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Research Paper

Harmonic-Arithmetic Index of Unicyclic Graphs with given Girth and Connected Graphs with Minimum Degree

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Abstract

Let G be the finite, simple, and connected graph with a vertex set as $V(G)$ and an edge set as $E(G)$. The harmonic-arithmetic index of graph G is defined as $HA(G) = \sum_{\rho\phi\in E(G)} \frac{4d_\rho d_\phi}{(d_\rho + d_\phi)^2}$ where d_ρ denotes the degree of the vertex ρ and $\rho\phi$ denotes the edge. Let $U_{\eta,\mathfrak{g}}$ be the set of unicyclic graphs with η vertices and given girth g. Let $G_{\eta,\delta}$ be the set of simple connected graphs with η vertices with minimum degree δ. In this article, we present the maximum and second-maximum harmonic-arithmetic index of unicyclic graphs with a given girth and determine their corresponding graphs. The obtained results remain valid when the analysis is confined to the class of chemical unicyclic graphs. Further, we obtain extremal graphs in $G_{\eta,\delta}$ for which the HA index reaches its smallest value, or we provide a lower bound, for $\delta \geq \lceil \delta_0 \rceil$, with $\delta_0 = p_0(\eta - 1)$, where $p_0 \approx 0.23606$ is the distinct positive root of the expression $p^2 + 4p - 1 = 0$. We demonstrate that the extremal graphs are regular graphs of degree δ when δ or η is even.

1 Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let m be the number of edges in graph G, and η be the number of vertices. For a vertex $z \in V(G)$, its neighborhood is defined as $N_G(z) = \{y \in V(G) : yz \in E(G)\}$. The degree of z is then given by $d_z = |N_G(z)|$. A vertex

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is called pendant if its degree is equal to one. A pendant edge is the edge that has a pendant vertex. The maximum and minimum degrees of G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. The length of the shortest path between the vertices y and z in G is denoted by $\mathrm{dis}(y, z)$. A chemical unicyclic graph is a unicyclic graph whose maximum degree does not exceed four. For more information, refer to [1–3].

Chemical graph theory [4] is a subfield of cheminformatics [5] that utilizes graph-theoretical concepts to model molecular structures. In chemical graph theory, atoms are represented as nodes or vertices, and chemical bonds are the links that bind these nodes together. With this approach, researchers can analyze and predict a variety of molecular properties using numerical descriptors known as topological indices, including the Balaban index, the Randić index, the Wiener index, the Harmonic index, and the Merrifield-Simmons index, and others.

A graph's topological index, also known as the graph invariant, is a numerical value that remains constant under graph isomorphism. Topological indices are a practical way to link the structures of chemical compounds to their physical and chemical properties, especially those related to medicine, drugs, toxicology, and similar characteristics. Vertex degrees, edge degrees, vertex distances, or graph spectra can all be used to determine these indices.

Graph-derived descriptors are used as input features in the QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) models to predict various chemical and biological properties. These models create associations between molecule structures and characteristics like solubility, toxicity, melting and boiling temperatures, and more by using statistical and machine learning approaches. By increasing its ability to recognize intricate patterns in huge datasets, machine learning helps improve prediction accuracy and facilitate the investigation of new chemicals.

Making molecular graphs and calculating pertinent descriptors and features in predictive modeling are necessary steps in integrating chemical graph theory with QSPR. In chemical and pharmaceutical research, this combination strategy becomes helpful since it expedites the creation and optimization of novel compounds. The property of an expression defined on the class of all graphs whose outcome is the same for all isomorphic graphs is known as graph invariance. Graph invariants include things like polynomials, numerical values, and sets of numbers.

Topological indices, associated with graph invariants, accept only numerical values [4, 6]. The topological indices known as Degree-based Topological Indices (DTI) [7, 8] are established using the following formulas [9, 10]

$$DTI_{\xi}(G) = \sum_{ch \in E(G)} \xi(d_c, d_h).$$

The equation $\xi(d_c, d_h) = \xi(d_h, d_c)$, where ξ is a positive function defined on the Cartesian product of the degree set.

