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ON HYPER ZAGREB INDEX OF CERTAIN GENERALIZED GRAPH STRUCTURES

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Abstract: Let $G = (V, E)$ be a graph with n vertices and m edges. The hyper Zagreb index of G, denoted by $HM(G)$, is defined as

$$HM(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2 ,$$

where $d_G(v)$ denotes the degree of a vertex v in G. In this paper we compute the hyper Zagreb index of certain generalized graph structures such as generalized thorn graphs and generalized theta graphs. Also,for the first time, we determine exact values for hyper Zagreb index of some cycle related graphs, namely cycle with parallel P_k chords, cycle with parallel C_k chords and shell type graphs.

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1. Introduction

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. In mathematical chemistry, molecules are often modeled by graphs named “molecular graphs. A molecular graph is a simple graph in which vertices are the atoms and edges are bonds between them. By IUPAC terminology, a topological index is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

In chemical graph theory, a graphical invariant is a number related to a graph which is structurally invariant. These invariant numbers are also known as the topological indices. The well-known Zagreb indices are one of the oldest graph invariants firstly introduced by Gutman and Trinajestić [13] more than forty years ago, where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structures, and this was elaborated on in [12].

Throughout this paper we consider only simple and connected graphs. For a graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$, the order (number of vertices) and size (number of edges) of G are denoted by n and m respectively. The degree of a vertex v in G is the number of edges incident to v and denoted by $d_G(v)$.

For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined as follows:

$$M_1 = M_1(G) = \sum_{v\in V(G)} d_G^2(v), \quad M_2 = M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

Also, $M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$. For more details on these indices see the recent papers [3, 4, 6, 7, 8, 11, 14, 18, 19, 29, 30, 31] and the references therein.

Miličevič et al. [20] in 2004 defined reformulated the Zagreb indices in terms of edge degrees instead of vertex degrees as:

$$EM_1(G) = \sum_{e\in E(G)} d(e)^2$$

and

$$EM_2(G) = \sum_{e\sim f} d(e)d(f),$$

where $d(e)$ represents the degree of the edge e in G, which is defined by $d(e) = d(u) + d(v) - 2$ with $e = uv$ and $e \sim f$ represents that the edges e and f are adjacent.

Shirdel et al. in [24] defined hyper Zagreb index, as:

$$HM(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^2$$

and discussed some graph operations of the hyper Zagreb index in [24].

Gao et al. [9]presented exact expressions for the hyper-Zagreb index of graph operations containing cartesian product and join of n graphs, splice, link and chain of graphs. Veylaki et al. [27] calculated third and hyper Zagreb coindices of graph operations containing the Cartesian product and composition. Suresh Elumalai et al. [25] obtained some bounds on the hyper Zagreb index. An excellent survey of several variants of Zagreb indices has been done by Gutman et al. in [10].

Vukičevič et al. [28] calculated the modified Wiener index of thorn graphs. In [32] Zhou et al. found an explicit formula to calculate the variable Wiener index of thorn graphs. Zhou et al.[33] derived the expression for Wiener-type polynomials of thorn graphs. Heydari et al. [15] calculated terminal Weiner index of thorn graphs. Nilanjan De et al. computed F-index of t-thorn graphs in [21]. For recent results on F-index, please refer [1, 2, 22]. K.M.Kathiresan et al.[17] obtained some bounds on the Wiener index of certain generalized thorn graphs. Venkatakrishnan et al. [26] computed eccentric connectivity index of the same structures.

1.1. Hyper Zagreb index of generalized thorn graphs

The *t-thorn graph* of a graph G, denoted by G^t, is a graph obtained by joining t copies of pendent edges known as thorns to each vertex of G.

In this section, we compute the Hyper Zagreb index of the following four types of generalized thorn graphs.

Let G be a graph of order n and size m respectively. Let $V(G) = \{v_1, v_2, \cdots, v_n\}$.

Generalized thorn graph of Type-I

Attach t_i copies of a path of order $r \geq 2$ at each vertex v_i of G by identifying the vertex v_i as the initial vertex of such paths. The resulting graph thus obtained is denoted by G_P.

Generalized thorn graph of Type-II

Attach t_i copies of a cycle of length r to each vertex v_i of G by identifying v_i as a vertex in each cycle. The resulting graph thus obtained is denoted by G_C.

Generalized thorn graph of Type-III

Attach t_i copies of a complete graph K_r of order $r \geq 3$ to each vertex v_i of G by identifying v_i as a vertex in K_r. The graph thus obtained is denoted by G_K.

Generalized thorn graph of Type-IV

Attach t_i copies of a complete bipartite graph $K_{r,s}$ to each vertex v_i of G by identifying v_i as a vertex in a partition of $K_{r,s}$ containing r vertices. The resulting graph thus obtained is denoted by G_A.

Generalized thorn graph of Type-V

Generalized thorn graph of Type-VI

To every vertex v_i of G, join t_i copies of K_p each by an edge. The graph thus obtained is denoted by $G_K^{'}$.

