Received: 01 June 2021 | Revised: 30 July 2021 | Accepted: 02 August 2021
DOI: 10.22034/ecc.2021.293152.1193
Eurasian Chemical Communications SAMI

FULL PAPER

Topological analysis of zigzag-edge coronoid graph by using M-polynomial

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The chemical graph theory is interrelated with the chemical structure of different compounds. This graph represents the molecule of the sub-stance. A chemical graph is rehabilitated into a real number by applying some mathematical tackles. This number can elaborate on the properties of the molecule. This number is called topological catalogs. Here, we find some topological catalogs *via* M-polynomial for the zigzag-edge coronoid graph.

KEYWORDS

Molecular graph; nanotube; M-polynomial; zigzag-edge coronoid; topological indices.

Introduction

Topological indices [1-10] in theoretical chemistry has drawn a great interest. The topological indices help us to recognize the different sorts of chemical substances. The topological index has a basic role that shows the chemical building to a mathematical number which is used to explain a molecule under testing.

Topological indices [11-18] are calculated from their definition; however, these are also calculated by using their M-polynomial. M-polynomial is also graph demonstrative mathematical object. By using M-polynomial, we work out various degree dependent topological invariant present in Table 2.

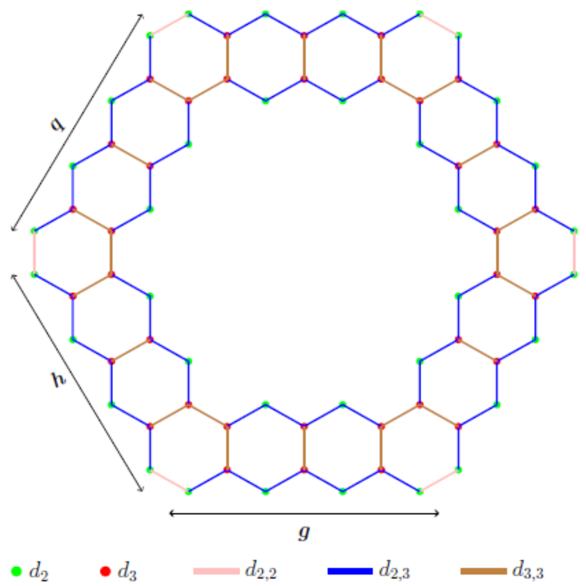


FIGURE 1 Zigzag-edge coronoid ZC(g,h,q)

The M-polynomial introduced for a graph G is defined as [19]:

$$M(G,x,y)=\sum_{\delta\le i\le j\le\Delta} m_{ij}(G)x^i y^j$$

Where $\delta=min\{d_v/v\in V(G)\}$, $\Delta=max\{d_v/v\in V(G)\}$ and $m_{ij}(G)$ is the number of edges vu∈E(G) such that $\{d_v;d_u\}=\{i;j\}$.

TABLE 1 Edge divider of zigzag-edge coronoid Graph ZC(g,h,q)

(d_u; d_v)	**Number of edges**
(2,2)	6
(2,3)	8(g +h+ q)-36
(3,3)	2(g+ h+ q)
Total edges	10(g +h+ q)-30

Table 3 represents some well-known degree based topological directories to compute through M-Polynomial. M-polynomial of many graphs were introduced in the past [20-30]. In the current work, we add M-polynomials and topological indices [31-33] of ZC(g,h,q), Figure 1, of the zigzag-edge coronoid ZC(g,h,q), can be considered as a structure obtained by fusing three linear polyenes of length *g*; *h* and *q*, respectively.

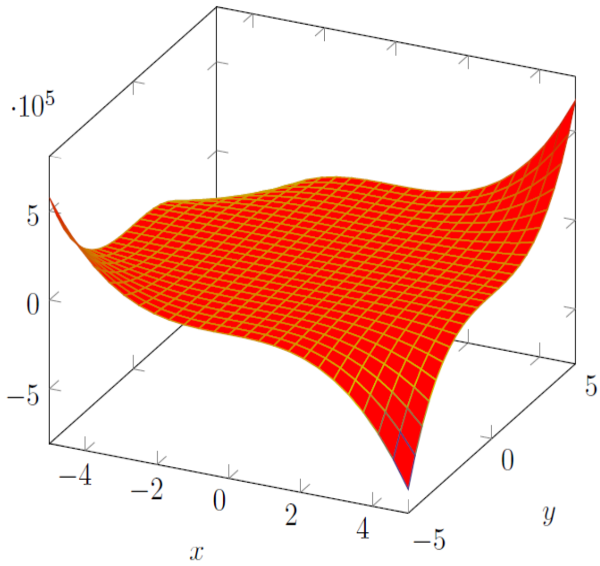


FIGURE 2 3D sketch the M-polynomial of the zigzag-edge coronoid ZC(g,h,q) for g=h=q=4

