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On Topological Polynomials of Silicate Network

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Abstract: The first and second Zagreb polynomials are defined as [1]: $M_1(G,x) = \sum_{uv \in E(G)} x^{d_u + d_v}$ and $M_2(G,x) = \sum_{uv \in E(G)} x^{d_u d_v}$, where d_u is degree of a vertex u. In this paper, Zagreb polynomials, fifth M-Zagreb polynomials, hyper fifth M-Zagreb polynomials, first, second K-Banhatti polynomials and general Zagreb polynomials of silicate network are studied.

Keywords: Degree, degree-sum, fifth M-Zagreb polynomial, hyper fifth M-Zagreb polynomial, K-Banhatti polynomial, Zagreb polynomial

1. Introduction

Let G = (V,E) be a graph with vertex set V(G) and edge set E(G). The degree of a vertex $u \in V(G)$ is denoted by d_u and is the number of vertices adjacent to u. The edge connecting the vertices u and v is denoted by uv [2]. A topological index is a numerical parameter mathematically derived from the graph structure. Many topological polynomials appear in the molecular topology [3-4]. Hosoya, Schultz, Modified Schultz polynomials and their indices of PAHs were studied in [5]. The Zagreb polynomial was studied for different molecular graphs in [6-12].M-Zagreb polynomials and corresponding degree-based topological indices have been considered in many papers such as [13-16]. Augmented Revan index and its polynomial of certain families of benzenoid systems, hyper-Revan indices and their polynomials of silicate networks and arithmetic-geometric reverse indices of certain networks were studied by V. R. Kulli [17-19].Degree-based topological indices and topological polynomials of silicate network have been computed in many papers [20-24].

The degree-based Zagreb polynomials are defined as [25-26]
$$\begin{split} M_1(G,x) &= \sum_{uv \in E(G)} x^{d_u + d_v}. \ (1) \\ M_2(G,x) &= \sum_{uv \in E(G)} x^{d_u \times d_v}. \ (2) \\ M_3(G,x) &= \sum_{uv \in E(G)} x^{|d_u - d_v|}. \ (3) \\ M_4(G,x) &= \sum_{uv \in E(G)} x^{d_u(d_u + d_v)}. \ (4) \\ M_5(G,x) &= \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}. \ (5) \end{split}$$

In addition, two polynomials related to first Zagreb index are defined as

 $M_1^*(G,x) = \sum_{v \in V(G)} d_v x^{d_v}$ and $M_0(G,x) = \sum_{v \in V(G)} x^{d_v}$ (6)

The fifth M-Zagreb polynomials are defined as [27-29]

$$M_{1}G_{5}(G,x) = \sum_{uv \in E(G)} x^{S_{u} \times S_{v}}.$$
 (7)
$$M_{2}G_{5}(G,x) = \sum_{uv \in E(G)} x^{S_{u} \times S_{v}}.$$
 (8)

The fifth hyper M-Zagreb polynomials are

$$HM_{1}G_{5}(G, x) = \sum_{uv \in E(G)} x^{(S_{u} + S_{v})^{2}}. (9)$$

$$HM_{2}G_{5}(G, x) = \sum_{uv \in E(G)} x^{(S_{u} \times S_{v})^{2}}. (10)$$

And general fifth M-Zagreb polynomials are defined as

$$M_{1}^{\alpha}G_{5}(G,x) = \sum_{uv \in E(G)} x^{(S_{u}+S_{v})^{\alpha}}.$$
 (11)
$$M_{1}^{\alpha}G_{5}(G,x) = \sum_{v \in E(G)} x^{(S_{u}\times S_{v})^{\alpha}}.$$
 (12)

 $M_{2}^{\alpha}G_{5}(G,x) = \sum_{uv \in E(G)} x^{(S_{u} \times S_{v})^{\alpha}}$, (12)

where α is a real number and $S_u = \sum_{v \in N_u} d_v$ with $N_u = \{u \in V(G) | uv \in E(G)\}$. We use the following lemma for defining $d_G(e)$.

Lemma 1. Let G be a graph with $u,v \in V(G)$ and $e = uv \in E(G)$ then $d_G(e) = d_e = d_u + d_v - 2$.