Generalized thorn graph of Type-VII

To every vertex v_i of G, join t_i copies of a complete bipartite graph $K_{r,s}$ each by an edge.

Theorem 1. $HM(G_P) = HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] \times (t_i + t_j) + \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + (16r - 35) + \sum_{i=1}^{n} t_i + \sum_{i=1}^{n} \left[t_i d(v_i)^2 + t_i^3 + 4t_i^2 + 2t_i^2 d(v_i) + 4t_i d(v_i)\right]$.

Proof. In the generalized thorn graph G_P of G, $d_{G_P}(v_i) = d(v_i) + t_i$, for any vertex $v_i \in V(G)$. Therefore,

$$\begin{aligned} HM(G_P) &= \sum_{v_iv_j \in E(G_P)} [d(v_i) + d(v_j)]^2 \\ &= \sum_{v_iv_j \in E(G_P)} [d(v_i) + t_i + d(v_j) + t_j]^2 \\ &\quad + \sum_{i=1}^{n} t_i \left[d(v_i) + t_i + 2\right]^2 + 16(r-3) \sum_{i=1}^{n} t_i + 9 \sum_{i=1}^{n} t_i \\ &= HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] (t_i + t_j) \end{aligned}$$

$$+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+\sum_{i=1}^{n}t_i\left[d(v_i)^2+(t_i+2)^2+2d(v_i)(t_i+2)\right]$$

$$+(16r-35)\sum_{i=1}^{n}t_i$$

$$=HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right](t_i+t_j)$$

$$+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+\sum_{i=1}^{n}\left[t_id(v_i)^2+t_i^3+4t_i^2+2t_i^2d(v_i)+4t_id(v_i)\right]$$

$$+(16r-35)\sum_{i=1}^{n}t_i.$$

□

Corollary 2. *If $t_i = t$, for all $1 \leq i \leq n$, then $HM(G_P) = HM(G) + 5tM_1(G) + 8mt^2 + nt^3 + 4nt^2 + 16mt + 16rnt - 35nt$.*

Example 3. **(i)** *If $G \cong P_n$ and $t_i = t$ for all $1 \leq i \leq n$, then $HM(G_P) = 16n + (12n-8)t^2 + 16nt(r+1) - 15nt - 46t - 30$. In particular, if $r = 2$, we get the thorn tree $\mathcal{T}$ (refer Figure 1) and $HM(\mathcal{T}) = 16n + (12n-8)t^2 + 33nt - 46t - 30$.*

(ii) *If $G \cong C_n$ and $t_i = t$ for all $1 \leq i \leq n$, then $HM(G_P) = 16n(rt+1) + nt + 12nt^2 + nt^3$.*

Theorem 4. $HM(G_C) = HM(G) + 4\sum_{v_iv_j\in E(G)}[d(v_i)+d(v_j)]$

$$\times(t_i+t_j)+4\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+2\sum_{i=1}^{n}t_id(v_i)^2$$

$$+8\sum_{i=1}^{n}\left[d(v_i)t_i^2+d(v_i)t_i+t_i^3+2t_i^2\right]+(16r-24)\sum_{i=1}^{n}t_i.$$

Proof.

$$HM(G_C)=\sum_{v_iv_j\in E(G_C)}\left[d(v_i)+d(v_j)\right]^2$$

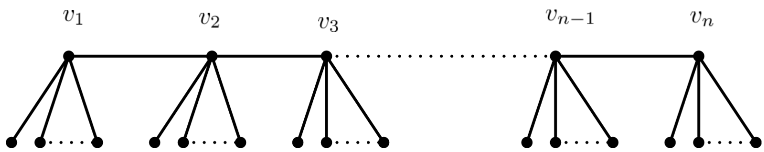

Figure 1: Thorn tree $\mathcal{T}$

$$
\begin{aligned}
&= \sum_{v_iv_j \in E(G)} [d(v_i)2t_i + d(v_j) + 2t_j]^2 \\
&= HM(G) + 4 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] (t_i + t_j) \\
&\quad +4 \sum_{i=1}^{n} (t_i + t_j)^2 + 2 \sum_{i=1}^{n} t_i (d(v_i)^2 + 4d(v_i)(t_i + 1) + 4t_i^2 \\
&\quad +8t_i + 4) + (16r - 32) \sum_{i=1}^{n} t_i \\
&= HM(G) + 4 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] (t_i + t_j) \\
&\quad +4 \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + 2 \sum_{i=1}^{n} t_i d(v_i)^2 \\
&\quad +8 \sum_{i=1}^{n} \left[d(v_i)t_i^2 + d(v_i)t_i + t_i^3 + 2t_i^2\right] + (16r - 24) \sum_{i=1}^{n} t_i
\end{aligned}
$$

□

Corollary 5. *If $t_i = t$, for all $1 \leq i \leq n$, then $HM(G_C) = HM(G) + 10tM_1(G) + 32mt^2 + 16mt + 8nt^3 + 16nt^2 + (16r - 24)nt$.*

Example 6. **(i)** *If $G \cong P_n$ and $t_i = t$ for all $1 \leq i \leq n$, then $HM(G_C) = 8nt^3 + 48nt^2 + 32nt + 16n(rt + 1) - 32t^2 - 76t - 30$.*

