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Extremal Values of The Harmonic Index of Graphs

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Abstract

For a graph Ω with vertex set $V(\Omega)$ and edge set $E(\Omega)$, its harmonic index is defined as $H(\Omega) = \sum_{uv \in E(\Omega)} \frac{2}{d_u + d_v}$, where d_u and d_v denote the degrees of vertices u and v, respectively. The harmonic index captures various structural characteristics of a graph, such as connectivity and the uniformity of its vertex degree distribution, and finds application in many fields, including molecular structure analysis, network layout optimization, and information dissemination analysis. In this paper, we first determine the extremal values of the harmonic index for chemical graphs, and chemical trees. Moreover, using some relevant operations, we fully characterize the trees with branch vertices that achieve the extremal values of the harmonic index.

Keywords: extremal value; extremal graph; tree; harmonic index.

1 Introduction

A topological index of a graph functions serves as a numerical characterization of the graph's structure. It converts the structural features of a graph into specific numerical values, thereby reflecting the graph's topological properties. Such indices play significant roles in multiple disciplines, including chemistry (especially in the study of molecular structures) and network analysis. As noted in [1, 5], investigating the operations of graphs, topological indices of a power graph for finite groups, and their Sombor polynomial enables a better understanding of the structural properties of molecules. For instance, these indices can distinguish between different graph structures through numerical differences or indicate certain inherent properties of a graph, such as connectivity and branching, via numerical magnitudes. This enables mathematical chemists to explore the biochemical properties of molecules, deduce the chemical structures of molecular graphs, and predict novel compounds. In 2021, Gutman [6] introduced the well-known Sombor index and proposed a general definition of topological indices based on vertex degrees, expressed as follows,

$$TI(\Omega) = \sum_{uv \in E(\Omega)} F(d_u, d_v) = \sum_{1 \le i \le j \le n-1} t_{ij} F_{ij},$$

where F is a function satisfying $F(x,y) = F(y,x)$, $d_\Omega(u)$ (simply written as d_u sometimes) denotes the degree of vertex u, Ω is a simple graph with vertex set $V(\Omega)$ and edge set $E(\Omega)$, t_{ij} represents the number of edges between vertices of degree i and vertices of degree j, and $F_{ij} = F_{ji}$ is a symmetric function on degrees i and j. When $F(d_u, d_v) = \dfrac{2}{d_u + d_v}$ $\left(\text{or equivalently } F_{ij} = \dfrac{2}{i+j}\right)$, the definition specializes to the harmonic index.

The harmonic index primarily quantifies topological characteristics of graphs, such as comparing structural differences between distinct graphs or analyzing their variations during dynamic processes (e.g., vertex/edge addition or deletion) to understand graph stability. First proposed in Fajtlowics [3], this index has garnered substantial scholarly attention, with a wealth of in-depth studies conducted around it. Specifically, Favaron et al. [4] delved into its intrinsic connections with the eigenvalues of graphs. Zhong [14] not only pinpointed the minimum and maximum harmonic index values for simple connected graphs, trees, and unicyclic graphs, but also provided clear characterizations of the extremal graphs that correspond to these boundary values in [15]. Li and Liu established robust links between the harmonic index and the matching number of trees in [10] and unicyclic graphs in [9]. For trees with a given order and total domination number, an upper bound on the harmonic index was determined in [2], alongside a characterization of corresponding extremal trees.

Jahangir et al. [7] identified the chemical trees with a specified number of maximum degree vertices that optimize the harmonic index. Li [8] presented conditions involving the harmonic index for some Hamiltonian properties of a graph, as well as an upper bound for the harmonic index of a graph. Rad et al. [11] generalized a lower bound for the harmonic index of cactus graphs in terms of order, the number of leaves, the number of cycles, and characterized all cactus graphs achieving equality for this bound. Saleh and Alsulami [12] introduced a new variant of the Randić index that incorporates intermolecular forces between bonded atoms, termed the entire Harmonic index, and proposed the entire harmonic polynomial of a graph. Sun et al. [13] established the condition under which a conjecture relating the harmonic index and the minimum degree of graphs holds, and constructed a counterexample to demonstrate the conjecture's failure under another condition.

This paper is organized as follows. In section 2, we completely characterize the chemical graphs and chemical trees with extremal harmonic index. In section 3, by introducing several graph operations, we determine the extremal trees with branching vertices for the harmonic index. In section 4, we propose a question that can be studied in the future.

2 Harmonic Index of Chemical Graphs and Chemical Trees

A graph Ω is referred to as a chemical graph if its maximum degree Δ satisfies $\Delta \leq 4$ and it contains no isolated vertices. Let Γ_n represent the set of chemical graphs with n vertices, and $\mathcal{F}_n$ denote the set of chemical trees with n vertices. For convenience, we define

$$\mathcal{A} = \{(k,l):\ 1 \leq k \leq l \leq 4\},$$

$$\mathcal{A}_1 = \mathcal{A} \setminus \{(4,4)\}, \qquad \mathcal{A}_2 = \mathcal{A} \setminus \{(1,1)\}, \qquad \mathcal{A}_3 = \mathcal{A} \setminus \{(1,1),(1,4),(4,4)\},$$

$$\mathcal{B}_1 = \{T \in \mathcal{F}_n : n_2 = n_3 = 0\}, \quad \mathcal{B}_2 = \{T \in \mathcal{F}_n : n_2 = 1, n_3 = 0\}, \quad \mathcal{B}_3 = \{T \in \mathcal{F}_n : n_2 = 0, n_3 = 1\}.$$

Four chemical trees in $\mathcal{B}_1, \mathcal{B}_2$ and $\mathcal{B}_3$ are depicted in Figures 1 and 2.

