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ABSTRACT

Recently, the δ -vertex degree concept was defined in Chemical Graph Theory. In this paper, we propose the first and second δ -Banhatti indices, first and second hyper δ -Banhatti indices and their corresponding polynomials of a molecular graph and compute exact formulas for silicate networks and hexagonal networks.

Keywords: δ -vertex degree, δ -Banhatti indices, hyper δ -Banhatti indices.

Mathematics Subject Classification: 05C05, 05C7, 05C09.

1. INTRODUCTION

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. In Chemical Graph Theory, graph indices have found to be useful in chemical documentation, isomer discrimination, structure property relationships, structure activity relationships and pharmaceutical drug design. There has been considerable interest in the general problem of computing graph indices, see [1, 2].

We consider only finite, simple, connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u . Let $\delta(G)$ denote the minimum degree among the vertices of G . We refer [3] for undefined terms and notations

Recently, the δ -vertex degree concept in Chemical Graph Theory is defined by Kulli in [4] as

$$\delta_u = d_G(u) - \delta(G) + 1.$$

The δ edge connecting the δ vertices u and v will be denoted by uv .

The first and second δ -Banhatti indices of a graph G are defined as

$$\delta B_1(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v), \quad \delta B_2(G) = \sum_{uv \in E(G)} \delta_u \delta_v.$$

Considering the first and second δ -Banhatti indices, we now define the first and second δ -Banhatti polynomials of a graph G as

$$\delta B_1(G, x) = \sum_{uv \in E(G)} x^{(\delta_u + \delta_v)}, \quad \delta B_2(G, x) = \sum_{uv \in E(G)} x^{\delta_u \delta_v}.$$

We introduce the δ -Banhatti vertex index of a graph G , defined as

$$\delta B_v(G) = \sum_{u \in V(G)} \delta_u^2.$$

Considering the δ -Banhatti vertex index, we define the δ -Banhatti vertex polynomial of a graph as

$$\delta B_v(G, x) = \sum_{u \in V(G)} x^{\delta_u^2}.$$

We now introduce the first and second hyper δ -Banhatti indices of a graph G and they are defined as

$$H\delta B_1(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v)^2, \quad H\delta B_2(G) = \sum_{uv \in E(G)} (\delta_u \delta_v)^2.$$

Considering the first and second hyper δ -Banhatti indices, we define the first and second hyper δ -Banhatti polynomials of a graph G as

$$H\delta B_1(G, x) = \sum_{w \in E(G)} x^{(\delta_u + \delta_v)^2}, \quad H\delta B_2(G, x) = \sum_{uv \in E(G)} x^{(\delta_u \delta_v)^2}.$$

For more discussion on topological indices, we encourage the readers to refer the papers [5, 6, 7, 8, 9, 10, 11, 12, 13, 14].

In this paper, we compute the first and second δ -Banhatti indices, first and second hyper δ -Banhatti indices and their corresponding polynomials of certain networks.

2. RESULTS FOR SILICATE NETWORKS

Silicate networks are obtained by fusing metal oxide or metal carbonates with sand. A silicate network is symbolized by SL_n , where n is the number of hexagons between the center and boundary of SL_n . A 2-D silicate network is presented in Figure 1.

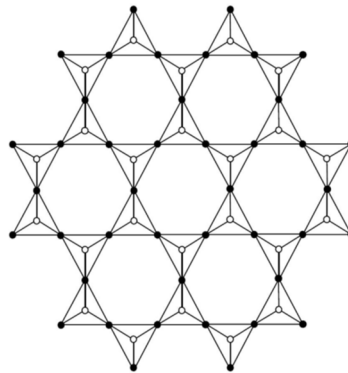


Figure 1. A 2-D silicate network

Let G be the graph of a silicate network SL_n . By calculation, we obtain that G has $15n^2 + 3n$ vertices and $36n^2$ edges. In G , there are two types of vertices as follows:

$$\begin{aligned} V_1 &= \{u \in V(G) \mid d_G(u) = 3\}, & |V_1| &= 6n^2 + 6n. \\ V_2 &= \{u \in V(G) \mid d_G(u) = 6\}, & |V_2| &= 9n^2 - 3n. \end{aligned}$$

Therefore, we have $\delta(G)=3$ and hence $\delta_u = d_G(u) - \delta(u) + 1 = d_G(u) - 2$. Thus there are two types of δ -vertices as given in Table 1.