(ii) *If $G \cong C_n$ and $t_i = t$ for all $1 \leq i \leq n$, then $HM(G_C) = 8nt^3 + 48nt^2 + 32nt + 16n(rt + 1)$.*

Theorem 7. $HM(G_K) = HM(G) + 2(r-1)\sum_{v_iv_j\in E(G)}[d(v_i)+d(v_j)]$
$\times (t_i+t_j) + (r-1)^2\sum_{v_iv_j\in E(G)}(t_i+t_j)^2 + (r-1)$
$\times \sum_{i=1}^{n} t_i d(v_i)^2 + 2(r-1)^2\sum_{i=1}^{n} d(v_i)t_i(t_i+1) + (r-1)^3\sum_{i=1}^{n}\left[t_i^3+2t_i^2+(2r-1)t_i\right].$

Proof.

$$\begin{aligned}
HM(G_K) &= \sum_{v_iv_j\in E(G_K)}[d(v_i)+d(v_j)]^2\\
&= \sum_{v_iv_j\in E(G)}[d(v_i)+t_i(r-1)+d(v_j)+t_j(r-1)]^2\\
&\quad +(r-1)\sum_{i=1}^{n} t_i\left[d(v_i)+t_i(r-1)+(r-1)\right]^2\\
&\quad +\frac{(r-1)(r-2)}{2}\sum_{i=1}^{n} t_i(2r-2)^2\\
&= HM(G)+2(r-1)\sum_{v_iv_j\in E(G)}[d(v_i)+d(v_j)]\,[t_i+t_j]\\
&\quad +(r-1)^2\sum_{v_iv_j\in E(G)}(t_i+t_j)^2\\
&\quad +(r-1)\sum_{i=1}^{n} t_i\left[d(v_i)^2+2(r-1)d(v_i)(t_i+1)+(r-1)^2(t_i+1)^2\right]\\
&\quad +2(r-1)^3(r-2)\sum_{i=1}^{n} t_i
\end{aligned}$$

$$\begin{aligned}
&= HM(G)+2(r-1)\sum_{v_iv_j\in E(G)}[d(v_i)+d(v_j)]\,[t_i+t_j]\\
&\quad +(r-1)^2\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+(r-1)\sum_{i=1}^{n} t_i d(v_i)^2\\
&\quad +2(r-1)^2\sum_{i=1}^{n} d(v_i)t_i(t_i+1)+(r-1)^3\sum_{i=1}^{n}\left[t_i(t_i+1)^2+2(r-2)t_i\right]
\end{aligned}$$

$$= HM(G) + 2(r-1) \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] [t_i + t_j]$$

$$+(r-1)^2 \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + (r-1) \sum_{i=1}^{n} t_i d(v_i)^2$$

$$+2(r-1)^2 \sum_{i=1}^{n} d(v_i) t_i (t_i + 1) + (r-1)^3 \sum_{i=1}^{n} \left[t_i^3 + 2t_i^2 + 2(r-1)t_i\right]$$

□

Corollary 8. *If* $t_i = t$*, for all* $1 \leq i \leq n$*,* $HM(G_K) = HM(G) + 5t(r-1)M_1(G) + 4mt(t+1)(r-1)^2 + n(r-1)^3(t^3 + 2t^2 + 2(r-1)t)$

Example 9. **(i)** *If* $G \cong P_n$ *and* $t_i = t$ *for all* $1 \leq i \leq n$*, then* $HM(G_K) = 16n - 30 + (20n-30)t(r-1) + (r-1)^2(n(r-1)t^3 + (2n-4)t^2 + (6n-4)t + 2nrt(r+t-2))$.

(ii) *If* $G \cong C_n$ *and* $t_i = t$ *for all* $1 \leq i \leq n$*, then* $HM(G) = 16n + 20nt(r-1) + 4nt(t+1)(r-1)^2 + n(r-1)^3(t^3 + 2t^2 + 2(r-1)t)$.

Theorem 10. $HM(G_A) = HM(G) + 2s \sum\limits_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] \times (t_i + t_j) + \sum\limits_{i=1}^{n} st_i \left[d(v_i) + r + s^2 + r^2 + st_i + 2rs\right]$.

Proof.

$$\begin{aligned} HM(G_A) &= \sum_{v_iv_j \in E(G_A)} [d(v_i) + d(v_j)]^2 \\ &= \sum_{v_iv_j \in E(G)} [d(v_i) + t_i s + d(v_j) + t_j s]^2 \\ &\quad + \sum_{i=1}^{n} st_i [d(v_i) + t_i s + r] + \sum_{i=1}^{n} t_i s (s+r)^2 \\ &= HM(G) + 2s \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] (t_i + t_j) \end{aligned}$$

$$+\sum_{i=1}^{n} st_i \left[d(v_i) + r + s^2 + r^2 + st_i + 2rs\right]$$

□

Corollary 11. *If $t_i = t$, for all $1 \leq i \leq n$, then $HM(G_A) = HM(G) + 4tsM_1(G) + 2mst + st(r + s^2 + r^2)n + s^2t^2n + 2rs^2tn$. Further, if $r = s$, then $HM(G_A) = HM(G) + 4tsM_1(G) + 2mst + ns^2t + ns^2t^2 + 2tns^3$.*