Theorem 2.1. *For any connected graph $\Omega \in \Gamma_n$, $H(\Omega) \leq \frac{n}{2}$. In particular, when graph Ω is regular, $H(\Omega) = \frac{n}{2}$.*

Proof. If $(k,l) \in \mathcal{A}_1$, then $\frac{2}{k+l} \leq \frac{k+l}{2kl}$. Hence, we get

$$\begin{aligned} H(\Omega) &= \sum_{(k,l)\in\mathcal{A}} \frac{2t_{kl}}{k+l} = \frac{t_{44}}{4} + \sum_{(k,l)\in\mathcal{A}_1} \frac{2t_{kl}}{k+l} = \frac{1}{4}\left(2n - 2\sum_{(k,l)\in\mathcal{A}_1} \frac{k+l}{kl} t_{kl}\right) + \sum_{(k,l)\in\mathcal{A}_1} \frac{2t_{kl}}{k+l} \\ &= \frac{n}{2} + \sum_{(k,l)\in\mathcal{A}_1} t_{kl}\left(\frac{2}{k+l} - \frac{k+l}{2kl}\right) \leq \frac{n}{2}. \end{aligned}$$

When the degree of each vertex in Ω is 2 or 3 or 4, a direct calculation shows that $H(\Omega) = \frac{n}{2}$. □

Theorem 2.2. *If n is an even number and $\Omega \in \Gamma_n$, then $H(\Omega) \leq H\left(\frac{n}{2}P_2\right) = \frac{n}{2}$.*

Proof. For any $(k,l) \in \mathcal{A}_2$, $\frac{2}{k+l} - \frac{k+l}{2kl} \leq 0$. Then, we have

$$\begin{aligned} H(\Omega) &= \sum_{(k,l)\in\mathcal{A}} \frac{2t_{kl}}{k+l} = t_{11} + \sum_{(k,l)\in\mathcal{A}_2} \frac{2t_{kl}}{k+l} = \frac{n}{2} - \frac{1}{2}\sum_{(k,l)\in\mathcal{A}_2} \frac{k+l}{kl} t_{kl} + \sum_{(k,l)\in\mathcal{A}_2} \frac{2t_{kl}}{k+l} \\ &= \frac{n}{2} + \sum_{(k,l)\in\mathcal{A}_2} t_{kl}\left(\frac{2}{k+l} - \frac{k+l}{2kl}\right) \leq \frac{n}{2}. \end{aligned}$$

If for any $(k,l) \in \mathcal{A}_2$, $t_{ij} = 0$, that is $\Omega \cong \frac{n}{2}P_2$, then $H(\Omega) = \frac{n}{2}$ always holds. □

Lemma 2.1. [14] *If T is a tree of order n, then $H(T) \leq H(P_n) = \frac{4}{3} + \frac{n-3}{2}$.*

Obviously, P_n is a chemical tree. Thus, Lemma 2.1 determines the maximum harmonic index of chemical trees. Now, if we denote n_i as the number of vertices of degree i, n as the order of graph Ω, then the following equations can be easily obtained,

$$\begin{cases} n_1 + n_2 + n_3 + n_4 + \cdots + n_{n-1} = n, \\ 2t_{11} + t_{12} + t_{13} + \cdots + t_{1,n-1} = n_1, \\ t_{12} + 2t_{22} + t_{23} + \cdots + t_{2,n-1} = 2n_2, \\ t_{13} + t_{23} + 2t_{33} + \cdots + t_{3,n-1} = 3n_3, \\ \vdots \\ t_{1,n-1} + t_{2,n-1} + \cdots + 2t_{n-1,n-1} = (n-1)n_{n-1}. \end{cases}$$

It is deduced that $n = \sum_{1\leq i\leq j\leq n-1} \frac{i+j}{ij} t_{ij}$. Moreover, if $T \in \mathcal{F}_n$, then $t_{11}(T) = 0$ and

$$\frac{5}{4}t_{14} + \frac{1}{2}t_{44} + \sum_{(k,l)\in\mathcal{A}_3} \frac{k+l}{kl} t_{kl} = n, \qquad t_{14} + t_{44} + \sum_{(k,l)\in\mathcal{A}_3} t_{kl} = n-1.$$

Therefore,

$$t_{14} = \frac{2n+2}{3} - \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 2\right)t_{kl}, \qquad t_{44} = \frac{n-5}{3} + \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 5\right)t_{kl}.$$

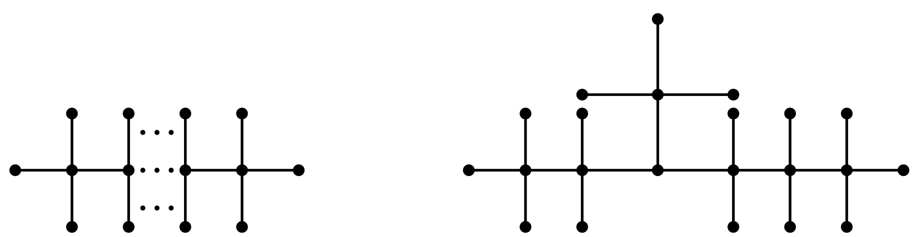

Figure 1: A chemical tree in $\mathcal{B}_1$ and a chemical tree of order 22 in $\mathcal{B}_3$.

Theorem 2.3. *If $T \in \mathcal{F}_n$, then $H(T) \geq \frac{4n+4}{15} + \frac{n-5}{12}$. Moreover, when $T \in \mathcal{B}_1$,*

$$H(T) = \frac{4n+4}{15} + \frac{n-5}{12}.$$

Proof. If $(k,l) \in \mathcal{A}_3$, then $\frac{2}{k+l} - \frac{k+l}{5kl} - \frac{3}{20} \geq 0$. Hence, we have

$$\begin{aligned} H(T) &= \sum_{(k.l)\in\mathcal{A}} \frac{2t_{kl}}{k+l} = \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} + \frac{2t_{14}}{5} + \frac{t_{44}}{4} \\ &= \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} + \frac{2}{5}\left[\frac{2n+2}{3} - \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 2\right)t_{kl}\right] \\ &\quad + \frac{1}{4}\left[\frac{n-5}{3} + \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 5\right)t_{kl}\right] \\ &= \frac{4n+4}{15} + \frac{n-5}{12} + \sum_{(k,l)\in\mathcal{A}_3} t_{kl}\left(\frac{2}{k+l} - \frac{k+l}{5kl} - \frac{3}{20}\right) \geq \frac{4n+4}{15} + \frac{n-5}{12}. \end{aligned}$$

