The 10th Conference on Mathematics in Engineering: Theory and Applications
Novi Sad, December 12-14th 2025

SOME VERTEX-DEGREE-BASED TOPOLOGICAL INDICES OF CATACONDENSED CORONOIDS

Lidija Čomić[1] and Nebojša Ralević[2]

https://doi.org/10.24867/META.2025.04 Short communication

Abstract. We compute several vertex-degree-based topological indices of graphs defined by catacondensed coronoid systems. We do this by using our recently proposed formulae for graphs defined by finite sets of hexagons of arbitrary topology in the hexagonal grid, and the associated M-polynomial.

AMS Mathematics Subject Classification (2020): 05C09, 05C92

Key words and phrases: topological graph indexes, vertex-degree-based indexes, M-polynomial, catacondensed coronoids

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 $\chi = \beta_0 - \beta_1$. 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, such sets are used to model molecules. Simply connected sets S are called benzenoid systems [6], and connected sets with one hole are coronoid systems [4].

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 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 number of boundary edges of type 3,3 is denoted by $m^*_{3,3}$. Non-boundary vertices are called interior. Their number is denoted by n_i.

A topological index of a graph G is a real number associated with G. The general form of a vertex-degree-based topological index $I(G)$ of a graph G is given by

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

[1]Department of Fundamental Sciences, Faculty of Technical Sciences, University of Novi Sad, e-mail: comic@uns.ac.rs

[2]Department of Fundamental Sciences, Faculty of Technical Sciences, University of Novi Sad, e-mail: nralevic@uns.ac.rs

where f is a real function such that $f(x,y) = f(y,x)$. Several dozens of well-known indices have been defined, varying over the choices of f. In chemical graph theory, graph indices have been repeatedly shown to be apt for describing and predicting chemical, physical and biological properties of associated chemical compounds.

We will consider five such indices, obtained by choosing f as follows:

1. $f(x,y) = x + y$ for the first Zagreb index M_1 [8],
2. $f(x,y) = xy$ for the second Zagreb index M_2 [7],
3. $f(x,y) = (xy)^\alpha$, $\alpha \in \mathbb{N}$, for the general Randić index R_α (variable second Zagreb index ${}^vM_2$ [9]),
4. $f(x,y) = 1/(xy)$ for the second modified Zagreb index ${}^mM_2$ (first order overall index [1]),
5. $f(x,y) = \frac{x^2+y^2}{xy} = \frac{x}{y} + \frac{y}{x}$ for the symmetric division deg index SDD [10].

It is well known [5] that these indices can alternatively be obtained from the M-polynomial

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

of G through differentiation or integration as follows

1. $M_1 = (D_x + D_y)(M(x,y))|_{x=y=1}$,
2. $M_2 = (D_xD_y)(M(x,y))|_{x=y=1}$,
3. $R_\alpha =^v M_2 = (D_x^\alpha D_y^\alpha)(M(x,y))|_{x=y=1}$,
4. ${}^mM_2 = (S_xS_y)(M(x,y))|_{x=y=1}$
5. $SDD = (D_xS_y + D_yS_x)(M(x,y))|_{x=y=1}$,

where

$$D_x(M(x,y)) = x\frac{\partial M(x,y)}{\partial x},\ D_y(M(x,y)) = y\frac{\partial M(x,y)}{\partial y},$$

and

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

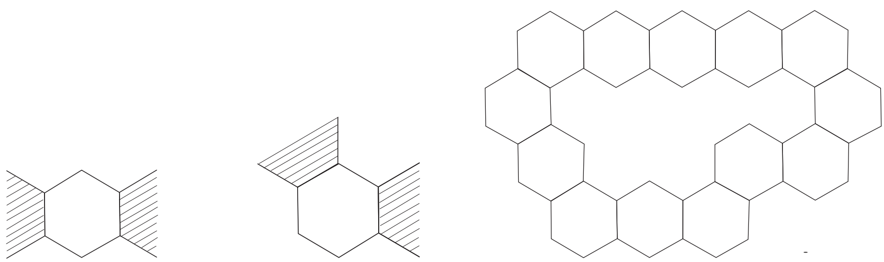
For simply connected sets S, there are different formulas for $m_{2,2}$, $m_{2,3}$ and $m_{3,3}$ in terms of other, easier to determine and chemically significant, graph invariants [6]. Interestingly, despite the long history and large body of research on vertex-degree-based topological indices for simply connected sets S, these formulae have only recently been extended to sets S of arbitrary topology by the present authors [2] as follows:

$$(1.1)\qquad \begin{aligned} m_{2,2} &= m^*_{3,3} + 6\chi \\ m_{2,3} &= 4h - 2n_i - 4\chi - 2m^*_{3,3} \\ m_{3,3} &= h + n_i - \chi + m^*_{3,3} \end{aligned}$$

Here, we further demonstrate the versatility of our formulae by determining the numbers $m_{2,2}$, $m_{2,3}$, $m_{3,3}$, the M-polynomial and the associated indices for catacondensed coronoid systems.

2. Vertex-degree-based topological indices of catacondensed coronoid systems

Catacondensed coronoid system S has exactly one hole and no inner vertices (thus, $\chi = 1 - 1 = 0$ and $n_i = 0$). The hexagons in S are in one of the two configurations, called L_2 (linear) and A_2 (angle or corner), as illustrated in Figure 1 (a). They can be cyclically ordered so that each hexagon shares an edge with the previous and the next one, and there are no more adjacencies among the hexagons in S (see Figure 1 (b)).



(a) (b)

Figure 1: (a) A linear (left) and corner (right) hexagon. (b) A coronoid system with $a = 8$ and $l = 5$.

We will obtain the M-polynomial and the associated indices of a catacondensed coronoid system with h hexagons, among which there are a corners and $l = h - a$ linear hexagons.

Theorem 2.1. *For the graph G of a catacondensed coronoid system with a corners and l linear hexagons, it holds*

$$M(G) = ax^2y^2 + (2a + 4l)x^2y^3 + (2a + l)x^3y^3.$$

Proof. We have that

$$\begin{aligned} m_{2,2} &= m^*_{3,3} = a \\ m_{2,3} &= 4h - 2m_{2,2} = 4h - 2a = 2a + 4l \\ m_{3,3} &= h + m_{2,2} = h + a = 2a + l \end{aligned}$$

The first equality follows from (1.1), and the fact that type 2,2 and type 3,3 edges come in pairs which belong to corner hexagons (see Figure 1 (a)). The second and third equalities follow from the first one and from (1.1).

□

Corollary 2.2. *For the graph of a catacondensed coronoid system, it holds*

$$\begin{aligned} M_1 &= (D_x + D_y)(M(x,y))|_{x=y=1} \\ &= 4a + 5(2a+4l) + 6(2a+l) \\ &= 26a + 26l, \end{aligned}$$

$$\begin{aligned} M_2 &= (D_x D_y)(M(x,y))|_{x=y=1} \\ &= D_x(2ax^2y^2 + 3(2a+4l)x^2y^3 + 3(2a+l)x^3y^3)|_{x=y=1} \\ &= (4ax^2y^2 + 6(2a+4l)x^2y^3 + 9(2a+l)x^3y^3)|_{x=y=1} \\ &= 34a + 33l, \end{aligned}$$

$$\begin{aligned} R_\alpha &= (D_x^\alpha D_y^\alpha)(M(x,y))|_{x=y=1} \\ &= D_x(2^\alpha ax^2y^2 + 3^\alpha(2a+4l) + 3^\alpha(2a+l)x^3y^3)|_{x=y=1} \\ &= (4^\alpha ax^2y^2 + 6^\alpha(2a+4l)x^2y^3 + 9^\alpha(2a+l)x^3y^3)|_{x=y=1} \\ &= (4^\alpha + 2\cdot 6^\alpha + 2\cdot 9^\alpha)a + (4\cdot 6^\alpha + 9^\alpha)l, \end{aligned}$$