Example 12. **(i)** *If $G \cong P_n$, $t_i = t$ for all $1 \leq i \leq n$ and $r = s$, then $HM(G_A) = 16n - 30 + 18nst - 26st + ns^2t + ns^2t^2 + 2tns^3$,*

(ii) *If $G \cong C_n$, $t_i = t$ for all $1 \leq i \leq n$ and $r = s$, then $HM(G_A) = 16n + 18nst + ns^2t + ns^2t^2 + 2tns^3$.*

Theorem 13. $HM(G_C^{'}) = HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)]$
$\times (t_i + t_j) + \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + M_1(G) + 2 \sum_{i=1}^{n} d(v_i)t_i$
$+ \sum_{i=1}^{n} \left[t_i^2 + (16r - 24)t_i\right] + 9n + 12m.$

Proof.

$$\begin{aligned}
HM(G_C^{'}) = & \sum_{v_iv_j \in E(G_C^{'})} \left[d_{G_C^{'}}(v_i) + d_{G_C^{'}}(v_j)\right]^2 \\
= & \sum_{v_iv_j \in E(G)} [d(v_i) + t_i + d(V_j) + t_j]^2 + \sum_{i=1}^{n} [d(v_i) + t_i + 3]^2 \\
& +50 \sum_{i=1}^{n} t_i + 16(r-2) \sum_{i=1}^{n} t_i \\
= & \, HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] (t_i + t_j) \\
& + \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + \sum_{i=1}^{n} d(v_i)^2
\end{aligned}$$

$$+2\sum_{i=1}^{n} d(v_i)(t_i+3)+\sum_{i=1}^{n}(t_i+3)^2+50\sum_{i=1}^{n} t_i+16(r-2)\sum_{i=1}^{n} t_i$$
$$=HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right](t_i+t_j)$$
$$+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+M_1(G)$$
$$+2\sum_{i=1}^{n} d(v_i)t_i+\sum_{i=1}^{n}\left[t_i^2+(16r-24)t_i\right]+9n+12m$$

□

Corollary 14. *If $t_i=t$, for all $1\le i\le n$, then* $HM(G_C^{'})=HM(G)+(4t+1)M_1(G)+4mt(t+1)+nt^2+nt(16r-24)+12m+9n.$

Example 15. **(i)** *If $G\cong P_n$ and $t_i=t$ for all $1\le i\le n$, then $HM(G_C^{'})=(5n-4)t^2+4nt(4r-1)+12(n-t)-44$,*

(ii) *If $G\cong C_n$ and $t_i=t$ for all $1\le i\le n$, then $HM(G_C^{'})=29n+nt(t-4)+16n(rt+1)$.*

Theorem 16. $HM(G_K^{'})=HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right]$
$\times(t_i+t_j)+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+\sum_{i=1}^{n} t_id(v_i)$
$+\sum_{i=1}^{n} t_i^2+(2r^4-6r^3-10r^2+15r)\sum_{i=1}^{n} t_i.$

Proof.

$$HM(G_K^{'})=\sum_{v_iv_j\in E(G_K^{'})}\left[d_{G_K^{'}}(v_i)+d_{G_K^{'}}(v_j)\right]^2$$
$$=\sum_{v_iv_j\in E(G)}\left[d(v_i)+t_i+d(v_j)+t_j\right]^2+\sum_{i=1}^{n} t_i\left[d(v_i)+t_i+r\right]$$
$$+2\sum_{i=1}^{n} t_i(2r-1)^2+\left[\frac{r(r-1)}{2}-2\right]\sum_{i=1}^{n} t_i(2r-2)^2$$
$$=HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right](t_i+t_j)+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2$$

$$+\sum_{i=1}^{n} t_i d(v_i)+\sum_{i=1}^{n} t_i^2+r\sum_{i=1}^{n} t_i+2r(r-1)^3\sum_{i=1}^{n} t_i$$
$$-8(r-1)^2\sum_{i=1}^{n} t_i = HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right](t_i+t_j)$$
$$+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2+\sum_{i=1}^{n} t_i d(v_i)+\sum_{i=1}^{n} t_i^2+\left[2r(r-1)^3-8(r-1)^2+r\right]\sum_{i=1}^{n} t_i.$$

Therefore,

$$HM(G_K^{'}) = HM(G)+2\sum_{v_iv_j\in E(G)}\left[d(v_i)+d(v_j)\right](t_i+t_j)$$
$$+\sum_{v_iv_j\in E(G)}(t_i+t_j)^2$$
$$+\sum_{i=1}^{n} t_i d(v_i)+\sum_{i=1}^{n} t_i^2+(2r^4-6r^3-10r^2+15r)\sum_{i=1}^{n} t_i.$$