The equality in the above formula holds if and only if for all $(k,l) \in \mathcal{A}_3$, $t_{kl} = 0$. Consequently $n_2 = n_3 = 0$, that is $T \in \mathcal{B}_1$. □

Corollary 2.1. *Let $n > 4$ and $n = 3s+2$, $s \geq 1$. If T has minimum harmonic index in $\mathcal{F}_n$, then $T \in \mathcal{B}_1$.*

Proof. If chemical tree $T \in \mathcal{B}_1$, the harmonic index of T is a constant, specifically,

$$H(T) = \frac{4n+4}{15} + \frac{n-5}{12}.$$

□

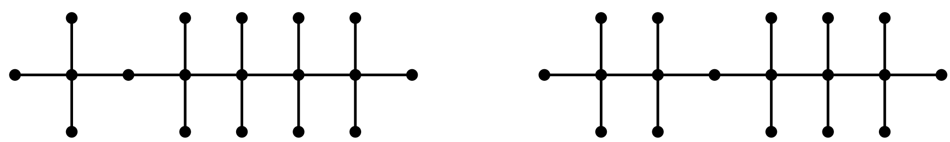

Figure 2: Two chemical trees of order 18 in $\mathcal{B}_2$.

Corollary 2.2. *Let $n \geq 9$ and $n = 3s$, $s \geq 3$. If T has minimum harmonic index in $\mathcal{F}_n$, then $T \in \mathcal{B}_2$ and $t_{12} = 0$.*

Proof. If $T \in \mathcal{B}_1 \cup \mathcal{B}_3$, then according to the Hand-shaking theorem, we have

$$2(n-1) = n_1 + 4n_4 \qquad \text{or} \qquad 2(n-1) = n_1 + 3n_3 + 4n_4.$$

This contradicts the assumption that $n = 3s$, $s \geq 1$. So $T \notin \mathcal{B}_1 \cup \mathcal{B}_3$. Let $h(k,l) = \dfrac{2}{k+l} - \dfrac{k+l}{5kl} - \dfrac{3}{20}$. Clearly, $h(1,3) > 0$, $h(3,3) > 0$, $h(3,4) > 0$, $h(1,2) > h(2,3) > h(2,4) > 0$, $h(2,2) > 2h(2,4)$. Therefore, from the definition of the harmonic index,

$$\begin{aligned}
H(T) &= \sum_{(k,l)\in\mathcal{A}} \frac{2t_{kl}}{k+l} = \frac{2t_{14}}{5} + \frac{t_{44}}{4} + \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} \\
&= \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} + \frac{2}{5}\left[\frac{2n+2}{3} - \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 2\right)t_{kl}\right] \\
&\quad + \frac{1}{4}\left[\frac{n-5}{3} + \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 5\right)t_{kl}\right] \\
&= \frac{4n+4}{15} + \frac{n-5}{12} + \sum_{(k,l)\in\mathcal{A}_3} t_{kl}\left(\frac{2}{k+l} - \frac{k+l}{5kl} - \frac{3}{20}\right) \\
&\geq \frac{4n+4}{15} + \frac{n-5}{12} + t_{12}h(1,2) + t_{22}h(2,2) + t_{23}h(2,3) + t_{24}h(2,4) \\
&> \frac{4n+4}{15} + \frac{n-5}{12} + (t_{12} + 2t_{22} + t_{23} + t_{24})h(2,4) = \frac{4n+4}{15} + \frac{n-5}{12} + 2n_2h(2,4).
\end{aligned}$$

If $n_2 = 0$, then $H(T) > \dfrac{4n+4}{15} + \dfrac{n-5}{12}$. Moreover, if $H(T) = \dfrac{4n+4}{15} + \dfrac{n-5}{12}$, then $T \in \mathcal{B}_1 \cup \mathcal{B}_3$, a contradiction. So, $n_2 \geq 1$. Since $h(2,4) > 0$, we have

$$H(T) \geq \frac{4n+4}{15} + \frac{n-5}{12} + 2n_2h(2,4) \geq \frac{4n+4}{15} + \frac{n-5}{12} + 2h(2,4).$$

The equality in the above formula holds if and only if,

$$t_{24} = 2, \qquad t_{12} = t_{22} = t_{13} = t_{23} = t_{33} = t_{34} = 0.$$

Furthermore, the harmonic index attains the minimum values if and only if $n_2 = 1, n_3 = 0$. So, if $n = 3s$ and $s \geq 3$, when $T \in \mathcal{B}_2$ and $t_{12} = 0$, the harmonic index attains the minimum value. □

Corollary 2.3. *Let $n \geq 13$ and $n = 3s+1$, $s \geq 4$. If T has minimum harmonic index in $\mathcal{F}_n$, then $T \in \mathcal{B}_3$ and $t_{13} = 0$.*

Proof. If $T \in \mathcal{B}_1 \cup \mathcal{B}_2$, then by the Hand-shaking theorem, we have

$$2(n-1) = n_1 + 4n_4 \qquad \text{or} \qquad 2(n-1) = n_1 + 2n_2 + 4n_4.$$

This contradicts the condition that $n = 3s+1$, $s \geq 4$. So $T \notin \mathcal{B}_1 \cup \mathcal{B}_2$. Consider the function,

$$h(k,l) = \frac{2}{k+l} - \frac{k+l}{5kl} - \frac{3}{20}.$$

Clearly, $h(1,3) > 0, h(3,3) > 0, h(2,2) > 0, h(2,4) > 0, h(1,2) > h(2,3) > h(3,4) > 0, h(3,3) > 2h(3,4)$. Thus, from the definition of harmonic index,

$$\begin{aligned}
H(T) &= \frac{2t_{14}}{5} + \frac{t_{44}}{4} + \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} \\
&= \sum_{(k,l)\in\mathcal{A}_3} \frac{2t_{kl}}{k+l} + \frac{2}{5}\left[\frac{2n+2}{3} - \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 2\right)t_{kl}\right] \\
&\quad + \frac{1}{4}\left[\frac{n-5}{3} + \frac{1}{3}\sum_{(k,l)\in\mathcal{A}_3}\left(4\frac{k+l}{kl} - 5\right)t_{kl}\right] \\
&= \frac{4n+4}{15} + \frac{n-5}{12} + \sum_{(k,l)\in\mathcal{A}_3} t_{kl}\left(\frac{2}{k+l} - \frac{k+l}{5kl} - \frac{3}{20}\right) \\
&\geq \frac{4n+4}{15} + \frac{n-5}{12} + t_{13}h(1,3) + t_{23}h(2,3) + t_{33}h(3,3) + t_{34}h(3,4) \\
&> \frac{4n+4}{15} + \frac{n-5}{12} + (t_{13} + t_{23} + 2t_{33} + t_{34})h(3,4) = \frac{4n+4}{15} + \frac{n-5}{12} + 3n_3h(3,4).
\end{aligned}$$