Harry Wiener developed the Wiener index in 1947 [11], and it is considered the first topological index.

$$W(G) = \sum_{\{c,h\} \subseteq V(G)} dis(c, h).$$

One of the earliest degree-based topological indices was the Randić index, which was initially presented by M. Randic in 1975 [12].

$$R(G) = \sum_{ch \in E(G)} \frac{1}{\sqrt{d_c d_h}}.$$

The harmonic index H(G) was proposed in [13], and is defined as:

$$H(G) = \sum_{ch \in E(G)} \frac{2}{d_c + d_h}.$$

Additionally, it is crucial to keep in mind that the SDD index [14] may be determined by comparing the arithmetic and harmonic means of the degrees of the end-vertices of the edges in G. Specifically, this suggests

$$SDD(G) = 4 \sum_{ch \in E(G)} \frac{(d_c + d_h)/2}{2d_c d_h/(d_c + d_h)} - 2\,|E(G)|\,.$$

Inspired by the aforementioned facts and the recently introduced inverse symmetric division degree (ISDD) index [15].
The HA index, which is extracted from the harmonic and arithmetic means of vertex degrees, was introduced and examined by Albalahi et al. (2023) [16]. This descriptor provides a distinctive perspective on molecular structure. Theoretical conclusions on the HA index are presented by the authors of [17], establishing connections and boundaries between other well-known topological indices and the HA index. The lower bounds for the HA index of trees with given pendant vertices are obtained in [18], and the lower and upper bounds of the HA index for trees of order n with given maximum degree are obtained in [19]. The extremal unicyclic graphs corresponding to the HA index have been characterized in [20]. Furthermore, in [18], by computing the HA index for monogenic semigroup graphs under two product operations, and in [21] and [19], by employing a regression model for benzenoid hydrocarbons, this research advances chemical graph theory and offers a practical method for analyzing real-world chemical structures. These findings advance our knowledge of the behavior of the HA index and its uses in molecular structure investigation. We employ a methodology that was initially presented in [22] and then again in [23].

$$HA(G) = \sum_{ch \in E(G)} \frac{2d_c d_h/(d_c + d_h)}{(d_c + d_h)/2} = \sum_{ch \in E(G)} \frac{4d_c d_h}{(d_c + d_h)^2}.$$

This article presents the first and second maximum HA index of unicyclic graphs $U_{\eta,\mathfrak{g}}$ with girth $\mathfrak{g}$, which is presented in the following Section 2. In Section 3, we present extremal graphs in $G_{n,\delta}$ that achieve the minimum value of the harmonic-arithmetic index or establish a lower bound for $\delta \geq \lceil \delta_0 \rceil$.

2 Maximum HA index of unicyclic graphs $U_{\eta,\mathfrak{g}}$ with a girth $\mathfrak{g}$

In this section, we define the maximum HA index of unicyclic graphs, $U_{\eta,\mathfrak{g}}$ with a girth $\mathfrak{g}$. The unicyclic graphs $U_{\eta,\mathfrak{g}}$ have η order and η edges. Let $\mathfrak{g}$ represent the girth, which is the length of the shortest cycle in the graph. Some papers related to unicyclic graphs with given girth are given in [24–26]. In a graph G, a non-trivial path $P : z_1 z_2 \cdots z_p$ is said to be a pendant path of G if the degree of the vertices z_1 and z_p in the graph G is one vertex having degree 1, while the other vertex has degree at least 3. Additionally, the degree of the vertex z_i is 2 for all indices i such that $2 \leq i \leq p-1$. This section concludes with a lemma that serves as the primary result of this paper:

Lemma 2.1. *Assume G be the graph with p pendant paths, then*

$$HA(G) \leq \left[\frac{24}{25} + \frac{8}{9}\right] p + |E(G)| - 2p.$$

Proof. Consider an edge ch on a graph G with η vertices. As a function of d_h, if d_c is fixed, then $\frac{4d_cd_h}{(d_c+d_h)^2}$ for $d_c \leq d_h \leq \eta - 1$ is decreasing.