TABLE 2 Degree dependent topological directories

Topological index	**Derivation from M(G; x, y)**		
First Zegreb index	$M_1[ZC(g,h,q)]$	=	$(D_x+D_y)[f(x;y)]_{x=y=1}$
Second Zagreb index	$M_2[ZC(g,h,q)]$	=	$(D_x.D_y)[f(x;y)]_{x=y=1}$
Modified second Zagreb index	$^mM_2[ZC(g,h,q)]$	=	$(S_xS_y)[f(x;y)]_{x=y=1}$
General Randić Index	$R_\alpha[ZC(g,h,q)]$	=	$(D_x^\alpha D_y^\alpha)[f(x;y)]_{x=y=1}$
Inverse Randić Index	$RR_\alpha[ZC(g,h,q)]$	=	$(S_x^\alpha S_y^\alpha)[f(x;y)]_{x=y=1}$
Symmetric division index	$SSD[ZC(g,h,q)]$	=	$(D_xS_y+S_xD_y)[f(x;y)]_{x=y=1}$
Harmonic index	$H[ZC(g,h,q)]$	=	$2S_xJ[f(x;y)]_{x=1}$
Inverse sum index	$I[ZC(g,h,q)]$	=	$S_xJD_xD_y[f(x;y)]_{x=1}$
Augmented Zagreb index	$A[ZC(g,h,q)]$	=	$S_x^3Q_{-2}JD_x^3D_y^3[f(x;y)]_{x=1}$

Where the operator used are defined as

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

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

$$Q_\alpha f(x,y) = x^\alpha f(x,y),$$

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

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

$$Jf(x,y) = f(x,x).$$

M-Polynomial of zigzag-edge coronoid graph

Theorem 3.1. If Zigzag-edge coronoid is denoted by ZC(g,h,q), then for g,h,q≥3, its M-polynomial is

M[ZC(g,h,q),x,y]

$=6x^2y^2+(8(g+h+q)-36)x^2y^3+2(g+h+q)x^3y^3$

Proof. Let ZC(g,h,q) be a Zigzag-edge coronoid, then from Table1 and figure1 the Edge partition of ZC(g,h,q) is

$E_{2;2}(ZC(g,h,q))=\{e=uv\in ZC(g,h,q):\ d_u=2;\ d_v=2\} \rightarrow |E_{2;2}ZC(g,h,q)|=6$

$E_{2;3}(ZC(g,h,q))=\{e=uv\in ZC(g,h,q):\ d_u=2;\ d_v=3\} \rightarrow |E_{2;3}ZC(g,h,q)|=(8(g+h+q)-36)$

$E_{3;3}ZC(g,h,q))=\{e=uv\in ZC(g,h,q):\ d_u=3;\ d_v=3\} \rightarrow |E_{3;3}ZC(g,h,q)|=2(g+h+q)$

$$M[ZC(g,h,q);x,y] = \sum_{\delta\le i\le j\le\Delta} m_{ij}[ZC(g,h,q)]x^i y^j = \sum_{2\le i\le j\le 3} m_{ij}[ZC(g,h,q)]x^i y^j$$

$$= \sum_{2\le 2} m_{22}[ZC(g,h,q)]x^2y^2 + \sum_{2\le 3} m_{23}[ZC(g,h,q)]x^2y^3 + \sum_{3\le 3} m_{33}[ZC(g,h,q)]x^3y^3$$

$M[ZC(g,h,q),x,y]=|E_{2;2}|x^2y^2+|E_{2;3}|x^2y^3+|E_{3;3}|x^3y^3$

$=6x^2y^2+(8(g+h+q)-36)x^2y^3+2(g+h+q)x^3y^3.$

The strategy of M-polynomial of ZC(g,h,q) is shown in Figure 2. ■

Topological indices of zigzag-edge coronoid

Theorem 4.1. Let ZC(*g, h, q*) be a Zigzag-edge coronoid

$M[ZC(g,h,q),x,y]=6x^2y^2+(8(g+h+q)-36)x^2y^3+2(g+h+q)x^3y^3$

$$[1.]M_1[ZC(g,h,q)] = 52(g+h+q)-156$$

$$[2.]M_2[ZC(g,h,q)] = 66(g+h+q)-192$$

$$[3.]^m M_2[ZC(g,h,q)] = \frac{14}{9}(g+h+q)-\frac{9}{2}$$

$$[4.]R_\alpha[ZC(g,h,q)] = [6^\alpha\times 8+9^\alpha\times 2](g+h+q)+[4^\alpha\times 6-6^\alpha\times 36]$$