Table 1. δ -vertex partition of SL_n

$\delta_u \setminus u \in V(G)$	1	4
Number of vertices	$6n^2 + 6n$	$9n^2 - 3n$

By calculation, in SL_n there are 3 types of edges based on degrees of end vertices of each edge as follows:

$$\begin{aligned} E_1 &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}, & |E_1| &= 6n. \\ E_2 &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, & |E_2| &= 18n^2 + 6n. \\ E_3 &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, & |E_3| &= 18n^2 - 12n. \end{aligned}$$

Hence there are 3 types of δ -edges as given in Table 2.

Table 2. δ -edge partition of SL_n

$\delta_u, \delta_v \setminus uv \in E(G)$	(1, 1)	(1, 4)	(4, 4)
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12$

Theorem 1. Let G be the graph of a silicate network SL_n . Then

- (i) $\delta B_v(SL_n) = 150n^2 - 42n$.
- (ii) $\delta B_v(SL_n, x) = (6n^2 + 6n)x + (9n^2 - 3n)x^{16}$.

Proof: (i) To compute $\delta B_v(SL_n)$, we see that

$$\begin{aligned} \delta B_v(SL_n) &= \sum_{u \in V(G)} \delta_u^2 \\ &= 1^2(6n^2 + 6n) + 4^2(9n^2 - 3n) \\ &= 150n^2 - 42n. \end{aligned}$$

- (ii) To compute $\delta B_v(SL_n, x)$, we see that

$$\begin{aligned} \delta B_v(SL_n, x) &= \sum_{u \in V(G)} x^{\delta_u^2} \\ &= (6n^2 + 6n)x^1 + (9n^2 - 3n)x^{16} \\ &= (6n^2 + 6n)x + (9n^2 - 3n)x^{16}. \end{aligned}$$

Theorem 2. Let G be the graph of a silicate network SL_n . Then

- (i) $\delta B_1(SL_n) = 234n^2 - 54n$.
- (ii) $\delta B_2(SL_n) = 360n^2 - 162n$.
- (iii) $\delta B_1(SL_n, x) = 6nx^2 + (18n^2 + 6n)x^5 + (18n^2 - 12n)x^8$.
- (iv) $\delta B_2(SL_n, x) = 6nx + (18n^2 + 6n)x^4 + (18n^2 - 12n)x^{16}$.

Proof: By using definitions and Table 2, we deduce

- (i)
$$\begin{aligned} \delta B_1(SL_n) &= \sum_{uv \in E(G)} (\delta_u + \delta_v) \\ &= (1+1)6n + (1+4)(18n^2 + 6n) + (4+4)(18n^2 - 12n) \\ &= 234n^2 - 54n. \end{aligned}$$

- (ii)
$$\begin{aligned} \delta B_2(SL_n) &= \sum_{uv \in E(G)} \delta_u \delta_v \\ &= (1 \times 1)6n + (1 \times 4)(18n^2 + 6n) + (4 \times 4)(18n^2 - 12n) \\ &= 360n^2 - 162n. \end{aligned}$$

- (iii)
$$\begin{aligned} \delta B_1(SL_n, x) &= \sum_{u \in V(G)} x^{\delta_u + \delta_v} \\ &= 6nx^{1+1} + (18n^2 + 6n)x^{1+4} + (18n^2 - 12n)x^{4+4} \\ &= 6nx^2 + (18n^2 + 6n)x^5 + (18n^2 - 12n)x^8. \end{aligned}$$

- (iv)
$$\delta B_2(SL_n, x) = \sum_{uv \in E(G)} x^{\delta_u \delta_v}$$

$$\begin{aligned}
 &= 6nx^{1 \times 1} + (18n^2 + 6n)x^{1 \times 4} + (18n^2 - 12n)x^{4 \times 4} \\
 &= 6nx + (18n^2 + 6n)x^4 + (18n^2 - 12n)x^{16}.
 \end{aligned}$$