Therefore, the contribution of the edge of a pendant path with length one in G to $HA(G)$ is relatively $\frac{4(3\cdot1)}{(3+1)^2} < 1 - 2 + \frac{4(2\cdot3)}{(3+2)^2} + \frac{4(2\cdot1)}{(2+1)^2}$, and thus p_k is the pendant path with length $k \geq 2$ in G contributing to $HA(G)$ at most $\frac{4(2\cdot3)}{25} + \frac{4(2\cdot1)}{9} + \frac{4(2\cdot2)}{16}(k-2) = k - 2 + \frac{24}{25} + \frac{8}{9}$. Consequently, $HA(G)$ is contributed to by the edges of a pendant path of length $k \geq 1$ in G at most $k - 2 + \frac{24}{25} + \frac{8}{9}$. Therefore, in graph G, there are p pendant paths, thus $HA(G) \leq \left[\frac{24}{25} + \frac{8}{9}\right] p + |E(G)| - 2p$. ■

2.1 First maximum HA index of unicyclic graphs $U_{\eta,\mathfrak{g}}$

Let $U_{\eta,\mathfrak{g}}$ represent the collection of all unicyclic graphs of order η with girth $\mathfrak{g}$, where $3 \leq \mathfrak{g} \leq \eta$. Let the class $U_{\eta,\eta}$ be composed of a single graph C_η. Similarly, the class $U_{\eta,\eta-1}$ is composed of a single graph. Specifically, the graph is created by joining any vertex of the cycle graph $C_{\eta-1}$ to one pendant vertex. The HA index of the cycle graph C_η is η. The η-order unicyclic graph of HA index with girth $\eta - 1$ is $\eta - \frac{33}{100}$. For $3 \leq \mathfrak{g} \leq \eta - 2$, let $U^*_{\eta,\mathfrak{g}}$ denote the η-order graph formed by connecting a pendant vertex of the $(\eta - \mathfrak{g})$-order path $P_{\eta-\mathfrak{g}}$ to a vertex of the $\mathfrak{g}$-order cycle $C_\mathfrak{g}$. The graph $U^*_{\eta,\mathfrak{g}}$ is depicted in Figure 1.

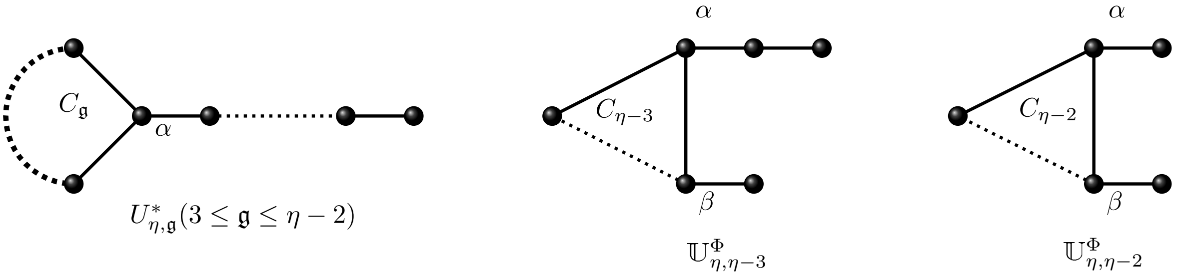


Figure 1: The graphs $U^*_{\eta,\mathfrak{g}}(3 \leq \mathfrak{g} \leq \eta - 2), \mathbb{U}^\Phi_{\eta,\eta-3}, \mathbb{U}^\Phi_{\eta,\eta-2}$.

Theorem 2.2. *Assume* $Z \in U_{\eta,\mathfrak{g}}$ *with* $3 \leq \mathfrak{g} \leq \eta - 2$, *then*

$$HA(Z) \leq \eta - \frac{52}{225},$$

equality is achieved if and only if $Z \cong U^*_{\eta,\mathfrak{g}}$.

Proof. The number of pendant paths for Z is denoted by p. For example, if $p = 1$, then $Z \cong U^*_{\eta,\mathfrak{g}}$, and

$$HA(Z) = \eta - \frac{52}{225}.$$

If $p \geq 2$, then Lemma 2.1 implies that

$$HA(Z) \leq \left[\frac{24}{25} + \frac{8}{9}\right] p + \eta - 2p \leq \left[\frac{24}{25} + \frac{8}{9}\right] 2 + \eta - 2(2) < \eta - \frac{52}{225}.$$

■

Corollary 2.3. *The graph* $U^*_{\eta,\mathfrak{g}}$ *uniquely attains the maximum HA index in the class of all chemical unicyclic graphs with n vertices and g girth for every* $3 \leq \mathfrak{g} \leq \eta - 2$.