$$[5.]RR_\alpha[ZC(g,h,q)] = [\frac{8}{6^\alpha}+\frac{2}{9^\alpha}](g+h+q)+[\frac{6}{4^\alpha}-\frac{36}{6^\alpha}].$$

$$[6.]SDD[ZC(g,h,q)] = \frac{64}{3}(g+h+q)-66$$

$$[7.]H[ZC(g,h,q)] = \frac{58}{15}(g+h+q)-\frac{57}{5}$$

$$[8.]I[ZC(g,h,q)] = \frac{63}{5}(g+h+q)-\frac{186}{5}$$

$$[9.]A[ZC(g,h,q)] = \frac{2777}{32}(g+h+q)-240$$

The following result obtained by applying the definition of M-polynomial

Proof. Let $M[ZC(g,h,q),x,y]=6x^2y^2+(8(g+h+q)-36)x^2y^3+2(g+h+q)x^3y^3$

The first Zagreb index

$$D_x f(x,y) = 12x^2y^2+2(8(g+h+q)-36)x^2y^3+6(g+h+q)x^3y^3$$

$$D_y f(x,y) = 12x^2y^2+3(8(g+h+q)-36)x^2y^3+6(g+h+q)x^3y^3$$

$$(D_x+D_y)f(x,y) = 24x^2y^2+5(8(g+h+q)-36)x^2y^3+12(g+h+q)x^3y^3$$

$$M_1[ZC(g,h,q)] = (D_x+D_y)f(x,y)_{x=y=1} = 52(g+h+q)-156$$

The second Zagreb index

$$D_y f(x,y) = 12x^2y^2 + 3(8(g+h+q)-36)x^2y^3 + 6(g+h+q)x^3y^3.$$

$$D_xD_y f(x,y) = 24x^2y^2 + 6(8(g+h+q)-36)x^2y^3 + 18(g+h+q)x^3y^3.$$

$$M_2[ZC(g,h,q)] = (D_xD_y)f(x,y)_{x=y=1} = 66(g+h+q)-192.$$

The modified second Zagreb index

$$S_y f(x,y) = 3x^2y^2 + \frac{1}{3}(8(g+h+q)-36)x^2y^3 + \frac{2}{3}(g+h+q)x^3y^3.$$

$$S_xS_y f(x,y) = \frac{3}{2}x^2y^2 + \frac{1}{6}(8(g+h+q)-36)x^2y^3 + \frac{2}{9}(g+h+q)x^3y^3.$$

$$^{m}M_2[ZC(g,h,q)] = (S_xS_y)f(x,y)_{x=y=1}. = \frac{14}{9}(g+h+q) - \frac{9}{2}.$$

The general Randić index

$$D_y^{\alpha} f(x,y) = 2^{\alpha}\cdot 6x^2y^2 + 3^{\alpha}\cdot(8(g+h+q)-36)x^2y^3 + 3^{\alpha}\cdot 2(g+h+q)x^3y^3.$$

$$D_x^{\alpha}D_y^{\alpha} f(x,y) = 4^{\alpha}\cdot 6x^2y^2 + 6^{\alpha}\cdot(8(g+h+q)-36)x^2y^3 + 9^{\alpha}\cdot 2(g+h+q)x^3y^3.$$

$$R_{\alpha}[ZC(g,h,q)] = (D_x^{\alpha}D_y^{\alpha})f(x,y)_{x=y=1} = [6^{\alpha}\cdot 8 + 9^{\alpha}\cdot 2](g+h+q) + [4^{\alpha}\cdot 6 - 6^{\alpha}\cdot 36].$$

The inverse Randić index

$$S_y^{\alpha} f(x,y) = \frac{6}{2^{\alpha}}x^2y^2 + \frac{1}{3^{\alpha}}(8(g+h+q)-36)x^2y^3 + \frac{2}{3^{\alpha}}(g+h+q)x^3y^3.$$

$$S_x^{\alpha}S_y^{\alpha} f(x,y) = \frac{6}{4^{\alpha}}x^2y^2 + \frac{1}{6^{\alpha}}(8(g+h+q)-36)x^2y^3 + \frac{2}{9^{\alpha}}(g+h+q)x^3y^3.$$

$$RR_{\alpha}[ZC(g,h,q)] = (S_x^{\alpha}S_y^{\alpha})[f(x,y)]_{x=y=1} = [\frac{8}{6^{\alpha}} + \frac{2}{9^{\alpha}}](g+h+q) + [\frac{6}{4^{\alpha}} - \frac{36}{6^{\alpha}}].$$

