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SOME CONNECTIVITY INDICES AND ZAGREB INDEX OF HONEYCOMB GRAPHS

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ABSTRACT: In this paper, we investigate several topological indices in honeycomb graphs: Randić connectivity index, sum-connectivity index, atom-bond connectivity index, geometric-arithmetic index, First and Second Zagreb indices and Zagreb polynomials. Formulas for computing the above topological descriptors in honeycomb graphs are given.

INTRODUCTION: In this paper, we only consider an undirected graph without loops and multiple edges. Let G be a graph, we denote $V(G)$ and $E(G)$ the vertex set and edge set of G, respectively. An edge uv is an $(s; t)$-edge if $d(u) = s$ and $d(v) = t$. In chemical graph theory, the vertices of the graph correspond to the atoms of molecules and the edges correspond to chemical bonds. The Wiener index $W(G)$ is defined as the sum of topological distances $d(u; v)$ between any two atoms in the molecular graph, which is introduced by the chemist Harold Wiener [1].

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$$W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$$

The Hosoya polynomial [8] of G is defined as

$$H(G,x)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} x^{d(u,v)}$$

The First Zagreb index $Zg_1(G)$ is defined as the sum of squares of the vertex degrees du and dv of vertices u and v in G [3, 4, 5]

$$Zg_1(G)=\sum_{v\in V(G)}(d_v)^2=\sum_{e=uv\in E(G)}(d_u+d_v)$$

The Second Zagreb index $Zg_2(G)$ is defined as the sum of squares of the vertex degrees du and dv of vertices u and v in G [3, 4, 5]

$$Zg_2(G)=\sum_{e=uv\in E(G)}(d_u d_v)$$

According to the above Zagreb indices, the First Zagreb polynomial $Zg_1(G; x)$ and the Second Zagreb polynomial $Zg_2(G; x)$ have been defined. They are defined as

$$Zg_1(G,x)=\sum_{e=uv\in E(G)} x^{d_u+d_v}$$

$$Zg_2(G,x)=\sum_{e=uv\in E(G)} x^{d_u d_v}$$

The Randić connectivity index [7] is defined on the ground of vertex degrees

$$\chi(G)=\sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

The sum-connectivity index is defined [12] as

$$X(G)=\sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}}$$

The Geometric-Arithmetic index [6] is defined as

$$GA(G)=\sum_{e=uv\in E(G)} \frac{2d_u d_v}{\sqrt{d_u+d_v}}$$

In 1998 by Estrada *et al.*, [2, 30] introduced the Atom-Bond Connectivity index is defined as

$$ABC(G)=\sum_{e=uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$$

Honeycomb Graph: The *n*-honeycomb graph *Hn* was studied in [10]. It is the graph shown in **Fig. 1**, where mean of vertex is vertex of the hexagons and mean of edges are the sides of the hexagons.

Definition 1: For any integer. Let P_1; P_2;…; P_k be *k* paths such that:

- When $n \equiv 0$ (mod 2), $P_i = v^i_{k-i+1} v^i_{k-i+2} \ldots v^i_{3k+i-1}$, *i*=1; 2;...; *k*;
- When $n \equiv 1$ (mod 2), $P_i = v^i_{k-i+1} v^i_{k-i+2} \ldots v^i_{3k+i-3}$, *i*=1; 2;...; *k*.

We first de ne a graph *H*, constructed by P_1; P_2;...;P_k and edges between P_i and P_i+1 for i = 1; 2;...;$k-1$ connected as follows:

- When $n \equiv 0$ (mod 2), for $j=k-i+1$; $k-i+2$;...;$3k+i-1$, $v^i_j v^{i+1}_j \in E(H)$, if $|i-j| \equiv 1$ (mod 2);
- When $n \equiv 1$ (mod 2), for $j=k-i+1$; $k-i+2$;...;$3k+i-3$, $v^i_j v^{i+1}_j \in E(H)$, if $i \equiv 1$ (mod 2) and $|j-k| \equiv 0$ (mod 2), or $i \equiv 0$ (mod 2) and $|j-k| \equiv 1$ (mod 2).