The following finding derive from Theorem 2.2, where $HA(C_\eta) = \eta$; specifically, the first of these two results was recently proved in [20].

Corollary 2.4. *([20]). For any integer $\eta \geq 3$, the cycle graph C_η is the only graph that achieves the maximum HA index among all unicyclic graphs of order η, then:*

$$HA(Z) \leq \eta,$$

equality is achieved if and only if $Z \cong C_\eta$.

2.2 Second maximum HA index of unicyclic graphs $U_{\eta,\mathfrak{g}}$

Lemma 2.5. *Let G be a simple graph with η vertices and m edges, then*

$$HA(G) = m - \sum_{ch \in E(Z)} \frac{(d_c - d_h)^2}{(d_c + d_h)^2}.$$

Proof. Assume that ch is an edge of the graph G and is denoted by e. Then, the definition of $HA(G)$ is achieved by assigning a weight $w^*(e)$ to the edge e:

$$w^*(e) = \frac{4d_c d_h}{(d_c + d_h)^2}.$$

To ensure that the harmonic-arithmetic index is a sum of the contributions made by edges:

$$HA(G) = \sum_{e \in E(G)} w^*(e).$$

For every edge, the weight $w^*(e)$ has a positive value e. Let G be a simple graph with m edges and $\eta \geq 2$ vertices. Let ϖ and σ be the degrees of the vertices d_c and d_h. An $(\varpi, \sigma)-$ is an edge of G that connects a vertex of degree ϖ with a vertex of degree σ. $e_{\varpi\sigma}$ will be used to indicate the number of $(\varpi, \sigma)-$ edges. $e_{\varpi\sigma} = e_{\sigma\varpi}$ and $\sum\limits_{1 \leqslant \varpi \leqslant \sigma \leqslant n-1} e_{\varpi\sigma} = m$ are clearly obvious.

$HA(G) = \dfrac{4\varpi\sigma}{(\varpi + \sigma)^2}$ can be rewritten as:

$$\begin{aligned} HA(G) &= \sum_{1 \leqslant \varpi \leqslant \sigma \leqslant \eta-1} \frac{4\varpi\sigma}{(\varpi + \sigma)^2} e_{\varpi\sigma} = \sum_{1 \leqslant \varpi \leqslant \sigma \leqslant \eta-1} \left[1 - \frac{(\varpi - \sigma)^2}{(\varpi + \sigma)^2} \right] e_{\varpi\sigma} \\ &= \sum_{1 \leqslant \varpi \leqslant \sigma \leqslant \eta-1} e_{\varpi\sigma} - \sum_{1 \leqslant \varpi \leqslant \sigma \leqslant \eta-1} \left[\frac{(\varpi - \sigma)^2}{(\varpi + \sigma)^2} \right] e_{\varpi\sigma}. \end{aligned}$$

As previously, let e be the graph G edge that joins the vertices c and h. The weight associated with the edge e is denoted as $w^{**}(e)$:

$$w^{**}(e) = \left[\frac{(\varpi - \sigma)^2}{(\varpi + \sigma)^2} \right].$$

In the case of connected graphs, which are without any isolated vertices,

$$HA(G) = m - \sum_{e \in E(G)} w^{**}(e).$$

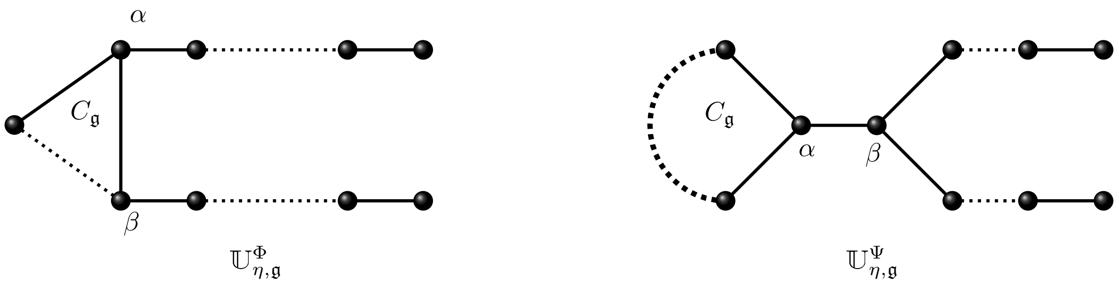
For unicyclic graphs U_η, which have η vertices and η edges. Thus,

$$HA(G) = \eta - \sum_{ch \in E(G)} \frac{(d_c - d_h)^2}{(d_c + d_h)^2}.$$

For a unicyclic graph G with η edges, we have $HA(G) = \eta - f(G)$, where $f(G) = \sum_{ch \in E(G)} \frac{(d_c - d_h)^2}{(d_c + d_h)^2}$. Consequently, $HA(G)$ is decreasing on $f(G)$ for a given η. ■

Next, we determine the graphs in the class $U_{\eta,\mathfrak{g}}$ that have the second-maximum HA index value. We first define specific graphs for this. In graph $U^*_{\eta,\mathfrak{g}}$, a is the unique vertex of degree 3 (see Figure 1). The class of the unique graph produced from $U^*_{\eta,\mathfrak{g}}$ is indicated by $\mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$ when $\mathfrak{g} \in \{\eta-3, \eta-2\}$. This may be accomplished by removing its distinct pendant vertex and placing it adjacent to one (let's say β) of those two neighbors of α that are on the cycle. Figure 1 also shows the graphs $\mathbb{U}^{\Phi}_{\eta,\eta-3}$ and $\mathbb{U}^{\Phi}_{\eta,\eta-2}$.

For $3 \leq \mathfrak{g} \leq \eta-4$, $\mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$ indicates the class of the graph(s) derived from the cycle $C_\mathfrak{g}$. The graph is achieved by connecting two pendant paths of length l_1 and l_2 at the vertices $\alpha, \beta \in V(C_\mathfrak{g})$ (one at α and the other at β), where $\min\{l_1, l_2\} \geq 2$ and $\alpha\beta \in E(C_\mathfrak{g})$. For $3 \leq \mathfrak{g} \leq \eta - 5$, $\mathbb{U}^{\Psi}_{\eta,\mathfrak{g}}$ indicates the class of the graph(s) derived from the cycle $C_\mathfrak{g}$ and the path $P_{\eta-\mathfrak{g}}$. This is achieved by connecting an edge between a vertex α of $C_\mathfrak{g}$ and a vertex β of $P_{\eta-\mathfrak{g}}$, where the distance between β and each of the pendant vertices of $P_{\eta-\mathfrak{g}}$ is at least 2. The general representations of the graphs that belong to $\mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$ and $\mathbb{U}^{\Psi}_{\eta,\mathfrak{g}}$ are given in Figure 2. According to $U'_{\eta,\mathfrak{g}} = \left(\cup_{\mathfrak{g}=3}^{\eta-4} \mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}\right) \cup \left(\cup_{\mathfrak{g}=3}^{\eta-5} \mathbb{U}^{\Psi}_{\eta,\mathfrak{g}}\right)$.



$\mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$ $\mathbb{U}^{\Psi}_{\eta,\mathfrak{g}}$

Figure 2: $\mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$ and $\mathbb{U}^{\Psi}_{\eta,\mathfrak{g}}$ are the general forms of graphs.