The first and second K-Banhatti polynomials are defined as [30-31]

 $KB_{1}(G,x) = \sum_{uv \in E(G)} x^{(d_{u}+d_{e})}. (13)$ $KB_{2}(G,x) = \sum_{uv \in E(G)} x^{(d_{u} \times d_{e})}. (14)$

General Zagreb polynomial is defined as $M_{a, b}(G, x) = \sum_{uv \in E(G)} x^{(ad_u + bd_v)}. (15)$

And modified general Zagreb polynomial is

 $M'_{a,b}(G,x) = \sum_{uv \in E(G)} x^{(d_u+a)(d_v+b)}$, (16) where a and b are suitably chosen real number parameters.

The complement of \overline{G} of a graph G is a graph whose vertex set is V(G) and two vertices of \overline{G} are adjacent if and only if they are nonadjacent in G [32-36]. Therefore \overline{G} has n vertices and $\binom{n}{2}$ - m edges. The degree of a vertex v in \overline{G} is $d_{\overline{G}}(v) = n - 1 - d_{\overline{G}}(v)$.

The first, second and third Zagreb polynomial of complement graph (\overline{G}) of G are defined as

- $M_1(\overline{G},x) = \sum_{uv \in E(G)} x^{d_{\overline{G}}(u) + d_{\overline{G}}(v)}.$ (17)
- $M_{2}(\overline{G},x) = \sum_{uv \in E(G)} x^{d_{\overline{G}}(u) \times d_{\overline{G}}(v)}.$ (18)

$$M_3(\overline{G},x) = \sum_{uv \in E(G)} x^{|d_{\overline{G}}(u) - d_{\overline{G}}(v)|}.$$
 (19)

In this paper, Zagreb-polynomials, fifth M-Zagreb polynomials, hyper fifth M-Zagreb polynomials, first, second K-Banhatti polynomials and Zagreb polynomials of complement graph (\overline{G}) of silicate network are studied. Our notations are standard and mainly taken from standard books of topology [37-39].

2. Materials and methods

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. Graph polynomials are polynomials assigned to molecular graphs. The molecular graph of silicate network

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of dimension two is shown figure (1). Let G be the graph of silicate network. It is observed from figure that there are $15n^2+3n$ vertices and $36n^2$ edges and the vertices either of degree 3 or 6. The (d_u, d_v) partition of silicate network is represented in table (1) and sum-degree partition in table (2). To compute K-Banhatti polynomials lemma number (1) is used.

3. Results and discussion

Zagreb polynomials of silicate network

It is observed from figure (1) that there are three edges corresponding to vertices with degree 3 and 6.The degree-based Zagreb polynomials can be computed as follows.

Theorem 1.1: First Zagreb polynomial of silicate network is $6nx^6+(18n^2+6n)x^9+(18n^2-12n)x^{12}$.

Proof. By using table (1) and figure (1), we have $M_{1}(G,x) = \sum_{uv \in E(G)} x^{d_{u}+d_{v}}$ $= \sum_{3,3 \in E(G)} x^{3+3} + \sum_{3,6 \in E(G)} x^{3+6} + \sum_{6,6 \in E(G)} x^{6+6}$ $= 6nx^{6} + (18n^{2} + 6n)x^{9} + (18n^{2} - 12n)x^{12}.$

Theorem 1.2.Second Zagreb polynomial of silicate network is $6nx^9+(18n^2+6n)x^{18}+(18n^2-12n)x^{36}$.

Proof: By using table (1) and figure (1), we have $M_{2}(G,x) = \sum_{uv \in E(G)} x^{d_{u} \times d_{v}}$ $= \sum_{3,3 \in E(G)} x^{3 \times 3} + \sum_{3,6 \in E(G)} x^{3 \times 6} + \sum_{6,6 \in E(G)} x^{6 \times 6}$ $= 6nx^{9} + (18n^{2} + 6n)x^{18} + (18n^{2} - 12n)x^{36}.$

Theorem 1.3: Addional first Zagreb polynomial of silicate network is $(18n^2+18n)x^3+(54n^2-18n)x^6$.