□

Corollary 17. *If $t_i = t$, for all $1 \le i \le n$, then $HM(G_K^{'}) = HM(G) + 4tM_1(G) + 4mt^2 + 2mt + nt^2 + (2r^4 - 6r^3 - 10r^2 + 15r)nt$.*

Example 18. **(i)** *If $G \cong P_n$ and $t_i = t$ for all $1 \le i \le n$, then $HM(G_K^{'}) = 16n - 30 + (18n - 10)t + (5n - 4)t^2 + (2r^4 - 6r^3 - 10r^2 + 15r)nt$,*

(ii) *If $G \cong C_n$ and $t_i = t$ for all $1 \le i \le n$, then $HM(G_K^{'}) = 16n + (5t + 18)nt + (2r^4 - 6r^3 - 10r^2 + 15r)nt$.*

Theorem 19. $HM(G_A^{'}) = HM(G) + \sum_{v_iv_j\in E(G)} [d(v_i) + d(v_j)]$
$\times (t_i + t_j) + \sum_{v_iv_j\in E(G)} (t_i + t_j)^2 + \sum_{i=1}^{n} t_i d(v_i)^2 + 2\sum_{i=1}^{n} t_i^2 d(v_i) + \sum_{i=1}^{n} t_i^3$
$+ 2(s + 1)\sum_{i=1}^{n} d(v_i)t_i + 2\sum_{i=1}^{n} t_i^2 + (s^2 + 3s + 2s(s + r)(s + r + 1) + 1)\sum_{i=1}^{n} t_i.$

Proof.

$$
\begin{aligned}
HM(G'_A) &= \sum_{v_iv_j \in E(G'_A)} \left[d_{G'_A}(v_i) + d_{G'_A}(v_j)\right]^2 \\
&= \sum_{v_iv_j \in E(G)} [d(v_i) + t_i + d(v_j) + t_j]^2 \\
&\quad + \sum_{i=1}^{n} t_i \, [d(v_i) + t_i + s + 1]^2 \\
&\quad + \sum_{i=1}^{n} t_i s \, [s + r + 1]^2 + \sum_{i=1}^{n} t_i s (s + r)^2 \\
&= HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] \, (t_i + t_j) \\
&\quad + \sum_{v_iv_j \in E(G)} (t_i + t_j)^2
\end{aligned}
$$

$$
\begin{aligned}
&+ \sum_{i=1}^{n} t_i \left[(d(v_i) + 1)^2 + (t_i + s)^2 + 2(d(v_i) + 1)(t_i + s)\right] \\
&+ \sum_{i=1}^{n} t_i s \left[(s + r + 1)^2 + (s + r)^2\right] \\
&= HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] \, (t_i + t_j) \\
&+ \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + \sum_{i=1}^{n} t_i \left[d(v_i)^2 + 2d(v_i) + 1\right] \\
&+ \sum_{i=1}^{n} \left[t_i(t_i^2 + 2st_i + s^2)\right] + 2 \sum_{i=1}^{n} [t_i(t_i + s)(d(v_i) + 1)] \\
&+ \sum_{i=1}^{n} t_i s \left\{\left[(s + r)^2 + 2(s + r) + 1\right] + (s + r)^2\right\} \\
&= HM(G) + 2 \sum_{v_iv_j \in E(G)} [d(v_i) + d(v_j)] \, (t_i + t_j) \\
&+ \sum_{v_iv_j \in E(G)} (t_i + t_j)^2 + \sum_{i=1}^{n} t_i d(v_i)^2
\end{aligned}
$$

$$+2\sum_{i=1}^{n} t_i^2 d(v_i) + \sum_{i=1}^{n} t_i^3 + 2(s+1)\sum_{i=1}^{n} d(v_i)t_i$$
$$+2(s+1)\sum_{i=1}^{n} t_i^2 + (s^2+3s+2s(s+r)(s+r+1)+1)\sum_{i=1}^{n} t_i$$

□

Corollary 20. *If $t_i = t$ for all $1 \leq i \leq n$, then $HM(G_A^{'}) = HM(G) + 3tM_1(G) + 8mt^2 + nt^3 + 4mt(s+1) + 2nt^2(s+1) + (s^2+3s+1)nt + 2s(s+r)(s+r+1)nt$.*

Example 21. **(i)** *If $G \cong P_n, t_i = t$ for all $1 \leq i \leq n$ and $r = s$, then $HM(G_A^{'}) = 16n - 30 + 17nt - 10t + 10nt^2 - 8t^2 + nt^3 + 11nst - 4st + 2nst^2 + 9ns^2t$. Further if $r = s = t$, then $HM(G_A^{'}) = 16n - 30 + 35nr + 12nr^3 + (21n-12)r^2 - 10r$.*

(ii) *If $G \cong C_n, t_i = t$ for all $1 \leq i \leq n$ and $r = s$, then $HM(G_A^{'}) = 16n + 17nt + 10nt^2 + 11nst + 9ns^2t + 2nst^2 + nt^3$. Further if $r = s = t$, then $HM(G_A^{'}) = 16n + 17nr + 21nr^2 + 12nr^3$.*

1.2. Hyper Zagreb index of generalized theta graphs

In this section, we compute the hyper Zagreb index of some generalized theta-graphs.