Now, let H' be a copy of *H*, and P_1'; P_2';...;P_k' are paths in H' corresponding to P_1; P_2;...;P_k. Let

- When $n \equiv 0$ (mod 2), $P_i' = u^i_{k-i+1} u^i_{k-i+2} \ldots u^i_{3k+i-1}$, *i* = 1; 2;...;*k*;
- When $n \equiv 1$ (mod 2), $P_i' = u^i_{k-i+1} u^i_{k-i+2} \ldots u^i_{3k+i-3}$, *i* = 1; 2;...;*k*.

A *n*-honeycomb graph H_n is then defined as: when $n \equiv 0$ (mod 2), H_n is the union of *H* and H' and edges $v_j^k u_j^k$ for $j \in \{1; 2;...;4k-1\}$ and $j \equiv 1$ (mod 2); when $n \equiv 1$ (mod 2), *G* is the union of *H* and $H'-P_1'$ and edges $v_j^k u_j^k$ for $j \in \{1; 2;...;4k-3\}$ and $j \equiv 1$ (mod 2).

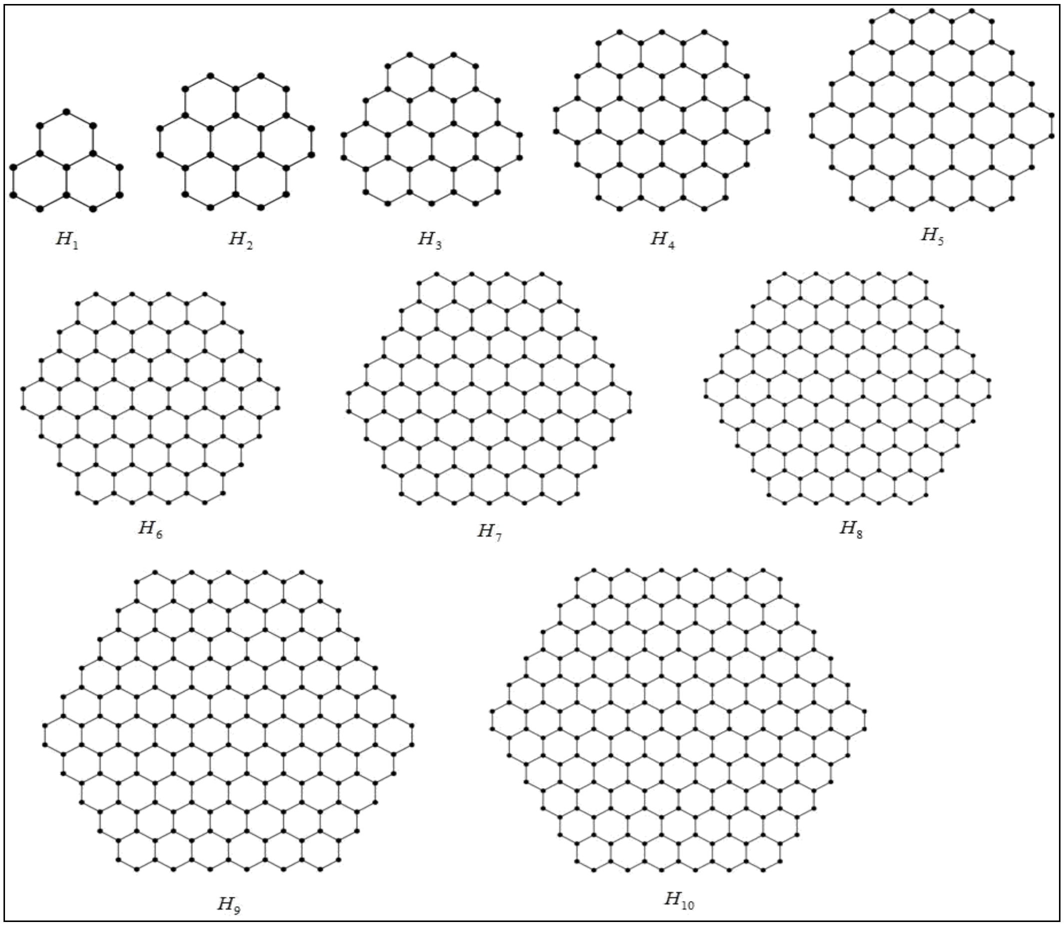


FIG. 1: THE *n*-HONEYCOMB GRAPH *Hn* WITH 1 ≤ *n* ≤ 10

We first give the Definition of this family of graphs as follows.