If $n_3 = 0$, then $H(T) > \frac{4n+4}{15} + \frac{n-5}{12}$. Moreover, if $H(T) = \frac{4n+4}{15} + \frac{n-5}{12}$, then $T \in \mathcal{B}_1 \cup \mathcal{B}_2$, a contradiction. So, $n_3 \geq 1$. Since $h(3,4) > 0$, we have

$$H(T) \geq \frac{4n+4}{15} + \frac{n-5}{12} + 3n_3h(3,4) \geq \frac{4n+4}{15} + \frac{n-5}{12} + 3h(3,4).$$

The equality holds if and only if $x_{34} = 3$, $t_{12} = t_{22} = t_{13} = t_{23} = t_{24} = t_{33} = 0$. Therefore, the harmonic index attains minimum value if and only if $n_2 = 0, n_3 = 1$. That is when $n = 3s+1$ and $s \geq 4$, if $T \in \mathcal{B}_3$ and $t_{13} = 0$, then T has minimum harmonic index. □

3 The Harmonic Index of Trees with Branches

In this section, a sequence of graph operations are first put forward, with which the extremal values of the harmonic index in trees possessing branching vertices are to be determined. Let

$\Psi(n,q)$ stand for the collection of trees that have n vertices and contain q branching vertices. Denote $R(t_1,t_2,\ldots,t_k)$ as star-like graph, which satisfies,

$$R(t_1,t_2,\ldots,t_k)-v=P_{t_1}\cup P_{t_2}\cup\ldots\cup P_{t_k},\qquad 1\le t_1\le t_2\le\cdots\le t_k,\qquad k\ge 3.$$

Let $S_{n,r}$ represent the family of all star-like graphs that have n vertices and a maximum degree of r where $r\ge 3$. Let r_i represent how many paths have length i, while s stands for the length of the longest path within tree T. Then,

$$\sum_{i=1}^{s} r_i=r,\qquad \sum_{i=1}^{s} ir_i=n-1. \tag{1}$$

Theorem 3.1. *If $T\in S_{n,r}$, then $TI(T)=r_1X_r+rY_r+(n-1)F_{22}$, where $X_r=F_{1r}+F_{22}-F_{12}-F_{2r}$, $Y_r=F_{12}+F_{2r}-2F_{22}$.*

Proof. If $T\in S_{n,r}$, then the degrees of the vertices in T are restricted to $1,2$, and r. According to the definition of the star-like graph, we have

$$t_{1r}=r_1,\qquad t_{12}=t_{2r}=r_2+\cdots+r_s,\qquad t_{22}=r_3+2r_4+\cdots+(s-2)r_s.$$

Thus, based on (1), we obtain

$$t_{1r}=r_1,\qquad t_{12}=t_{2r}=r-r_1,\qquad t_{22}=n-1+r_1-2r.$$

From the general definition of the topological index, we know that,

$$\begin{aligned}TI(T)&=t_{12}F_{12}+t_{1r}F_{1r}+t_{22}F_{22}+t_{2r}F_{2r}\\&=(r-r_1)F_{12}+r_1F_{1r}+(n-1+r_1-2r)F_{22}+(r-r_1)F_{2r}\\&=r_1\left(F_{1r}+F_{22}-F_{12}-F_{2r}\right)+r\left(F_{12}+F_{2r}-2F_{22}\right)+(n-1)F_{22}\\&=r_1X_r+rY_r+(n-1)F_{22}.\end{aligned}$$

We complete the proof of this theorem. □

Corollary 3.1. *If $T\in S_{n,r}$ and $X_r\ge 0$, then $TI(T)$ reaches its maximum value precisely when*

$$T\cong R(\overbrace{1,\ldots,1}^{r-1},n-r).$$

Proof. Arbitrarily take two trees T_1 and T_2 in $S_{n,r}$. According to Theorem 3.1, we have

$$TI(T_1)-TI(T_2)=(r_1(T_1)-r_1(T_2))X_r.$$

Therefore, $TI(T)$ achieves its maximum if and only if T contains the largest number of vertices with degree 1, which means $T\cong R(\overbrace{1,\ldots,1}^{r-1},n-r)$. □

Lemma 3.1. *Let xy be a non-pendant cut edge of graph Ω. Remove the edge xy, merge vertices x and y into a single vertex x, and then add a new pendant edge xy connected to vertex x. Let the resulting graph be denoted as $\Omega'=\Omega\cdot(xy)+xy$ (see Figure 3), then $H(\Omega')<H(\Omega)$.*

Proof. Denote $N_\Omega(x) = \{y, x_1, \ldots, x_p\}$ and $N_\Omega(y) = \{x, y_1, \ldots, y_q\}$. According to the definition of harmonic index,

$$H(\Omega) - H(\Omega') = \frac{2}{(p+1)+(q+1)} + \sum_{i=1}^{p} \frac{2}{p+1+d_\Omega(x_i)} + \sum_{j=1}^{q} \frac{2}{q+1+d_G(y_j)}$$
$$- \left(\frac{2}{(p+q+1)+1} + \sum_{i=1}^{p} \frac{2}{p+q+1+d_\Omega(x_i)} + \sum_{j=1}^{q} \frac{2}{p+q+1+d_\Omega(y_j)} \right) > 0.$$

We complete the proof of this lemma. □

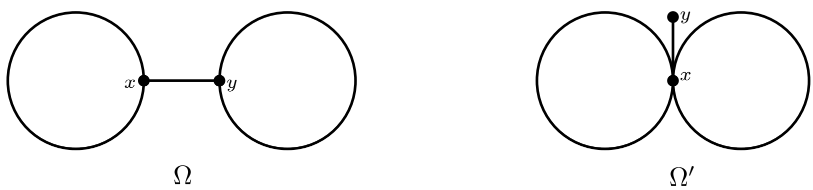

Figure 3: Graphs in Lemma 3.1.