Theorem 3. Let G be the graph of a silicate network SL_n . Then

- (i) $H\delta B_1(SL_n) = 1602n^2 - 594n$.
- (ii) $H\delta B_2(SL_n) = 4896n^2 - 2970n$.
- (iii) $H\delta B_1(SL_n, x) = 6nx^4 + (18n^2 + 6n)x^{25} + (18n^2 - 12n)x^{64}$.
- (iv) $H\delta B_2(SL_n, x) = 6nx + (18n^2 + 6n)x^{16} + (18n^2 - 12n)x^{256}$.

Proof: From definitions and by using Table 2, we derive

$$\begin{aligned}
 \text{(i)} \quad H\delta B_1(SL_n) &= \sum_{uv \in E(G)} (\delta_u + \delta_v)^2 \\
 &= (1+1)^2 6n + (1+4)^2 (18n^2 + 6n) + (4+4)^2 (18n^2 - 12n) \\
 &= 1602n^2 - 594n.
 \end{aligned}$$

$$\begin{aligned}
 \text{(ii)} \quad H\delta B_2(SL_n) &= \sum_{uv \in E(G)} (\delta_u \delta_v)^2 \\
 &= (1 \times 1)^2 6n + (1 \times 4)^2 (18n^2 + 6n) + (4 \times 4)^2 (18n^2 - 12n) \\
 &= 4896n^2 - 2970n.
 \end{aligned}$$

$$\begin{aligned}
 \text{(iii)} \quad H\delta B_1(SL_n, x) &= \sum_{uv \in E(G)} x^{(\delta_u + \delta_v)^2} \\
 &= 6nx^{(1+1)^2} + (18n^2 + 6n)x^{(1+4)^2} + (18n^2 - 12n)x^{(4+4)^2} \\
 &= 6nx^4 + (18n^2 + 6n)x^{25} + (18n^2 - 12n)x^{64}.
 \end{aligned}$$

$$\begin{aligned}
 \text{(iv)} \quad H\delta B_2(SL_n, x) &= \sum_{uv \in E(G)} x^{(\delta_u \delta_v)^2} \\
 &= 6nx^{(1 \times 1)^2} + (18n^2 + 6n)x^{(1 \times 4)^2} + (18n^2 - 12n)x^{(4 \times 4)^2} \\
 &= 6nx + (18n^2 + 6n)x^{16} + (18n^2 - 12n)x^{256}.
 \end{aligned}$$

3. RESULTS FOR HEXAGONAL NETWORKS

It is known that there exist three regular plane tilings with composition of same kind of regular polygons such as triangular, hexagonal and square. Triangular tiling is used in the construction of hexagonal networks. This network is denoted by HX_n , where n is the number of vertices in each side of hexagon. A hexagonal network dimension six is presented in Figure 2.

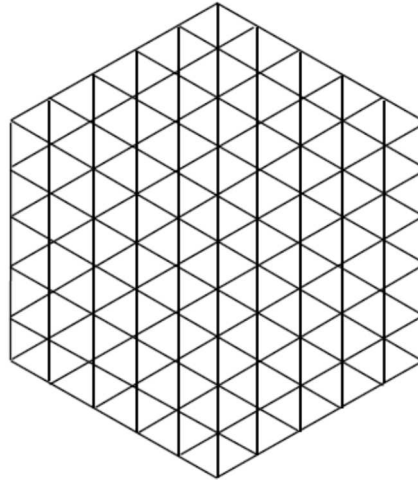


Figure 2. Hexagonal network of dimension six

Let G be the graph of a hexagonal network HX_n . By calculation, G has $3n^2 - 3n + 1$ vertices and $9n^2 - 15n + 6$ edges. In HX_n , there are three types of vertices as follows:

$$\begin{aligned} V_1 &= \{u \in V(G) \mid d_G(u) = 3\}, & |V_1| &= 6. \\ V_2 &= \{u \in V(G) \mid d_G(u) = 4\}, & |V_2| &= 6n - 12. \\ V_3 &= \{u \in V(G) \mid d_G(u) = 6\}, & |V_3| &= 3n^2 - 9n + 7. \end{aligned}$$

Thus $\delta(G)=3$ and hence $\delta_u = d_G(u) - \delta(u) + 1 = d_G(u) - 2$. Therefore there are three types of δ -vertices as given in Table 3.