By the Definition, $|V(P_i)|=2k+2_i-1$ when $n \equiv 0 \pmod 2$, and $|V(H_n)|=\frac{3n^2+12n+12}{2}$, when $n \equiv 1 \pmod 2$.

Therefore, $P_i' = u^i_{k-i+1}u^i_{k-i+2}\ldots u^i_{3k+i-1}$ when $n \equiv 0 \pmod 2$, and $|V(H_n)|=\frac{3n^2+12n+11}{2}$, when $n \equiv 1 \pmod 2$.

For an *n*-honeycomb graph H_n, we denote by $H_n(i;\ i+1)$ the sub-graph induced by $V(P_i)\cup V(P_{i+1}), i=1,2,\ldots,k-1, k=\left\lceil \frac{n}{2} \right\rceil +1.$ In particular, we use $H_n(k)$ to denote the sub-graph induced by $V(P_k)\cup V(P_k')$ (*e.g.* for H_5 and H_6 see **Fig. 2**).

If *n* is even, the graph H_n is the Circumcoronene series of Benzenoid [11-29].

In this paper, we will use $E_{s;\,t}^{n}$ to denote the set $E_{s;t}$ in Hn, *e.g.* $E^5_{2,2}=\{v_{1,4}v_{1,5}, v_{1,11}v_{1,12}, v_{4,1}u_{4,1}, u_{2,3}u_{2,4}, u_{2,12}u_{2,13}\}$.

RESULT:

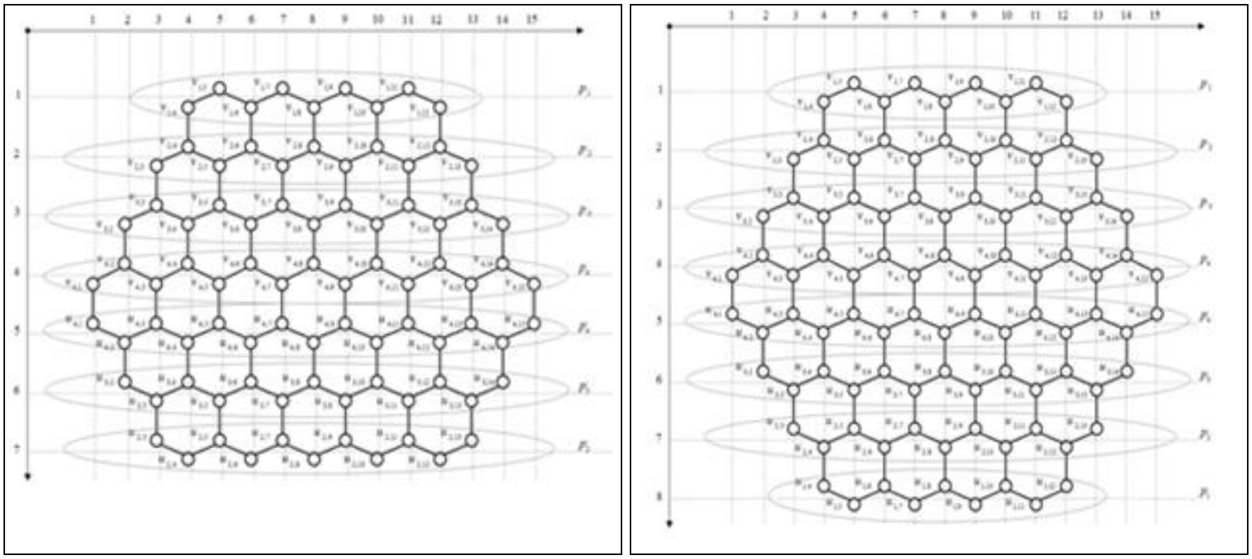
Lemma 1:

- If *n* is even, then $|E_2{}^n;_2|=6$, $|E_2{}^n;_3|=6n$ and $|E^n_{3,3}|=\frac{9n^2+6n}{4}$.
- If *n* is odd, then $|E_2{}^n;_2|=6$, $|E_2{}^n;_3|=6n$ and $|E^n_{3,3}|=\frac{9n^2+6n-3}{4}$.