The following conclusion can be directly derived from Corollary 3.1 and Lemma 3.1.

Theorem 3.2. *If $T \in \Psi(n, 1)$, then,*

$$2 - \frac{2}{n} \leq H(T) \leq \frac{5}{3} - \frac{4}{r+1} + \frac{2}{r+2} + \frac{n-r}{2},$$

the left-hand side equality holds precisely when $T \cong S_n$, while the right-hand side equality holds exactly when $T \cong R(\overbrace{1, \ldots, 1}^{r-1}, n-r)$.

The star graph of order k is literally denoted by S_k. Based on this, we denote $DS(p, q)$ as the double-star graph, which can be constructed by adding a new edge between the centers of two star graphs S_{p+1} and S_{q+1}, where $p + q + 2 = n$.

Theorem 3.3. *If $T \in \Psi(n, 2)$, then $H(T) \geq \frac{2}{n} + 3 - \frac{4}{n-2}$, and the equality holds precisely when $T \cong DS(n-4, 2)$.*

Proof. In accordance with Lemma 3.1, for any $T \in \Psi(n, 2)$,

$$H(T) \geq H(DS(p, q)) = \frac{2p}{p+2} + \frac{2q}{q+2} + \frac{2}{n}.$$

When $\left\lceil \frac{n-2}{2} \right\rceil \leq x \leq n-4$, the function,

$$f(x) = 4 - \frac{4}{x+2} - \frac{4}{n-x} + \frac{2}{n},$$

is strictly decreasing. Thus, $f(x)_{\min} = f(n-4) = \frac{2}{n} + 3 - \frac{4}{n-2}$, and at this time,

$$T \cong DS(n-4, 2).$$

□

Let $P = uu_1u_2 \dots u_k$ be a path in Ω such that $d_u \geq 3$, $d_{u_k} = 1$ and $d_{u_i} = 2$ for $1 \leq i < k$. Then, it is called a pendant path in Ω, u and k are called the origin and the length of P, respectively.

Lemma 3.2. *Let $T \in \Psi(n, 2)$, x be the branching vertex of T. If $d_x \geq 4$ and there are two pendant paths P_1 and P_2 of length ≥ 2 attached to the vertex x, then there exists $T' \in \Psi(n, 2)$ satisfying $H(T') > H(T)$.*

Proof. Let $xu \in E(P_1)$, v be the pendant vertex of P_2, and define $T' = T - xu + uv$.

$$H(T') - H(T) = \sum_{y \in N_T(x)\setminus\{u\}} \left(\frac{2}{d_T(x) - 1 + d_T(y)} - \frac{2}{d_T(x) + d_T(y)} \right) + \frac{1}{2} + \frac{1}{2} - \frac{2}{1+2} - \frac{2}{d_T(x)+2} > 0.$$

So, $H(T') > H(T)$. □

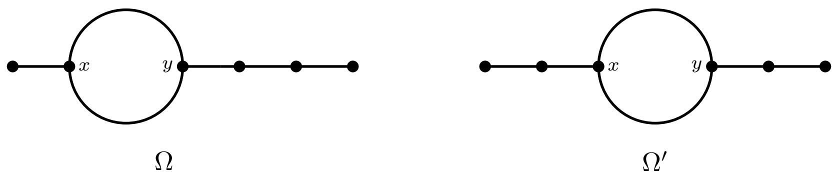

Figure 4: Graphs Ω and Ω' in Lemma 3.3.

Let x and y be two pendant vertices in a path of length $\mathbf{l} \geq 2$. Specifically, attaching two paths (each of length $p \geq 2$ and $q \geq 2$) onto x, and attaching two paths (each of length $r \geq 2$ and $s \geq 2$) onto y respectively. The graph obtained through this construction will be denoted as $Q(p, q; \mathbf{l}; r, s)$ in the subsequent context.

Lemma 3.3.

(1) *Let Ω and Ω' be the two graphs in Figure 4 respectively. If $d_\Omega(x) \geq 3$, then $H(\Omega) < H(\Omega')$.*

(2) *Let $T = Q(p, q; \mathbf{l}; r, s)$ and $T' = Q(p+1, q; \mathbf{l} - 1; r, s)$ be two trees in $\Psi(n, 2)$, with $p \geq 2$, $q \geq 2$, $r \geq 2$, $s \geq 2$, and $\mathbf{l} \geq 2$. Then $H(T) \leq H(T')$.*

Proof.

(1) When $t \geq 3$, function $\sigma(t) = \dfrac{2}{t+2} - \dfrac{2}{t+1}$ is strictly increasing. According to the definition of harmonic index,

$$H(\Omega') - H(\Omega) = \frac{2}{d_\Omega(x)+2} - \frac{2}{d_\Omega(x)+1} - \left(\frac{2}{4} - \frac{2}{3} \right) > \sigma(3) - \sigma(2) > 0.$$

(2) When $\mathbf{l} \geq 3$, $H(T) = H(T')$. Now, assume $\mathbf{l} = 2$. Through direct computation, we find that $H(T) - H(T') = \sigma(3) - \sigma(4) < 0$.