Definition 22. ([5]) The generalized theta-graph $\Theta(l_1, l_2, \cdots, l_k)$ consists of two vertices u and v joined by internally disjoint paths of lengths $l_1, l_2, \cdots, l_k$.

A particular case of this structure can be found in [23].

Definition 23. A book B_k is a generalized theta-graph $\Theta(2, 2, \cdots, 2)$ that consists of k internally disjoint paths of length 2.

Definition 24. The hanging generalized theta-graph $\mathcal{G}_\Theta = G(\Theta_1, \Theta_2, \cdots, \Theta_r; u_1, u_2, \cdots, u_r)$, where $\Theta_i = \Theta(l_{i1}, l_{i2}, \cdots, l_{ik_i})$; $1 \leq i \leq r$, is a graph obtained by attaching a generalized theta-graph Θ_i to a vertex u_i of the path $P_r =< u_1, u_2, \cdots, u_r >$ of length $r-1$ after identifying u_i as a vertex of Θ_i.

Theorem 25. *For a generalized theta-graph* $\Theta = \Theta(l_1, l_2, \cdots, l_k)$, $HM(\Theta) = 2k(k+2)^2 + 16\sum_{i=1}^{k}(l_i - 2)$.

Proof. Let u and v be two vertices of Θ which are joined internally by k disjoint paths of lengths $l_1, l_2, \cdots, l_k$ respectively. Then $deg_\Theta(u) = deg_\Theta(v) = k$,

$$HM(\Theta) = \sum_{xy\in E(\Theta)} (deg(x) + deg(y))^2$$
$$= 2k(k+2)^2 + 16\sum_{i=1}^{k}(l_i - 2).$$

□

Corollary 26. *If* $l_1 = l_2 = \cdots = l_k = n-1$, *then* $HM(\Theta) = 2k(k+2)^2 + 16k(n-3)$.

Example 27. *For a book graph* B_k, $HM(B_k) = 2k(k+2)^2$.

Theorem 28. *For a hanging theta-graphs* $\mathcal{G}_\Theta$,
$HM(\mathcal{G}_\Theta) = 2\sum_{i=1}^{r} k_i(k_i+3)^2 + 16\sum_{i=1}^{r}\sum_{j=1}^{k_i}(l_{ij} - 2)$
$+ (k_1 + k_2 + 3)^2 + (k_{r-1} + k_r + 3)^2 + \sum_{i=2}^{r-2}(k_i + k_{i+1} + 4)^2$,
where $r \geq 2$.

Proof. In $\mathcal{G}_\Theta$, $d(u_1) = k_1 + 1,\ d(u_r) = k_r + 1$ and $\dot{(u_i)} = k_i + 2,\ for\ 2 \leq i \leq r-1$. So,

$$HM(\mathcal{G}_\Theta) = \sum_{xy\in E(\mathcal{G}_\Theta)} (d(x) + d(y))^2$$
$$= 2\sum_{i=1}^{4} k_i(k_i+3)^2 + 16\sum_{i=1}^{r}\sum_{j=1}^{k_i}(l_{ij} - 2)$$
$$+ (k_1 + k_2 + 3)^2 + (k_{r-1} + k_r + 3)^2 + \sum_{i=2}^{r-2}(k_i + k_{i+1} + 4)^2.$$

□

Corollary 29. *If* $l_{ij} = n-1$,*for all* $1 \le j \le k_i$ *and* $1 \le i \le r$, *then* $HM(\mathcal{G}_\Theta) = 2\sum_{i=1}^{r} k_i(k_i+2)^2 + 16(n-3)\sum_{i=1}^{r} k_i + (k_1+k_2+3)^2 + (k_r+k_{r-1}+3)^2 + \sum_{i=2}^{r-2}(k_i+k_{i+1}+4)^2$.

Corollary 30. *If* $l_{ij} = n-1$,*for all* $1 \le j \le k_i$ *and* $1 \le i \le r$ *and* $k_1 = k_2 = \cdots = k_r = k$, *then* $HM(\mathcal{G}_\Theta) = [2rk+4r-16](k+2)^2 + 16rk(n-3) + 2(2k+3)^2$.

1.3. Hyper Zagreb index of some cycle related graphs

In this section we compute exact values for hyper Zagreb index of cycle related graphs such as cycle with parallel P_k chords, cycle with parallel C_k chords and shell type graphs. The definitions which we use in this section are taken from [16].

1.3.1. Cycle with parallel P_k chords

Definition 31. A cycle with parallel P_k chords, denoted by, $C(n, P_k)$ ia a graph obtained from a cycle $C_n : \langle v_0, v_1, \cdots, v_{n-1}v_0\rangle$ of order $n \ge 6$ by adding disjoint paths P_k of order k between the pairs of vertices $(v_1, v_{n-1}), (v_2, v_{n-2}), \cdots, (v_\alpha, v_\beta)$ of C_n where $\alpha = \left\lfloor \frac{n}{2} \right\rfloor - 1$ and $\beta = \left\lfloor \frac{n}{2} \right\rfloor + 1$, if n is even and $\beta = \left\lfloor \frac{n}{2} \right\rfloor + 2$, if n is odd.