Proof: i) If *n* is even, we can see that

$$|E^n_{2,2}|=\{v_{1,\frac{n}{2}+1}v_{1,\frac{n}{2}+2}, v_{1,\frac{3n}{2}+3}v_{1,\frac{3n}{2}+4}, v_{\frac{n}{2}+1,1}u_{\frac{n}{2}+1,1}, v_{\frac{n}{2}+1,2n+3}u_{\frac{n}{2}+1,2n+3}, u_{1,\frac{n}{2}+1}u_{2,\frac{n}{2}+2}, u_{1,\frac{3n}{2}+3}u_{1,\frac{3n}{2}+4}\},$$

then we have $|E_2{}^n{}_{;2}| = 6$. It can be seen that the boundary of H_n forms the set $E_2{}^n{}_{;2} \cup E_2{}^n{}_{;3}$. Note that $|E_{2,2}^n \cup E_{2,3}^n| = 6n+6$. Therefore, we have $|E_{2,3}^n| = 6n+6-|E_{2,2}^n| = 6n$.



A B

FIG. 2: (A) THE VERTICES IN *H₅*; (B) THE VERTICES IN *H₆*

Note that $E(H_n) = E_{2,2}^n \cup E_{2,3}^n \cup E_{3,3}^n$, and $\sum_{v\in V(H_n)} = \frac{9n^2+30n+24}{2} = 2|E(H_n)|$.

Since $|E_{2;2}|=6$ and $|E_{2;3}|=6n$, we have $|E_{3;3}|=4$.

ii) If n is odd, we can see that

$$|E_{2,2}^n| = \{v_{1,\frac{n+1}{2}+1}v_{1,\frac{n+1}{2}+2}, v_{1,\frac{3n}{2}+3}v_{1,\frac{3n+1}{2}+4}, v_{\frac{n+1}{2}+1,1}u_{\frac{n+1}{2}+1,1}, v_{\frac{n+1}{2}+1,2n+5}u_{\frac{n+1}{2}+1,2n+5}, u_{2,\frac{n+1}{2}}u_{2,\frac{n+1}{2}+1}, u_{2,\frac{3n+1}{2}+4}u_{2,\frac{3n+1}{2}+5}\},$$

then we have $|E_{2,2}^n| = 6$.

It can be seen that the boundary of Hn forms the set Note that

$$|E_{2,2}^n \cup E_{2,3}^n| = 3(|E(P_1)|-1) + 3(|E(P_2')|-1) = 6|E(P_1)| = 6n+6.$$

Therefore, we have $|E_{2,3}^n| = 6n+6-|E_{2,2}^n| = 6n.$

Note that $E(H_n) = E_{2,2}^n \cup E_{2,3}^n \cup E_{3,3}^n$, and $\sum_{v\in V(H_n)} = \frac{9n^2+30n+21}{2} = 2|E(H_n)|$.

Since $|E_{2;2}|=6$ and $|E_{2;3}|=6n$, we have $|E_{3,3}^n| = \frac{9n^2+6n-3}{4}$.

Theorem 1: If n is even, then

$$\text{a) } ABC(H_n) = \frac{3n^2+2n+6\sqrt{2}}{2}$$

$$\text{b) } Zg_1(H_n) = \frac{27n^2+78n+48}{2}$$

$$\text{c) } Zg_2(H_n) = \frac{81n^2+198n+96}{4}$$

d) $\chi(H_n) = \frac{3n^2 + (2+4\sqrt{6})n + 12}{4}$

e) $X(H_n) = \frac{3\sqrt{6}}{8}n^2 + (\frac{6\sqrt{6}}{8} + \frac{6\sqrt{5}}{5})n + 3$

f) $GA(H_n) = \frac{27\sqrt{6}}{4}n^2 + (\frac{72\sqrt{5}}{5} + \frac{9\sqrt{6}}{2})n + 24$

g) $Zg_1(H_n, x) = 6x^4 + 6nx^5 + \frac{9n^2 + 6n}{4}x^6$

h) $Zg_2(H_n, x) = 6x^4 + 6nx^6 + \frac{9n^2 + 6n}{4}x^9$

Proof: a) By Lemma 1, we have if *n* is even,

$$ABC(H_n) = \sum_{uv \in E_{2,2}^n} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} + \sum_{uv \in E_{2,3}^n} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} + \sum_{uv \in E_{3,3}^n} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$= 6\frac{\sqrt{2}}{2} + \frac{2}{3}(\frac{9n^2 + 6n}{4}) = \frac{3n^2 + 2n + 6\sqrt{2}}{2}.$$