□

Theorem 3.4. *For any tree $T \in \Psi(n,2)$ with $n \geq 10$, the inequality $H(T) \leq \frac{23}{5} + \frac{1}{2}(n-10)$ holds. Equality is achieved if and only if $T \cong Q(p,q;\mathbf{1};r,s)$, where $p \geq 2$, $q \geq 2$, $r \geq 2$, and $s \geq 2$.*

Proof. Since every edge of any tree is a cut edge, according to Lemma 3.1, Lemma 3.3 (1) and $n \geq 10$, if $H(T)$ attains the maximum harmonic index value in $\Psi(n,2)$, then except for the two branches, there are no vertices of degree greater than 2 in T, and then leaves are not adjacent to the branching vertices. If there are two pendant paths of length no less than 2 attached to the branching vertex u in T, then by Lemma 3.2, there exists a tree $T_1 = Q(a,b;\mathbf{x};c,d) \in \Psi(n,2)$ such that $H(T_1) > H(T)$. If $\mathbf{x} \geq 2$, then by Lemma 3.3, one can find a tree $T \in \Psi(n,2)$ satisfying,

$$H(T) \leq H(T').$$

Therefore, when the harmonic index attains the maximum value, $T \cong Q(p,q;\mathbf{1};r,s)$ with $p \geq 2$, $q \geq 2$, $r \geq 2$, $s \geq 2$, that is $H(T) \leq \frac{23}{5} + \frac{1}{2}(n-10)$. □

By summarizing the consequences in Theorem 3.3 and Theorem 3.4, one can see that the graphs $DS(n-2,2)$ and $Q(2,2;\mathbf{1};2,n-8)$ attain the extremal harmonic index in $\Psi(n,2)$, see these two graphs in Figure 5.

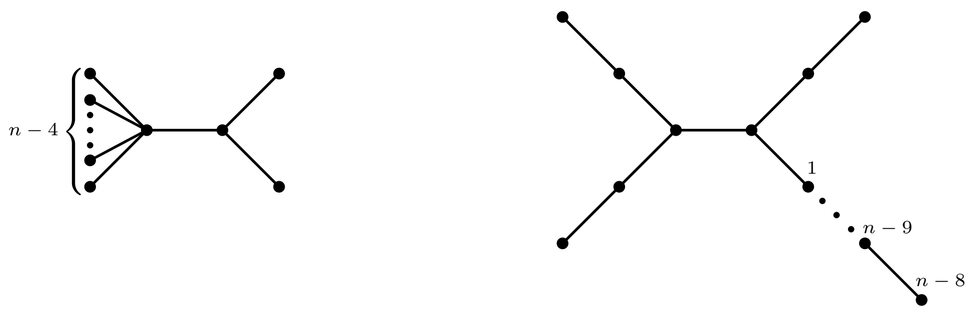

Figure 5: Extremal trees with two branches.

Denote $Q(p_1,\ldots,p_a;\mathbf{k};q_1,\ldots,q_b;\mathbf{l};r_1,\ldots,r_c)$ as the tree with three branchs in Figure 6.

$$\Psi(n,3) = \Big\{Q(p_1,\ldots,p_a;\mathbf{k};q_1,\ldots,q_b;\mathbf{l};r_1,\ldots,r_c) : p_i,q_j,r_t \geq 1, \quad 1 \leq i \leq a, \quad 1 \leq j \leq b, \\ 1 \leq t \leq c, \quad a,b,c \geq 2, \quad \sum p_i + \sum q_j + \sum r_t + k + l + 1 = n\Big\}.$$

In the special case that $p_1 = \ldots = p_r = p$, the three branched denoted by,

$$Q(p_1,\ldots,p_a;\mathbf{k};q_1,\ldots,q_b;\mathbf{l};r_1,\ldots,r_c),$$

is re-expressed as $Q(p^a;\mathbf{k};q_1,\ldots,q_b;\mathbf{l};r_1,\ldots,r_c)$. A comparable simplification applies when q_1 to q_b are equal, as well as when all r_1 to r_c are equal.

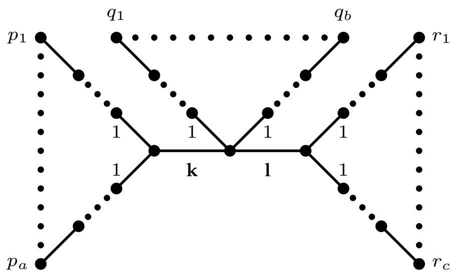

Figure 6: Tree with three branches.

We can immediately obtain the following lemma by repeatedly applying Lemma 3.1.

Lemma 3.4. *If $H(T)$ attains maximum value in $\Psi(n,3)$, then $T \cong Q(1^r;\mathbf{1};1^s;\mathbf{1};1^t)$ for some r,s,t.*

Lemma 3.5. *Let $T = Q(1^a;\mathbf{1};1^b;\mathbf{1};1^c)$ and $T' = Q(1^{a-1};\mathbf{1};1^b;\mathbf{1};1^{c+1})$ are two trees in $\Psi(n,3)$. If $3 \leq a < c+1$, then $H(T) > H(T')$.*

Proof. When $x \geq 3$ and $y > 0$, the second derivation of the function $f(x) = \dfrac{2x}{x+2} + \dfrac{2}{x+y+3}$ is $f''(x) = -\dfrac{8}{(x+2)^3} + \dfrac{4}{(x+y+3)^3} < 0$. Thus, the function $f'(x)$ is strictly decreasing. Consider the function $g(x) = f(x) - f(x-1)$ for $x \geq 3$. Then,

$$g'(x) = \frac{4}{(x+2)^2} - \frac{2}{(x+y+3)^2} - \left[\frac{4}{(x+1)^2} - \frac{2}{(x+y+2)^2}\right] < 0.$$

So, when $x \geq 3$, the function $g(x)$ is strictly decreasing. Furthermore, when $a < c+1$, we have $f(a)-f(a-1) = g(a) > g(c+1) = f(c+1)-f(c) > 0$. According to the definition of the harmonic index,

$$\begin{aligned}
H(T) - H(T') &= \frac{2a}{a+2} + \frac{2c}{c+2} + \frac{2}{a+b+3} + \frac{2}{c+b+3} \\
&\quad - \left[\frac{2(a-1)}{a+1} + \frac{2(c+1)}{c+3} + \frac{2}{a+b+2} + \frac{2}{c+b+4}\right] \\
&= f(a) + f(c) - f(a-1) - f(c+1) \\
&= f(a) - f(a-1) - [f(c+1) - f(c)] > 0.
\end{aligned}$$

Therefore, $H(T) > H(T')$. □

Lemma 3.6. *Let $T = Q(1^2;\mathbf{1};1^b;\mathbf{1};1^c)$, $T' = Q(1^2;\mathbf{1};1^{b-1};\mathbf{1};1^{c+1})$, $T'' = Q(1^2;\mathbf{1};1^{b+1};\mathbf{1};1^{c-1})$. When $2 \leq b \leq c$, $H(T) > H(T')$; when $b > c \geq 2$, $H(T) > H(T'')$.*

Proof. Now, we consider function $f(x) = \dfrac{2x}{x+2} - \dfrac{2(x-1)}{x+1}$, where $x \geq 3$. By derivation, we have $f'(x) = \dfrac{4}{(x+2)^2} - \dfrac{4}{(x+1)^2} < 0$. This indicates that when $x \geq 3$, $f(x)$ is strictly decreasing.