Theorem 32. $$HM[C(n,P_k)] = \begin{cases} (16k+2)\left\lfloor \frac{n}{2} \right\rfloor + 36n - 16k - 46, \\ \textit{if } n \textit{ is even}, \\ (16k+2)\left\lfloor \frac{n}{2} \right\rfloor + 36n - 16k - 66, \\ \textit{if } n \textit{ is odd}. \end{cases}$$

Proof. **Case 1: n is even.**
First, we observe the following edge partition in $C(n, P_k)$

Edge uv with $(d(u), d(v))$	**Number of edges**
(2,2)	$\alpha(k-3)$
(2,3)	$2\left\lfloor \frac{n}{2} \right\rfloor + 2$
(3,3)	n-4

where $\alpha = \left\lfloor \frac{n}{2} \right\rfloor - 1$.

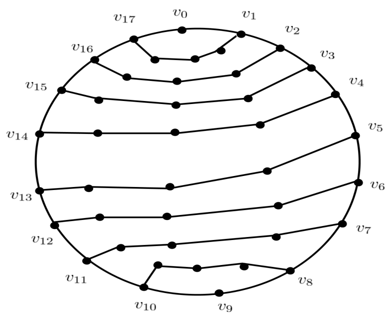

Figure 2: Cycle $C(18, P_5)$ with parallel P_5 chords

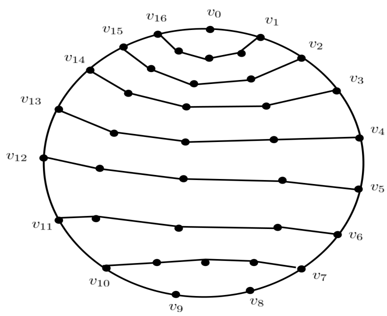

Figure 3: Cycle $C(17, P_5)$ with parallel P_5 chords

Now,

$$\begin{aligned} HM\left[C(n,P_k)\right] &= 16\alpha(k-3) + 50\left(\left\lfloor \frac{n}{2} \right\rfloor + 1\right) + 36(n-4) \\ &= (16k+2)\left\lfloor \frac{n}{2} \right\rfloor + 36n - 16k - 46. \end{aligned}$$

Case 2: n is odd.
In this case, we have the following edge partition

Edge uv with $(d(u), d(v))$	**Number of edges**
$(2,2)$	$\alpha(k-3)+1$
$(2,3)$	$2\left\lfloor \frac{n}{2} \right\rfloor + 2$
$(3,3)$	$n-5$

where $\alpha = \left\lfloor \frac{n}{2} \right\rfloor - 1$.

Using the above edge partition and by usual calculations, we get

$$HM\left[C(n,P_k)\right] = 16\left[\alpha(k-3)+1\right] + 25\left[2\left\lfloor\frac{n}{2}\right\rfloor + 2\right] + 36(n-5)$$
$$= (16k+2)\left\lfloor\frac{n}{2}\right\rfloor + 36n - 16k - 66.$$

□

1.3.2. Cycle with parallel C_k chords

In this section we determine the exact value for hyper Zagreb index of a cycle with parallel C_k chord and it is defined as follows.

Definition 33. Let $C_n : v_1, v_2, \cdots, v_n$ be a cycle of order n and C_k be another cycle of length k. Then a cycle with parallel C_K chords, denoted by $C(n, C_k)$ is a graph obtained from C_n by adding a cycle C_k of length k between every pair of non-adjacent vertices $(v_2, v_n), (v_3, v_{n-1}), \cdots, (v_a, v_b)$ where $a = \left\lfloor\frac{n}{2}\right\rfloor$ and $b = \left\lfloor\frac{n}{2}\right\rfloor + 2$, if n is even and $a = \left\lfloor\frac{n}{2}\right\rfloor$ and $b = \left\lfloor\frac{n}{2}\right\rfloor + 3$, if n is odd.

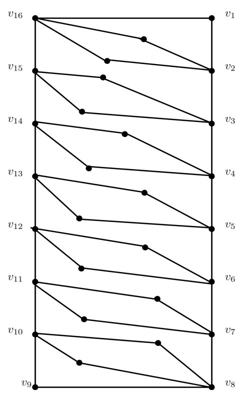

Figure 4: Cycle $C(16, C_4)$ with parallel C_4 chords

Theorem 34. $HM\left[C(n,C_k)\right] = \begin{cases} (16k+80)\left\lfloor\frac{n}{2}\right\rfloor - 16k + 64n - 192, \\ \textit{if } n \textit{ is even}, \\ (16k+80)\left\lfloor\frac{n}{2}\right\rfloor - 16k + 64n - 240, \\ \textit{if } n \textit{ is odd}. \end{cases}$