The symmetric division index

$$S_y f(x,y) = 3x^2y^2 + \frac{1}{3}(8(g+h+q)-36)x^2y^3 + \frac{2}{3}(g+h+q)x^3y^3.$$

$$D_xS_y f(x,y) = 6x^2y^2 + \frac{2}{3}(8(g+h+q)-36)x^2y^3 + 2(g+h+q)x^3y^3.$$

$$D_y f(x,y) = 12x^2y^2 + 3(8(g+h+q)-36)x^2y^3 + 6(g+h+q)x^3y^3.$$

$$S_xD_y f(x,y) = 6x^2y^2 + \frac{3}{2}(8(g+h+q)-36)x^2y^3 + 2(g+h+q)x^3y^3.$$

$$(D_xS_y + S_xD_y)f(x,y) = 12x^2y^2 + \frac{13}{6}(8(g+h+q)-36)x^2y^3 + 4(g+h+q)x^3y^3.$$

$$SDD[ZC(g,h,q)] = (D_xS_y + S_xD_y)f(x,y)_{x=y=1} = \frac{64}{3}(g+h+q) - 66.$$

The harmonic index

$$Jf(x,y)=6x^4+(8(g+h+q)-36)x^5+2(g+h+q)x^6.$$

$$S_xJf(x,y)=\frac{3}{2}x^4+\frac{1}{5}(8(g+h+q)-36)x^5+\frac{1}{3}(g+h+q)x^6.$$

$$2S_xJf(x,y)=3x^4+\frac{2}{5}(8(g+h+q)-36)x^5+\frac{2}{3}(g+h+q)x^6.$$

$$H[ZC(g,h,q)]=2S_xJf(x,y)f(x,y)_{x=1}=\frac{58}{15}(g+h+q)-\frac{57}{5}.$$

The inverse sum index

$$D_yf(x,y)=12x^2y^2+3(8(g+h+q)-36)x^2y^3+6(g+h+q)x^3y^3.$$

$$D_xD_yf(x,y)=24x^2y^2+6(8(g+h+q)-36)x^2y^3+18(g+h+q)x^3y^3.$$

$$JD_xD_yf(x,y)=24x^4+6(8(g+h+q)-36)x^5+18(g+h+q)x^6.$$

$$S_xJD_xD_yf(x,y)=6x^4+\frac{6}{5}(8(g+h+q)-36)x^5+3(g+h+q)x^6.$$

$$I[ZC(g,h,q)]=(S_xJD_xD_y)f(x,y)_{x=1}=\frac{63}{5}(g+h+q)-\frac{186}{5}.$$

The augmented Zagreb index

$$D_y^3f(x,y)=48x^2y^2+27(8(g+h+q)-36)x^2y^3+54(g+h+q)x^3y^3.$$

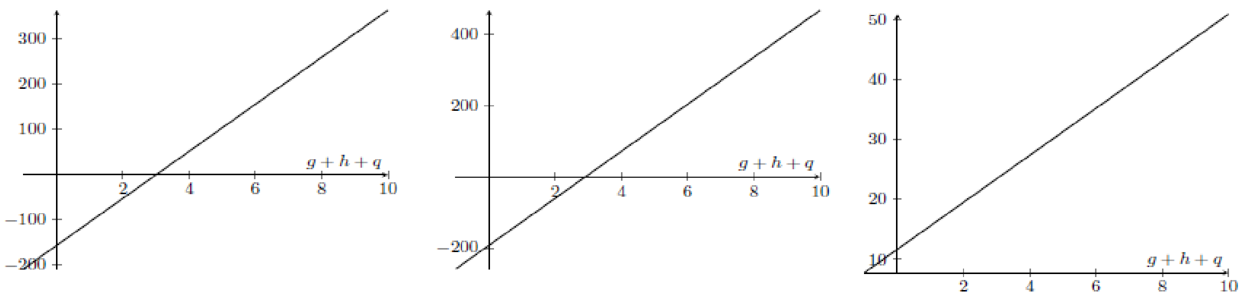
$$D_x^3D_y^3f(x,y)=384x^2y^2+216(8(g+h+q)-36)x^2y^3+1458(g+h+q)x^3y^3.$$