(1) If $2 \le b \le c$, then $f(b) \ge f(c)$. According to the definition of the harmonic index,

$$\begin{aligned}
H(T) - H(T') &= \frac{2}{b+5} + \frac{2b}{b+3} + \frac{2c}{c+2} - \frac{2}{b+4} - \frac{2(b-1)}{b+2} - \frac{2(c+1)}{c+3} \\
&= \frac{2}{b+5} + \frac{2b}{b+3} - \frac{2}{b+4} - \frac{2(b-1)}{b+2} - f(c+1) \\
&\ge \frac{2}{b+5} + \frac{2b}{b+3} - \frac{2}{b+4} - \frac{2(b-1)}{b+2} - f(b+1) \\
&= \frac{2}{b+5} + \frac{2b}{b+3} - \frac{2}{b+4} - \frac{2(b-1)}{b+2} + \frac{2b}{b+2} - \frac{2(b+1)}{b+3} \\
&= \left(\frac{2}{b+5} - \frac{2}{b+4}\right) - \left(\frac{2}{b+3} - \frac{2}{b+2}\right) > 0.
\end{aligned}$$

(2) When $x \ge 2$, the functions,

$$f(x) = \frac{2x}{x+2} - \frac{2(x-1)}{x+1}, \qquad \text{and} \qquad g(x) = \frac{2}{x+5} + \frac{2}{x+1} + x\left(\frac{2}{x+3} - \frac{2}{x+1}\right),$$

are strictly decreasing. Then, from the definition of the harmonic index and $b \ge c \ge 2$,

$$\begin{aligned}
H(T) - H(T'') &= \frac{2}{b+5} + \frac{2b}{b+3} + \frac{2c}{c+2} - \left[\frac{2}{b+6} + \frac{2(b+1)}{b+4} + \frac{2(c-1)}{c+1}\right] \\
&= \frac{2}{b+5} + \frac{2b}{b+3} - \frac{2}{b+6} - \frac{2(b+1)}{b+4} + f(c) \\
&\ge \frac{2}{b+5} + \frac{2b}{b+3} - \frac{2}{b+6} - \frac{2(b+1)}{b+4} + f(b) \\
&= \frac{2}{b+5} + \frac{2}{b+1} + b\left(\frac{2}{b+3} - \frac{2}{b+1}\right) \\
&\quad - \left[\frac{2}{b+6} + \frac{2}{b+2} + (b+1)\left(\frac{2}{b+4} - \frac{2}{b+2}\right)\right] \\
&= g(b) - g(b+1) > 0.
\end{aligned}$$

Consequently, $H(T) > H(T'')$.

□

Theorem 3.5. *If $T \in \Psi(n,3)$, then $H(T) \ge \frac{11}{6} + \frac{2(n-6)}{n-4} + \frac{2}{n-2}$. The equality condition is satisfied precisely when $T \cong S(1^2; \mathbf{1}; 1; \mathbf{1}; 1^{n-6})$.*

Proof. We only need to compare the harmonic indices of $B = Q(1^2; \mathbf{1}; 1^{n-7}; \mathbf{1}; 1^2)$ and

$$C = Q(1^2; \mathbf{1}; 1; \mathbf{1}; 1^{n-6}).$$

Since $n \ge 8$, we have

$$H(C) - H(B) = \frac{11}{6} + \frac{2(n-6)}{n-4} + \frac{2}{n-2} - \left[2 + \frac{2(n-7)}{n-4} + \frac{4}{n-2}\right] \le 0.$$

Therefore, for any $T \in \Psi(n,3)$, $H(T) \ge H(Q(1^2; \mathbf{1}; 1; \mathbf{1}; 1^{n-6})) = \frac{11}{6} + \frac{2(n-6)}{n-4} + \frac{2}{n-2}$. □

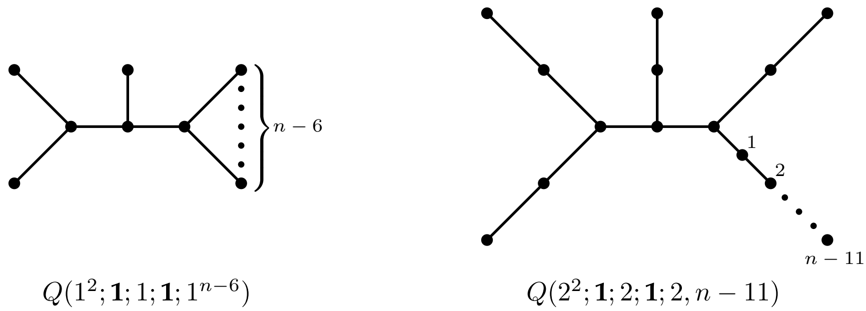

Figure 7: Trees with Extremal values in $\Psi(n,3)$.

The trees with extremal harmonic indices in $\Psi(n,3)$ are shown in Figure 7.