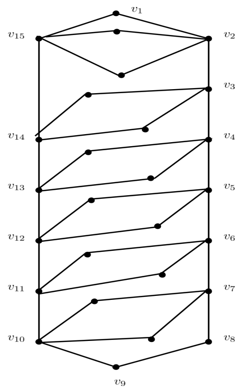

Figure 5: Cycle $C(15, C_4)$ with parallel C_4 chords

Proof. **Case** 1**:** n **is even**.
The following table gives the edge partition of $C(n, C_k)$ when n is even:

Edge uv with $(d(u), d(v))$	Number of edges
$(2, 2)$	$(k-4)(\left\lfloor \frac{n}{2} \right\rfloor - 1)$
$(2, 4)$	$4 \left\lfloor \frac{n}{2} \right\rfloor$
$(4, 4)$	$n-4$

By means of this table, one can easily obtain the required result that

$$\begin{aligned} HM\left[C(n, C_k)\right] &= (k-4)(\left\lfloor \frac{n}{2} \right\rfloor - 1)(16) + 4\left\lfloor \frac{n}{2} \right\rfloor (36) + (n-4)(64) \\ &= (16k + 80)\left\lfloor \frac{n}{2} \right\rfloor - 16k + 64n - 192. \end{aligned}$$

Case 2**:** n **is odd.**

Edge uv with $(d(u), d(v))$	Number of edges
$(2, 2)$	$(k-4)\left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right) + 1$
$(2, 4)$	$4 \left\lfloor \frac{n}{2} \right\rfloor$
$(4, 4)$	$n-5$

Now,

$$\begin{aligned} HM\left[C(n, C_k)\right] &= \left[(k-4)\left(\left\lfloor \frac{n}{2} \right\rfloor\right) + 1\right](16) + 4\left\lfloor \frac{n}{2} \right\rfloor (36) + (n-5)(64) \\ &= (16k + 80)\left\lfloor \frac{n}{2} \right\rfloor - 16k + 64n - 240. \end{aligned}$$

□

1.3.3. Shell type graph $Sh(n, k)$

In this section, we compute the hyper Zagreb index of shell graph $C(n, n-3)$ and shell type graph $Sh(n, k)$.

Definition 35. A shell graph $C(n, k)$ represents a cycle C_n of order n with k chords sharing a common end point called the apex.

Theorem 36. *For a shell graph $C(n, n-3)$, $HM\left[C(n, n-3)\right] = n^3 + 3n^2 + 32n - 104$.*

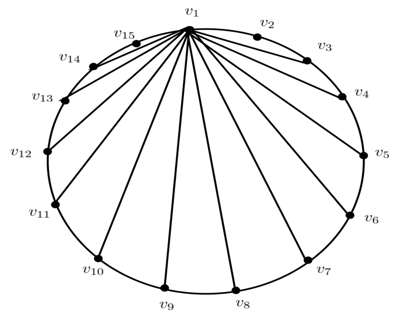

Figure 6: Shell graph $C(15, 12)$ with apex v_1

Proof. The proof of this result is straight forward with the help of the following edge partition of $C(n, n-3)$.

Edge uv with $(d(u), d(v))$	Number of edges
$(2, n-1)$	2
$(3, n-1)$	$n-3$
$(2, 3)$	2
$(3, 3)$	$n-4$

□

Generalizing this definition, we get the shell type graph as follows:

Definition 37. A shell type graph $Sh(n,k)$ is a graph formed using a cycle C_n of order n in which $n-3$ paths P_k of order $k \geq 3$ share a common end point called apex.

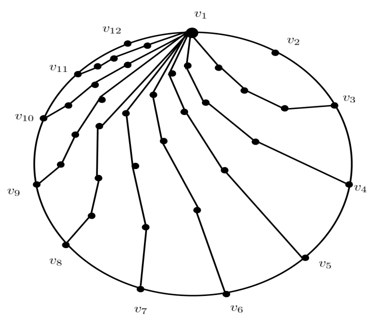

Figure 7: Shell type graph $Sh(12,5)$ with apex v_1

Theorem 38. $HM\left[Sh(n,k)\right] = 16kn + 12n - 48k + n^2 + n^3 - 26.$

Proof. One can easily observe the following edge partition of $Sh(n,k)$.

Edge uv with $(d(u),d(v))$	Number of edges
$(2,2)$	$(k-3)(n-3)$
$(2,3)$	$n-1$
$(3,3)$	$n-4$
$(2,n-1)$	$n-1$

Using the above edge partition we get

$$\begin{aligned} HM\left[Sh(n,k)\right] &= (k-3)(n-3)(16) + 25(n-1) + 36(n-4) \\ &\quad +(n-1)(n+1)^2 \\ &= 16kn + 12n - 48k + n^2 + n^3 - 26. \end{aligned}$$

□

2. Conclusions

The hyper Zagreb index of certain generalized graph structures such as generalized thorn graphs and generalized theta graphs are computed in this paper. Also, some cycle related graphs namely, cycle with parallel P_k chords, cycle with parallel C_k chords, shell type graphs have been studied for the first time in the area of Topological indices. However, computing reformulated Zagreb index of generalized thorn graphs and generalized theta graphs still remain open and challenging problem for researchers.

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