Table 3. δ -vertex partition of HX_n

$\delta_u \setminus u \in V(G)$	1	2	4
Number of vertices	6	$6n - 12$	$3n^2 - 9n + 7$

By calculation, in HX_n there are five types of edges based on degrees of end vertices of each edge as follows:

$$\begin{aligned} E_1 &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}, & |E_1| &= 12. \\ E_2 &= \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 6\}, & |E_2| &= 6. \\ E_3 &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 4\}, & |E_3| &= 6n - 18. \\ E_4 &= \{uv \in E(G) \mid d_G(u) = 4, d_G(v) = 6\}, & |E_4| &= 12n - 24. \\ E_5 &= \{uv \in E(G) \mid d_G(u) = d_G(v) = 6\}, & |E_5| &= 9n^2 - 33n + 30. \end{aligned}$$

Thus there are five types of δ -edges as given in Table 4.

Table 4. δ -edge partition of HX_n

$\delta_u, \delta_v \setminus uv \in E(G)$	(1, 2)	(1, 4)	(2, 2)	(2, 4)	(4, 4)
Number of edges	12	6	$6n - 18$	$12n - 24$	$9n^2 - 33n + 30$

Theorem 4. Let G be the graph of a hexagonal network HX_n . Then

- (i) $\delta B_v(HX_n) = 48n^2 - 120n + 70$.
- (ii) $\delta B_v(HX_n, x) = 6x + (6n - 12)x^4 + (3n^2 - 9n + 7)x^{16}$.

Proof:

- (i) To compute $\delta B_v(HX_n)$, we see that

$$\begin{aligned}\delta B_v(HX_n) &= \sum_{u \in V(G)} \delta_u^2 \\ &= 1^2 \times 6 + 2^2(6n-12) + 4^2(3n^2-9n+7) \\ &= 48n^2 - 120n + 70.\end{aligned}$$

(ii) To compute $\delta B_v(HX_n, x)$, we see that

$$\begin{aligned}\delta B_v(HX_n, x) &= \sum_{u \in V(G)} x^{\delta_u^2} \\ &= 6x^1 + (6n-12)x^2 + (3n^2-9n+7)x^4 \\ &= 6x + (6n-12)x^4 + (3n^2-9n+7)x^{16}.\end{aligned}$$

Theorem 5. Let G be the graph of a hexagonal network HX_n . Then

- (i) $\delta B_1(HX_n) = 72n^2 - 168n + 90$.
 (ii) $\delta B_2(HX_n) = 144n^2 - 408n + 364$.
 (iii) $\delta B_1(HX_n, x) = 12x^3 + 6x^5 + (6n-18)x^4 + (12n-24)x^6 + (9n^2-33n+30)x^8$.
 (iv) $\delta B_2(HX_n, x) = 12x^2 + (6n-12)x^4 + (12n-24)x^8 + (9n^2-33n+30)x^{16}$.

Proof: From definitions and by using Table 4, we obtain

$$\begin{aligned}\text{(i)} \quad \delta B_1(HX_n) &= \sum_{uv \in E(G)} (\delta_u + \delta_v) \\ &= (1+2)12 + (1+4)6 + (2+2)(6n-18) + (2+4)(12n-24) + (4+4)(9n^2-33n+30) \\ &= 72n^2 - 168n + 90.\end{aligned}$$

$$\begin{aligned}\text{(ii)} \quad \delta B_2(HX_n) &= \sum_{uv \in E(G)} \delta_u \delta_v \\ &= (1 \times 2)12 + (1 \times 4)6 + (2 \times 2)(6n-18) + (2 \times 4)(12n-24) + (4 \times 4)(9n^2-33n+30) \\ &= 144n^2 - 408n + 364.\end{aligned}$$