Lemma 3.7. *Let $\Omega_{n,1}$ and $\Omega_{n,i}$ are the two graphs in Figure 8, and $d_x \geq 3$ in graph $\Omega_{n,1}$. When $2 \leq i \leq \left\lceil \frac{n}{2} \right\rceil$, $H(\Omega_{n,1}) > H(\Omega_{n,i})$.*

Proof. If $3 \leq i \leq \left\lceil \frac{n}{2} \right\rceil$, then based on the definition of the harmonic index and $d_x \geq 3$, we have

$$H(\Omega_{n,1}) - H(\Omega_{n,i}) \geq \frac{2}{3} + \frac{2}{d_x+2} + \frac{n-3}{2} - \left(\frac{4}{3} + \frac{2}{d_x+3} + \frac{2}{d_x+3} + \frac{n-5}{2}\right) + \sum_{u \in N_H(x)} \left(\frac{2}{d_x+d_u} - \frac{2}{d_x+1+d_u}\right) > 0.$$

If $i = 2$, then,

$$H(\Omega_{n,1}) - H(\Omega_{n,i}) = \frac{2}{d_x+2} + \frac{2}{3} + \frac{n-3}{2} - \left(\frac{2}{d_x+2} + \frac{2}{d_x+3} + \frac{2}{3} + \frac{n-4}{2}\right) + \sum_{u \in N_H(x)} \left(\frac{2}{d_x+d_u} - \frac{2}{d_x+1+d_u}\right) > 0.$$

Therefore, if $2 \leq i \leq \left\lceil \frac{n}{2} \right\rceil$, then $H(\Omega_{n,1}) > H(\Omega_{n,i})$. □

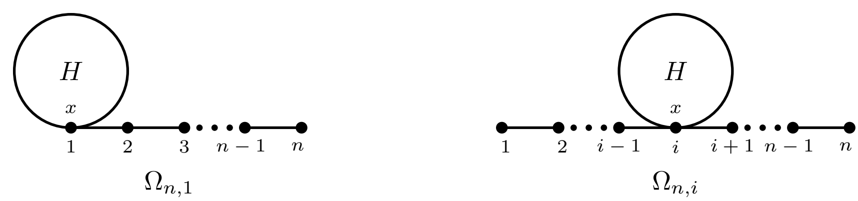

Figure 8: Graphs $\Omega_{n,1}$ and $\Omega_{n,i}$ in Lemma 3.7.

Lemma 3.8. *Suppose $n \geq 15$. If $T = Q(p,q;\mathbf{k};r;\mathbf{l};s,t) \in \Psi(n,3)$ attains maximum harmonic index, then all pendant paths have lengths exceeding 1.*

Proof. Assume that there is a pendant path of length 1 in T. Without loss of generality, let $p = 1$. Then, by Lemma 3.3 (1), we have $q \le 2$, $r \le 2$, $s \le 2$, $t \le 2$. Therefore, $\mathbf{k} + \mathbf{l} \ge 5$, which means $\mathbf{k} > 2$ or $\mathbf{l} > 2$. Without loss of generality, assume $\mathbf{k} > 2$, let $D = Q(2, q; \mathbf{k} - \mathbf{1}; r; \mathbf{l}; s, t)$. Then,

$$H(T) - H(D) = \frac{\mathbf{k} - 1}{2} + \frac{4}{5} - \left(\frac{2}{3} + \frac{\mathbf{k} - 3}{2} + \frac{6}{5}\right) < 0.$$

This contradicts the fact that $T \in \Psi(n, 3)$ has the maximum harmonic index. □

According to Lemma 3.8, if $T \in \Psi(n, 3)$ has the maximum harmonic index, then T must be in the form of $Q(p, q; \mathbf{k}; r; \mathbf{l}; s, t)$, where $p \ge 2$, $q \ge 2$, $r \ge 2$, $s \ge 2$, and $t \ge 2$.

Lemma 3.9. *If $\mathbf{k} + \mathbf{l} \ge 3$, for trees $T = Q(p, q; \mathbf{k}; r; \mathbf{l}; s, t)$ and $T' = Q(p, q; \mathbf{1}; r; \mathbf{k} + \mathbf{l} - 1; s, t)$, it holds that $H(T) \le H(T')$.*

Proof. By direct calculation, if $\mathbf{k} + \mathbf{l} = 3$, then $H(T) = H(T')$. If $\mathbf{k} \ge 2$ and $\mathbf{l} \ge 2$, then,

$$H(T) - H(T') = \frac{\mathbf{k} + \mathbf{l} - 4}{2} + \frac{8}{5} - \left(\frac{\mathbf{k} + \mathbf{l} - 3}{2} + \frac{4}{5} + \frac{1}{3}\right) < 0.$$

Therefore, $H(T) \le H(T')$. □

Theorem 3.6. *Let $n \ge 15$. For any $T \in \Psi(n, 3)$, the harmonic index satisfied $H(T) \le \frac{n}{2} - \frac{1}{2}$. Equality holds if and only if $T \cong Q(p, q; \mathbf{1}; r; \mathbf{1}; s, t)$, where*

$$p \ge 2, \quad q \ge 2, \quad r \ge 2, \quad s \ge 2, \quad t \ge 2 \quad \textit{and} \quad p + q + r + s + t = n - 3.$$

Proof. For two trees $T' = Q(p', q', \mathbf{1}; r', \mathbf{l}; s', t')$ and $T = Q(p, q; \mathbf{1}; r; \mathbf{1}; s, t)$, we have

$$\begin{aligned} t_{22}(T') &= n - 14, & t_{23}(T') &= 7, & t_{33}(T') &= 1, & t_{12}(T') &= 5, \\ t_{22}(T) &= n - 13, & t_{23}(T) &= 5, & t_{33}(T) &= 2, & t_{12}(T) &= 5. \end{aligned}$$

Then,

$$H(T') - H(T) = \frac{10}{3} + \frac{n - 14}{2} + \frac{14}{5} + \frac{1}{3} - \left(\frac{10}{3} + \frac{n - 13}{2} + 2 + \frac{2}{3}\right) < 0.$$

Therefore, $H(T') < H(T)$. □

4 Conclusions

In this paper, we determine the extremal values of the harmonic index for chemical graphs and chemical trees with branches, and corresponding graphs with these extremal values are also characterized. However, since the extremal graphs corresponding to the harmonic index with respect to numerous graph parameters have not yet been characterized, we propose a research question regarding the number of vertices n and the number of edges m as follows.

Question: How to determine the extremal values of harmonic index for $(n, m)-$graphs?

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Conflicts of Interest The authors declare no conflict of interest.

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