Theorem 2.6. *Let* $Z \in U_{\eta,\mathfrak{g}}$ *such that* $Z \ncong U^*_{\eta,\mathfrak{g}}$.

i) If $3 \leq \mathfrak{g} \leq \eta - 4$, *then*

$$HA(Z) \leq \eta - \frac{86}{225}. \tag{1}$$

If $3 \leq \mathfrak{g} \leq \eta - 5$, *then Equality 1 is achieved if and only if* $Z \in U'_{\eta,\mathfrak{g}}$ *(see Figure 2). If* $\mathfrak{g} = \eta - 4$, *then Equality 1 is achieved if and only if* $Z \in \mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$.

ii) If $\mathfrak{g} = \eta - 3$, *then*

$$HA(Z) \leq \eta - \frac{433}{900},$$

equality is achieved if and only if $Z \in \mathbb{U}^{\Phi}_{\eta,\eta-3}$.

iii) If $\mathfrak{g} = \eta - 2$*, then*

$$HA(Z) \leq \eta - \frac{29}{50},$$

equality is achieved if and only if $Z \in \mathbb{U}^{\Phi}_{\eta,\eta-2}$.

Proof. Suppose that p is the number of pendant paths in Z. Given that $Z \ncong U^{*}_{\eta,\mathfrak{g}}$, where $p \geq 2$.
(i) Since $3 \leq \mathfrak{g} \leq \eta - 4$ and $p \geq 3$, then Lemma 2.1 implies that

$$HA(Z) \leq \left[\frac{24}{25} + \frac{8}{9}\right] p + \eta - 2p \leq \left[\frac{24}{25} + \frac{8}{9}\right] 3 + \eta - 2(3) < \eta - \frac{86}{225}.$$

Now, consider the case where $p = 2$. In this scenario, the graph Z is one of the three classes depicted in Figure 3, namely $Z \in U^{I}_{\eta,\mathfrak{g}} \cup U^{II}_{\eta,\mathfrak{g}} \cup U^{III}_{\eta,\mathfrak{g}}$. The definitions of these classes are as follows.

The class $U^{I}_{\eta,\mathfrak{g}}$ includes graph(s) formed by augmenting the $\mathfrak{g}$-order cycle $C_{\mathfrak{g}}$ with two pendant paths, each connected to a different vertex $\alpha, \beta \in V(C_{\mathfrak{g}})$ (one at α and the other at β). The lengths of the pendant paths are u and v, respectively, where $u \geq v \geq 1$ and $u + v = \eta - \mathfrak{g}$. The class $U^{II}_{\eta,\mathfrak{g}}$ includes graph(s) formed by augmenting the $\mathfrak{g}$-order cycle $C_{\mathfrak{g}}$ with two pendant paths connected to a single vertex $\alpha \in V(C_{\mathfrak{g}})$. One of the pendant paths has a length of u, while the other has a length of v, where $u \geq v \geq 1$ and $u + v = \eta - \mathfrak{g}$. The class $U^{III}_{\eta,\mathfrak{g}}$ includes graph(s) formed by augmenting the $\mathfrak{g}$-order cycle graph $C_{\mathfrak{g}}$ and the $(u+1)$-order path graph P_{u+1}.

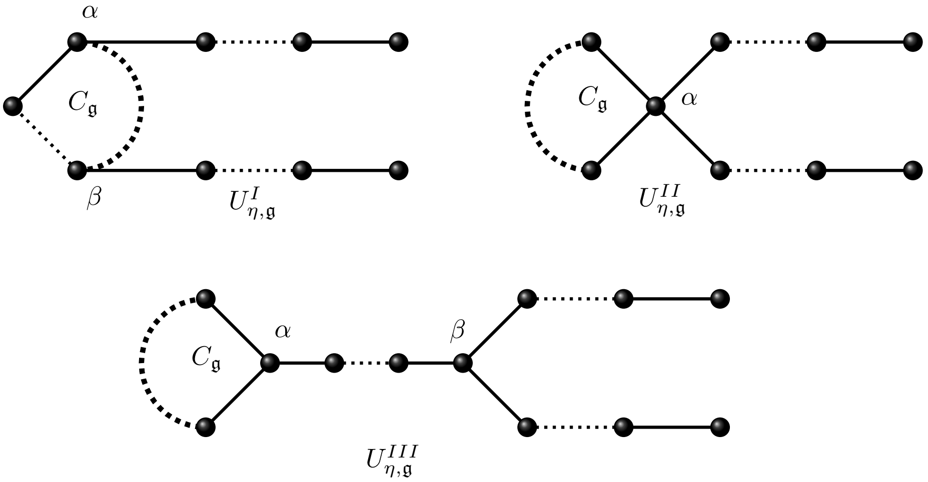


Figure 3: The classes $U^{I}_{\eta,\mathfrak{g}}$, $U^{II}_{\eta,\mathfrak{g}}$, and $U^{III}_{\eta,\mathfrak{g}}$ are the general forms of graphs.