Proof. Silicate network with $15n^2+3n$ vertices and $36n^2$ edges, has vertices either of degree 3 or 6.By using equation (6) and figure (1), we have $M_1^*(G,x) = \sum_{v \in V(G)} d_v x^{d_v} = \sum_{3 \in V(G)} 3 \times x^3 + \sum_{6 \in V(G)} 6 \times x^6$ $= (18n^2+18n)x^3+(54n^2-18n)x^6.$

Fifth M-Zagreb polynomials of silicate network

Theorem 2.1: Fifth M₁-Zagreb polynomial of silicate network is $6nx^{30} + 24x^{39} + 24(n-1)x^{42} + 12(n-1)x^{45} + (18n^2 - 30n + 12)x^{48} + 12x^{51} + 6(2n-3)x^{54} + 12(n-1)x^{57} + (18n^2 - 36n + 18)x^{60}.$

Proof: By using equation (7) and table (2), we have $M_{1}G_{5}(G,x) = \sum_{uv \in E(G)} x^{S_{u}+S_{v}} = \sum_{15,15 \in E(G)} x^{15+15} + \sum_{15,24 \in E(G)} x^{15+24} + \sum_{15,27 \in E(G)} x^{15+27} + \sum_{18,27 \in E(G)} x^{18+27} + \sum_{18,30 \in E(G)} x^{18+30} + \sum_{24,27 \in E(G)} x^{24+27} + \sum_{27,27 \in E(G)} x^{27+27} + \sum_{27,30 \in E(G)} x^{27+30} + \sum_{30,30 \in E(G)} x^{30+30} = 6nx^{30} + 24x^{39} + 24(n-1)x^{42} + 12(n-1)x^{45} + (18n^2 - 30n + 12)x^{48} + 12x^{51} + 6(2n-3)x^{54} + 12(n-1)x^{57} + (18n^2 - 36n + 18)x^{60}.$ **Theorem 2.2:** The fifth hyper M₁-Zagreb polynomial of silicate network is $6nx^{900} + 24x^{1521} + 24(n-1)x^{1764} + 12(n-1)x^{2025} + (18n^2 - 30n + 12)x^{2304} + 12x^{2601} + 6(2n-3)x^{2916} + 12(n-1)x^{3249} + (18n^2 - 36n + 18)x^{3600}$.

Proof: By using equation (9) and table (2), we have $HM_1G_5(G,x) = \sum_{uv \in E(G)} x^{(S_u+S_v)^2}$ $= \sum_{15,15 \in E(G)} x^{(15+15)^2} + \sum_{15,24 \in E(G)} x^{(15+24)^2} + \sum_{15,27 \in E(G)} x^{(18+27)^2} + \sum_{18,27 \in E(G)} x^{(18+27$

 $\begin{array}{l} \sum_{18,30\in E(G)} x^{(18+30)^2} &+ \sum_{24,27\in E(G)} x^{(24+27)^2} &+ \\ \sum_{27,27\in E(G)} x^{(27+27)^2} &+ \sum_{27,30\in E(G)} x^{(27+30)^2} &+ \\ \sum_{30,30\in E(G)} x^{(30+30)^2} &= \\ = 6nx^{900} + 24x^{1521} + 24(n-1)x^{1764} + 12(n-1)x^{2025} &+ (18n^2 - 30n + 12)x^{2304} + 12x^{2601} &+ \\ 6(2n-3)x^{2916} &+ 12(n-1)x^{3249} &+ (18n^2 - 36n + 18)x^{3600}. \end{array}$

K-Banhatti polynomials of silicate network

Theorem 3.1: First K-Banhatti polynomial of silicate network is $6nx^{14}$ + $(18n^2+6n)x^{23}$ + $(18n^2-12n)x^{32}$.

Proof: By equation (13) and using table (3), we have first K-Banhatti polynomial

$$\begin{split} \text{KB}_1(\text{G}, \textbf{x}) &= \sum_{uv \in \text{E}(\text{G})} \textbf{x}^{(d_u + d_e)} \\ &= \sum_{3,3 \in \text{E}(\text{G})} \textbf{x}^{(3+4) + (3+4)} + \sum_{3,6 \in \text{E}(\text{G})} \textbf{x}^{(3+7) + (6+7)} + \\ &\sum_{6,6 \in \text{E}(\text{G})} \textbf{x}^{(6+10) + (6+10)} \\ &= 6n\textbf{x}^{14} + (18n^2 + 6n)\textbf{x}^{23} + (18n^2 - 12n)\textbf{x}^{32}. \end{split}$$

Theorem 3.2: Second K-Banhatti polynomial of silicate network is $6nx^{24}$ + $(18n^2+6n)x^{63}$ + $(18n^2-12n)x^{120}$.