$$\begin{aligned} {}^mM_2 &= (S_x S_y)(M(x,y))|_{x=y=1} \\ &= S_x(\int_0^y (ax^2t + (2a+4l)x^2t^2 + (2a+l)x^3t^2)dt)|_{x=y=1} \\ &= S_x((\tfrac{1}{2}ax^2y^2 + \tfrac{1}{3}(2a+4l)x^2y^3 + \tfrac{1}{3}(2a+l)x^3y^3))|_{x=y=1} \\ &= (\int_0^x (\tfrac{1}{2}aty^2 + \tfrac{1}{3}(2a+4l)ty^3 + \tfrac{1}{3}(2a+l)t^2y^3)dt)|_{x=y=1} \\ &= (\tfrac{1}{4}ax^2y^2 + \tfrac{1}{6}(2a+4l)x^2y^3 + \tfrac{1}{9}(2a+l)x^3y^3))|_{x=y=1} \\ &= \tfrac{29}{36}a + \tfrac{7}{9}l, \end{aligned}$$

$$\begin{aligned} SDD &= (D_xS_y + D_yS_x)(M(x,y))|_{x=y=1} \\ &= (D_x(\tfrac{1}{2}ax^2y^2 + \tfrac{1}{3}(2a+4l)x^2y^3 + \tfrac{1}{3}(2a+l)x^3y^3) + \\ &\quad D_y(\tfrac{1}{2}ax^2y^2 + \tfrac{1}{2}(2a+4l)x^2y^3 + \tfrac{1}{3}(2a+l)x^3y^3))|_{x=y=1} \\ &= (ax^2y^2 + \tfrac{2}{3}(2a+4l)x^2y^3 + (2a+l)x^3y^3 + \\ &\quad ax^2y^2 + \tfrac{3}{2}(2a+4l)x^2y^3 + (2a+l)x^3y^3))|_{x=y=1} \\ &= (a + \tfrac{2}{3}(2a+4l) + (2a+l) + a + \tfrac{3}{2}(2a+4l) + (2a+l) \\ &= \tfrac{31}{3}a + \tfrac{32}{3}l. \end{aligned}$$

3. Discussion

We have determined several vertex-degree-based indices of catacondensed coronoid systems using our recently proposed formulae [2] and the associated M-polynomial. In that way, we extended our previous work on a special class of such systems, called fenestrenes [3]. We are currently working on developing analogous formulae for other chemically significant grids, which have been completely neglected in this regard despite considerable amount of attention given to the hexagonal grid.

Acknowledgement

This work has been partially supported by the Science Fund of the Republic of Serbia, #GRANT no. 7632, the project "Mathematical Methods in Image Processing under Uncertainty" MaMIPU and by the project "Socio-technological aspects of improving the teaching process in the English language in fundamental disciplines".

References

[1] D. Bonchev, "Overall connectivity - a next generation molecular connectivity", *Journal of Molecular Graphics and Modelling*, 20, pp. 65-75, 2001.

[2] L. Čomić and N. Ralević, "Vertex-Degree-Based Topological Indices of Arbitrary Sets of Hexagons in the Regular Hexagonal Grid", *Applicable Analysis and Discrete Mathematics*, 2024.

[3] L. Čomić, N. Ralević, and S. Tošić, "Vertex-degree-based topological indices of fenestrene", In *The 6th Conference on Mathematics in Engineering: Theory and Applications, Novi Sad*, pp. 75-79, 2021.

[4] S. J. Cyvin, J. Brunvoll, and B. N. Cyvin, , *Theory of Coronoid Hydrocarbons*, volume 54 of *Lecture Notes in Chemistry*, Springer-Verlag, Berlin Heidelberg, 1991.

[5] E. Deutsch and S. Klavžar, "M-Polynomial and Degree-Based Topological Indices", *Iranian Journal of Mathematical Chemistry*, 6(2), pp. 93-102, 2015.

[6] I. Gutman and S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, 1989.

[7] I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes", *Journal of Chemical Physics*, 62, pp. 3399-3405, 1975.

[8] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons", *Chemical Physics Letters*, 17, pp. 535-538, 1972.

[9] A. Miličević and S. Nikolić, "On Variable Zagreb Indices", *Croatica Chemica Acta*, 77(1-2), pp. 97-101, 2004.

[10] D. Vukičević and M. Gašperov, "Bond Additive Modeling 1. Adriatic Indices", *Croatica Chemica Acta*, 83(3), pp. 243-260, 2010.