + \frac{3\sqrt{6}}{2}pr + \frac{\sqrt{6}}{2}qr \frac{3\sqrt{6}}{2}r^2;$

14.  $\chi_{\alpha}(G) = ((3p+2n+q)(3r-2)-9r^2-3r+12)6^{\alpha}+4(3p+2n+q-3r-6)5^{\alpha}+6\cdot4^{\alpha};$ 

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

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

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

*Proof.* Using Proposition 5. we have that

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

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,

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

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

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

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

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

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

- $15. \ GA(G) = 18 \frac{48\sqrt{6}}{5} + (-4 + \frac{16\sqrt{6}}{5})k + (-4 + \frac{16\sqrt{6}}{5})p + (-4 + \frac{16\sqrt{6}}{5})q + (-3 \frac{24\sqrt{6}}{5})r + 6kr + 6pr + 6qr 9r^2;$
- 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.  $F(G) = -48 + 32k + 32p + 32q 210r + 108kr + 108pr + 108qr 162r^2;$
- $\begin{array}{l} 21. \ SO(G) = 48\sqrt{2} 24\sqrt{13} + (-12\sqrt{2} + 8\sqrt{13})k + (-12\sqrt{2} + 8\sqrt{13})p + (-12\sqrt{2} + 8\sqrt{13})p + (-12\sqrt{2} + 8\sqrt{13})q + (-9\sqrt{2} 12\sqrt{13})r + 18\sqrt{2}kr + 18\sqrt{2}pr + 18\sqrt{2}qr 27\sqrt{2}r^2; \end{array}$
- 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.  ${}^{m}M_{1}(G) = -\frac{3}{2} + k + p + q \frac{13}{6}r + \frac{4}{9}kr + \frac{4}{9}pr + \frac{4}{9}qr \frac{2}{3}r^{2};$
- 26.  ${}^{m}M_2(G) = -\frac{7}{6} + \frac{8}{9}k + \frac{8}{9}p + \frac{8}{9}q \frac{7}{3}r + \frac{2}{3}kr + \frac{2}{3}pr + \frac{2}{3}qr r^2;$
- 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  $(K_1(k, p, q, r) \text{ and } K_2(k, p, q, r))$  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.

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