$$\begin{aligned}\text{(iii)} \quad \delta B_1(HX_n, x) &= \sum_{uv \in E(G)} x^{\delta_u + \delta_v} \\ &= 12x^{1+2} + 6x^{1+4} + (6n-18)x^{2+2} + (12n-24)x^{2+4} + (9n^2-33n+30)x^{4+4} \\ &= 12x^3 + 6x^5 + (6n-18)x^4 + (12n-24)x^6 + (9n^2-33n+30)x^8.\end{aligned}$$

$$\begin{aligned}\text{(iv)} \quad \delta B_2(HX_n, x) &= \sum_{uv \in E(G)} x^{\delta_u \delta_v} \\ &= 12x^{1 \times 2} + 6x^{1 \times 4} + (6n-18)x^{2 \times 2} + (12n-24)x^{2 \times 4} + (9n^2-33n+30)x^{4 \times 4} \\ &= 12x^2 + (6n-12)x^4 + (12n-24)x^8 + (9n^2-33n+30)x^{16}.\end{aligned}$$

Theorem 6. Let G be the graph of a hexagonal network HX_n . Then

- (i) $H\delta B_1(HX_n) = 576n^2 - 1584n + 1026$.
 (ii) $H\delta B_2(HX_n) = 2304n^2 - 7584n + 6000$.
 (iii) $H\delta B_1(HX_n, x) = 12x^9 + 6x^{25} + (6n-18)x^{16} + (12n-24)x^{36} + (9n^2-33n+30)x^{64}$.
 (iv) $H\delta B_2(HX_n, x) = 12x^4 + (6n-12)x^{16} + (12n-24)x^{64} + (9n^2-33n+30)x^{256}$.

Proof: By using definitions and Table 4, we have

$$\begin{aligned}
 \text{(i)} \quad H\delta B_1(HX_n) &= \sum_{uv \in E(G)} (\delta_u + \delta_v)^2 \\
 &= (1+2)^2 12 + (1+4)^2 6 + (2+2)^2 (6n-18) + (2+4)^2 (12n-24) + (4+4)^2 (9n^2 - 33n + 30) \\
 &= 576n^2 - 1584n + 1026.
 \end{aligned}$$

$$\begin{aligned}
 \text{(ii)} \quad H\delta B_2(HX_n) &= \sum_{uv \in E(G)} (\delta_u \delta_v)^2 \\
 &= (1 \times 2)^2 12 + (1 \times 4)^2 6 + (2 \times 2)^2 (6n-18) + (2 \times 4)^2 (12n-24) + (4 \times 4)^2 (9n^2 - 33n + 30) \\
 &= 2304n^2 - 7584n + 6000.
 \end{aligned}$$

$$\begin{aligned}
 \text{(iii)} \quad H\delta B_1(HX_n, x) &= \sum_{uv \in E(G)} x^{(\delta_u + \delta_v)^2} \\
 &= 12x^{(1+2)^2} + 6x^{(1+4)^2} + (6n-18)x^{(2+2)^2} + (12n-24)x^{(2+4)^2} + (9n^2 - 33n + 30)x^{(4+4)^2} \\
 &= 12x^9 + 6x^{25} + (6n-18)x^{16} + (12n-24)x^{36} + (9n^2 - 33n + 30)x^{64}
 \end{aligned}$$

$$\begin{aligned}
 \text{(iv)} \quad H\delta B_2(HX_n, x) &= \sum_{uv \in E(G)} x^{(\delta_u \delta_v)^2} \\
 &= 12x^{(1 \times 2)^2} + 6x^{(1 \times 4)^2} + (6n-18)x^{(2 \times 2)^2} + (12n-24)x^{(2 \times 4)^2} + (9n^2 - 33n + 30)x^{(4 \times 4)^2} \\
 &= 12x^4 + (6n-12)x^{16} + (12n-24)x^{64} + (9n^2 - 33n + 30)x^{256}.
 \end{aligned}$$

4. CONCLUSION

In this study, we have determined the δ -Banhatti indices, hyper δ -Banhatti indices of silicate and hexagonal networks. Furthermore we have computed the δ -Banhatti polynomials, hyper δ -Banhatti polynomials of silicate and hexagonal networks.

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