$$JD_x^3D_y^3f(x,y)=384x^4+216(8(g+h+q)-36)x^5+1458(g+h+q)x^6.$$

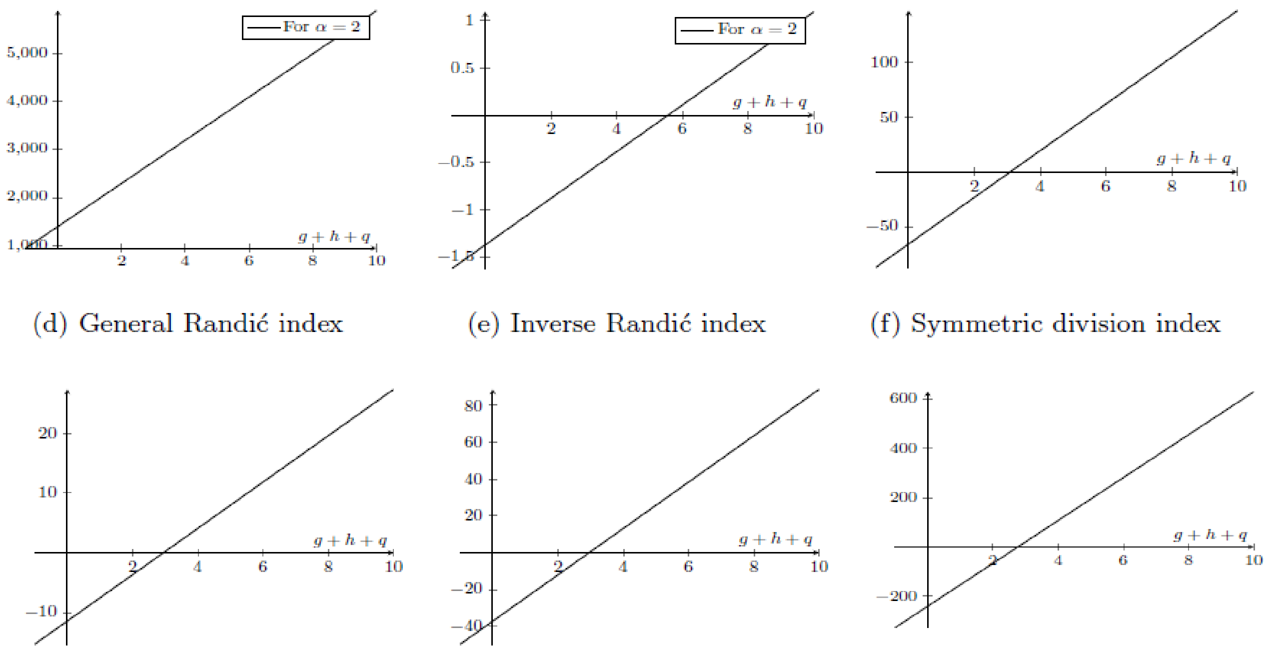
$$Q_{-2}JD_x^3D_y^3f(x,y)=384x^2+216(8(g+h+q)-36)x^3+1458(g+h+q)x^4.$$

$$S_x^3Q_{-2}JD_x^3D_y^3f(x,y)=48x^2+8(8(g+h+q)-36)x^3+\frac{729}{32}(g+h+q)x^4.$$

$$A[ZC(g,h,q)]=S_x^3Q_{-2}JD_x^3D_y^3f(x,y)_{x=1}=\frac{2777}{32}(g+h+q)-240.$$



(a) First Zagreb index (b) Second Zagreb index (c) Modified Zagreb index



(d) General Randić index (e) Inverse Randić index (f) Symmetric division index

(g) Harmonic index (h) Inverse sum index (i) Augmented Zagreb index

FIGURE 3 The plot of topological indices of ZC(g,h,q)

Conclusion

In this study, we calculated the closed-form of M-polynomial for the graph Zigzag-edge coronoid, and then we derivative several degree-based topological indices as well, which supports shrinking the number of experiments. These topological indices can help characterize biological, chemical, and physical features of a molecule. So topological index has a fundamental role that represents the chemical structure of a molecule to a real number and is used to precise the molecule which is being tested. These outcomes are very supportive in accepting and forecasting the physico-chemical properties of these chemical structures. Distance-related graph indices for these imperative chemical graphs is still open to further research.

Acknowledgments

The authors extend their real appreciation to the reviewers for their insightful comments and technical suggestions to enhance quality of the article.

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How to cite this article: Muhammad Ehsan, Sumera Sattar, Faryal Chaudhry, Farkhanda Afzal*, Mohammad Reza Farahani, Murat Cancan. Topological analysis of zigzag-edge coronoid graph by using M-polynomial. *Eurasian Chemical Communications*, 2021, 3(9), 590-597. **Link:** http://www.echemcom.com/article_1346