Proof: By equation (14) and using table (3), we have second K-Banhatti polynomial

$$\begin{split} & \mathsf{KB}_2(\mathsf{G},\!x) = \sum_{uv \in \mathsf{E}\,(\,\mathsf{G}\,)} x^{(\mathsf{d}_u \times \mathsf{d}_e)} \\ & = \sum_{3,3 \in \mathsf{E}(\mathsf{G})} x^{(3 \times 4) + (3 \times 4)} + \sum_{3,6 \in \mathsf{E}(\mathsf{G})} x^{(3 \times 7) + (6 \times 7)} + \\ & \sum_{6,6 \in \mathsf{E}(\mathsf{G})} x^{(6 \times 10) + (6 \times 10)} \\ & = 6nx^{24} + (18n^2 + 6n)x^{63} + (18n^2 - 12n)x^{120}. \end{split}$$

General Zagreb polynomials of silicate network

Theorem 4.1: General Zagreb polynomial of silicate network is $6nx^{3a+3b} + (18n^2 + 6n)x^{3a+6b} + (18n^2 - 12n)x^{6a+6b}$.

Proof. By using equation (15) and table (1), we have $M_{a,b}(G,x) = \sum_{uv \in E(G)} x^{(ad_u + bd_v)}$ $= \sum_{3,3 \in E(G)} x^{a3+b3} + \sum_{3,6 \in E(G)} x^{a3+b6} + \sum_{6,6 \in E(G)} x^{a6+b6}$ $= 6nx^{3a+3b} + (18n^2 + 6n)x^{3a+6b} + (18n^2 - 12n)x^{6a+6b}.$

Theorem 4.2: Modified general Zagreb polynomial of silicate network is $6nx^{(3+a)(3+b)} + (18n^2 + 6n)x^{(3+a)(6+b)} + (18n^2 - 12n)x^{(6+a)(6+b)}$.

Proof. By using equation (16) and table (1), we have $M'_{a,b}(G,x) = \sum_{uv \in E(G)} x^{(d_u+a)(d_v+b)}$

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 $\sum_{3,6\in E(G)} x^{(3+a)(6+b)} +$ $\sum_{3,3\in E(G)} x^{(3+a)(3+b)} +$ = $\sum_{6,6\in E(G)} x^{(6+a)(6+b)}$ $6nx^{(3+a)(3+b)} + (18n^2 + 6n)x^{(3+a)(6+b)} + (18n^2 - 6n)x^{(3+a)(6+b)}$ $12n)x^{(6+a)(6+b)}$

Zagreb polynomial of complement graph(\overline{G})

Theorem 5.1. First Zagreb polynomial of complement graph (G) of silicate network is $6nx^{(2n-8)} + (18n^2 + 6n)x^{(2n-11)} + (18n^2 - 12n)x^{(2n-14)}.$

Proof. By using equation (17) and table (1), we have $M_1(\overline{G},x) = \sum_{uv \in E(G)} x^{d_{\overline{G},(u)} + d_{\overline{G},(v)}}$
$$\begin{split} & \sum_{3,3 \in E(G)} x^{(n-1-3)+(n-1-3)} + \\ & \sum_{3,6 \in E(G)} x^{(n-1-3)+(n-1-6)} + \sum_{6,6 \in E(G)} x^{(n-1-6)+(n-1-6)} \\ & = 6nx^{(2n-8)} + (18n^2 + 6n)x^{(2n-11)} \\ & + (19n^2) \end{split}$$



Figure 1: Silicate network of dimension two.

Table 1: (d_u, d_v) partition of silicate network					
(d_{u}, d_{v})	(3,3)	(3,6)	(6,6)		
Number of edges	6n	6n(3n+1)	6n(3n-2)		

Table 2: (S_u, S_v) partition of silicate network.									
$(S_{u,} S_{v})$	(15,15)	(15,24)	(15,27)	(18,27)	(18,30)	(24,27)	(27,27)	(27,30)	(30,30)
Number of edges	6n	24	24(n-1)	12(n-1)	18n ² -30n+12	12	6(2n-3)	12(n-1)	18n ² -36n+18

Table 3: Edge partition of silicate network for K-Banhatti polynomial.