b) By Lemma 1, we have if *n* is even,

$$Zg_1(H_n) = \sum_{uv \in E_{2,2}^n} (d_u + d_v) + \sum_{uv \in E_{2,3}^n} (d_u + d_v) + \sum_{uv \in E_{3,3}^n} (d_u + d_v)$$

$$= 24 + 30n + \frac{6(9n^2 + 6n)}{4} = \frac{27n^2 + 78n + 48}{2}.$$

c) By Lemma 1, we have if *n* is even,

$$Zg_2(H_n) = \sum_{uv \in E_{2,2}^n} (d_u d_v) + \sum_{uv \in E_{2,3}^n} (d_u d_v) + \sum_{uv \in E_{3,3}^n} (d_u d_v)$$

$$= 24 + 36n + \frac{9(9n^2 + 6n)}{4} = \frac{81n^2 + 198n + 96}{4}.$$

d) By Lemma 1, we have if *n* is even,

$$\chi(H_n) = \sum_{uv \in E_{2,2}^n} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{2,3}^n} \frac{1}{\sqrt{d_u d_v}} + \sum_{uv \in E_{3,3}^n} \frac{1}{\sqrt{d_u d_v}}$$

$$= 3 + 6n\frac{1}{\sqrt{6}} + \frac{\frac{1}{3}(9n^2 + 6n)}{4} = \frac{3n^2 + (2+4\sqrt{6})n + 12}{4}.$$

e) By Lemma 1, we have if *n* is even,

$$X(H_n) = \sum_{uv \in E_{2,2}^n} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv \in E_{2,3}^n} \frac{1}{\sqrt{d_u + d_v}} + \sum_{uv \in E_{3,3}^n} \frac{1}{\sqrt{d_u + d_v}}$$

$$= 3 + 6n\frac{1}{\sqrt{5}} + \frac{\frac{1}{\sqrt{6}}(9n^2 + 6n)}{4} = \frac{3\sqrt{6}}{8}n^2 + (\frac{6\sqrt{6}}{8} + \frac{6\sqrt{5}}{5})n + 3.$$

f) By Lemma 1, we have if *n* is even,

$$GA(H_n)=\sum_{uv\in E_{2,2}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{2,3}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{3,3}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}$$
$$=24+6n\frac{12}{\sqrt{5}}+\frac{\frac{18}{\sqrt{6}}(9n^2+6n)}{4}=\frac{27\sqrt{6}}{4}n^2+(\frac{72\sqrt{5}}{5}+\frac{9\sqrt{6}}{2})n+24.$$

g) Since in the graph H_n, $d_u+d_v=4$ if and only if $d_u=d_v=2$, $d_u+d_v=6$ if and only if $d_u=d_v=3$, $d_u+d_v=5$ if and only if $\{d_u; d_v\}=\{2; 3\}$, we have $Zg_1(H_n,x)=6x^4+6nx^5+\frac{9n^2+6n}{4}x^6$.

h) Since in the graph H_n, $d_ud_v=4$ if and only if $d_u=d_v=2$, $d_ud_v=9$ if and only if $d_u=d_v=3$, $d_ud_v=6$ if and only if $\{d_u; d_v\}=\{2; 3\}$, we have $Zg_z(H_n,x)=6x^4+6nx^6+\frac{9n^2+6n}{4}x^9$.

Theorem 2: If n is odd, then

a) $ABC(H_n)=\frac{3n^2+2n-1+6\sqrt{2}}{2}$

b) $Zg_1(H_n)=\frac{27n^2+78n+39}{2}$

c) $Zg_2(H_n)=\frac{81n^2+198n+69}{4}$

d) $\chi(H_n)=\frac{3n^2+(2+4\sqrt{6})n+11}{4}$

e) $X(H_n)=\frac{3\sqrt{6}}{8}n^2+(\frac{6\sqrt{6}}{8}+\frac{6\sqrt{5}}{5})n+3-\frac{\sqrt{6}}{8}$

f) $GA(H_n)=\frac{27\sqrt{6}}{4}n^2+(\frac{72\sqrt{5}}{5}+\frac{9\sqrt{6}}{2})n+24-\frac{9\sqrt{6}}{4}$

g) $Zg_1(H_n,x)=6x^4+6nx^5+\frac{9n^2+6n-3}{4}x^6$

h) $Zg_2(H_n,x)=6x^4+6nx^6+\frac{9n^2+6n-3}{4}x^9$

Proof:

a) By Lemma 1, we have if *n* is odd,

$$ABC(H_n)=\sum_{uv\in E_{2,2}^n}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{uv\in E_{2,3}^n}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{uv\in E_{3,3}^n}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$
$$=6\frac{\sqrt{2}}{2}+\frac{2}{3}(\frac{9n^2+6n-3}{4})=\frac{3n^2+2n-1+6\sqrt{2}}{2}.$$

b) By Lemma 1, we have if n is even,

$$Zg_1(H_n)=\sum_{uv\in E_{2,2}^n}(d_u+d_v)+\sum_{uv\in E_{2,3}^n}(d_u+d_v)+\sum_{uv\in E_{3,3}^n}(d_u+d_v)$$
$$=24+30n+\frac{6(9n^2+6n-3)}{4}=\frac{27n^2+78n+39}{2}.$$

c) By Lemma 1, we have if n is even,

$$Zg_2(H_n)=\sum_{uv\in E_{2,2}^n}(d_ud_v)+\sum_{uv\in E_{2,3}^n}(d_ud_v)+\sum_{uv\in E_{3,3}^n}(d_ud_v)$$
$$=24+36n+\frac{9(9n^2+6n-3)}{4}=\frac{81n^2+198n+69}{4}$$

d) By Lemma 1, we have if n is even,

$$\chi(H_n)=\sum_{uv\in E_{2,2}^n}\frac{1}{\sqrt{d_ud_v}}+\sum_{uv\in E_{2,3}^n}\frac{1}{\sqrt{d_ud_v}}+\sum_{uv\in E_{3,3}^n}\frac{1}{\sqrt{d_ud_v}}$$
$$=3+6n\frac{1}{\sqrt{6}}+\frac{\frac{1}{3}(9n^2+6n-3)}{4}=\frac{3n^2+(2+4\sqrt{6})n+11}{4}.$$

e) By Lemma 1, we have if n is even,

$$X(H_n)=\sum_{uv\in E_{2,2}^n}\frac{1}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{2,3}^n}\frac{1}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{3,3}^n}\frac{1}{\sqrt{d_u+d_v}}$$
$$=3+6n\frac{1}{\sqrt{5}}+\frac{\frac{1}{\sqrt{6}}(9n^2+6n-3)}{4}=\frac{3\sqrt{6}}{8}n^2+(\frac{6\sqrt{6}}{8}+\frac{6\sqrt{5}}{5})n+3-\frac{\sqrt{6}}{8}$$

f) By Lemma 1, we have if n is even,

$$GA(H_n)=\sum_{uv\in E_{2,2}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{2,3}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}+\sum_{uv\in E_{3,3}^n}\frac{2d_ud_v}{\sqrt{d_u+d_v}}$$
$$=24+6n\frac{12}{\sqrt{5}}+\frac{\frac{18}{\sqrt{6}}(9n^2+6n-3)}{4}=\frac{27\sqrt{6}}{4}n^2+(\frac{72\sqrt{5}}{5}+\frac{9\sqrt{6}}{2})n+24-\frac{9\sqrt{6}}{4}.$$

g) Since in the graph H_n, $d_u+d_v=4$ if and only if $d_u=d_v=2$, $d_u+d_v=6$ if and only if $d_u=d_v=3$, $d_u+d_v=5$ if and only if $\{d_u; d_v\}=\{2; 3\}$, we have $Zg_1(H_n,x)=6x^4+6nx^5+\frac{9n^2+6n-3}{4}x^6$.

h) Since in the graph H_n, $d_ud_v=4$ if and only if $d_u=d_v=2$, $d_ud_v=9$ if and only if $d_u=d_v=3$, $d_ud_v=6$ if and only if $\{d_u; d_v\}=\{2; 3\}$, we have $Zg_z(H_n,x)=6x^4+6nx^6+\frac{9n^2+6n-3}{4}x^9$.

CONCLUSION: In this paper, we computed topological indices "Randić connectivity index, sum-connectivity index, atom-bond connectivity index, geometric-arithmetic index, First and Second Zagreb indices and Zagreb polynomials" of a honeycomb graph Hk. Formulas for computing the above topological descriptors in honeycomb graphs are given and such results of other types of chemical graphs.

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