(du,dv)	(3,3)	(3,6)	(6,6)
d _G (e)	4	7	10
Number of edges	6n	18n ² +6n	18n ² -12n

Table 4: $M_3(G_x)$, $M_4(G_x)$, $M_5(G_x)$, $M_0(G_x)$, $M_2G_5(G_x)$, $HM_2G_5(G_x)$, $M_1^{\alpha}G_5(G_x)$, $M_2^{\alpha}G_5(G_x)$, $M_2(\overline{G}_x)$ and $M_3(\overline{G}_x)$ polynomials of silicate network

polynomials of sineare network				
Topological	Polynomial for silicate network			
polynomial				
$M_3(G,x)$	$(18n^2-6n)+(18n^2+6n)x^3$			
M4(G,x)	$6nx^{18} + (18n^2 + 6n)x^{27} + (18n^2 - 12n)x^{72}$			
$M_5(G,x)$	$6nx^{18} + (18n^2 + 6n)x^{54} + (18n^2 - 12n)x^{72}$			
$M_0(G,x)$	$(6n^2+6n)x^3+(9n^2-3n)x^6$			
$M_2G_5(G,x)$	$6nx^{225} + 24x^{360} + 24(n-1)x^{405} + 12(n-1)x^{486} + (18n^2 - 30n + 12)x^{540} + 12x^{648}$			
	$+ 6(2n-3)x^{729} + 12(n-1)x^{810} + (18n^2 - 36n + 18)x^{900}$			
$HM_2G_5(G,x)$	$6nx^{50625} + 24x^{129600} + 24(n-1)x^{164025} + 12(n-1)x^{236196} + (18n^2 - 30n + 12)x^{291600}$			
	$+ 12x^{419904} + 6(2n-3)x^{531441} + 12(n-1)x^{656100} + (18n^2 - 36n + 18)x^{810000}$			
$M_1^{\alpha}G_5(G,x)$	$6nx^{(30)^{\alpha}} + 24x^{(39)^{\alpha}} + 24(n-1)x^{(42)^{\alpha}} + 12(n-1)x^{(45)^{\alpha}} + (18n^2 - 30n + 12)x^{(48)^{\alpha}} + 12x^{(51)^{\alpha}}$			
	$+ 6(2n-3)x^{(54)^{\alpha}} + 12(n-1)x^{(57)^{\alpha}} + (18n^2 - 36n + 18)x^{(60)^{\alpha}}$			
$M_2^{\alpha}G_5(G,x)$	$6nx^{(225)^{\alpha}} + 24x^{(360)^{\alpha}} + 24(n-1)x^{(405)^{\alpha}} + 12(n-1)x^{(486)^{\alpha}} + (18n^2 - 30n + 12)x^{(540)^{\alpha}} + 12x^{(648)^{\alpha}} + 12$			
	$+ 6(2n-3)x^{(729)^{\alpha}} + 12(n-1)x^{(810)^{\alpha}} + (18n^2 - 36n + 18)x^{(900)^{\alpha}}$			
$M_2(\overline{G},x)$	$6nx^{(n-4)^2} + (18n^2 + 6n)x^{(n^2 - 11n + 28)} + (18n^2 - 12n)x^{(n-7)^2}$			
$M_3(\overline{G},x)$	$(18n^2 - 6n) + (18n^2 + 6n)x^3$			

4. Conclusion

The degree-based Zagreb polynomials, fifth M-Zagreb polynomials, K-Banhatti polynomials, general Zagreb polynomials, Zagreb polynomials of complement graph (G) and additional two polynomials related to first Zagreb index are obtained for silicate network. Some topological polynomials: $M_3(G,x)$, $M_4(G,x)$, $M_5(G,x)$, $M_0(G,x)$, $M_2G_5(G,x), \ HM_2G_5(G,x), M_1^{\alpha}G_5(G,x), \ M_2^{\alpha}G_5(G,x), \ M_2(\overline{G},x)$ and $M_3(\overline{G}_x)$ are computed. Third Zagreb polynomial of molecular graph (G) and complement graph (\overline{G}) have the same value for silicate network.

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