The result is achieved by connecting a path of length v between a vertex $\alpha \in V(C_{\mathfrak{g}})$ and a non-pendant vertex $\beta \in V(P_{u+1})$, where $u \geq 2$, $v \geq 1$, and $u + v = \eta - \mathfrak{g}$. Based on Lemma 2.5, the corresponding HA values are presented in the Table 1. The integers u and v are unable to be equal to 1 at the same time, as $n - 4 \geq \mathfrak{g}$. As a result, we have Table 1. By collecting the HA index values obtained in each of the previously discussed cases and doing a simple comparison, we arrive at the expected conclusion of this section. Consequently, we have

$$HA(G_1^2) = HA(G_1^8) = \eta - 0.382222 > HA\left(G_1^i\right),$$

Table 1: Classification of the graphs G_1^i along with their corresponding conditions and HA index values.

Class	**Graphs**	**Conditions**	e_{12}	e_{13}	e_{14}	e_{22}	e_{23}	e_{24}	e_{33}	**HA**
$U^{I}_{\eta,\mathfrak{g}}$	G_1^1	$u > v = 1, \alpha\beta \in E(G)$	1	1	0	$\eta - 6$	3	0	1	$\eta - 0.481111$
	G_1^2	$u \geq v > 1, \alpha\beta \in E(G)$	2	0	0	$\eta - 7$	4	0	1	$\eta - 0.382222$
	G_1^3	$u > v = 1, \alpha\beta \notin E(G)$	1	1	0	$\eta - 7$	5	0	0	$\eta - 0.561111$
	G_1^4	$u \geq v > 1, \alpha\beta \notin E(G)$	2	0	0	$\eta - 8$	6	0	0	$\eta - 0.462222$
$U^{II}_{\eta,\mathfrak{g}}$	G_1^5	$u > v = 1$	1	0	1	$\eta - 5$	0	3	0	$\eta - 0.804444$
	G_1^6	$u \geq v > 1$	2	0	0	$\eta - 6$	0	4	0	$\eta - 0.666667$
$U^{III}_{\eta,\mathfrak{g}}$	G_1^7	$v = 1$, one pendant vertex is adjacent to β	1	1	0	$\eta - 6$	3	0	1	$\eta - 0.481111$
	G_1^8	$v = 1$, no pendant vertex is adjacent to β	2	0	0	$\eta - 7$	4	0	1	$\eta - 0.382222$
	G_1^9	$v > 1$, two pendant vertices is adjacent to β	0	2	0	$\eta - 6$	4	0	0	$\eta - 0.66$
	G_1^{10}	$v > 1$, one pendant vertex is adjacent to β	1	1	0	$\eta - 7$	5	0	0	$\eta - 0.561111$
	G_1^{11}	$v > 1$, no pendant vertex is adjacent to β	2	0	0	$\eta - 8$	6	0	0	$\eta - 0.462222$

for every $i \in \{1, 3, 4, 5, 6, 7, 9, 10, 11\}$, as desired. Hence, $HA(H) \leq \eta - 0.382222$ with equality is achieved if and only if $H = G_1^2$ & $G_1^8 \in U'_{\eta,\mathfrak{g}}$(for $3 \leq \mathfrak{g} \leq \eta - 5$) and if $H = G_1^2 \in \mathbb{U}^{\Phi}_{\eta,\mathfrak{g}}$(for $\mathfrak{g} = \eta - 4$)(see Figure 2).

(ii) Given that $\mathfrak{g} = \eta - 3$, we have $p \in \{2, 3\}$.

Case 1. $p = 3$.

Graph Z is one of the three graph classes, as shown in Figure 4, its standard forms are $H \in \mathbb{U}^{I}_{\eta,\mathfrak{g}} \cup \mathbb{U}^{II}_{\eta,\mathfrak{g}} \cup \mathbb{U}^{III}_{\eta,\mathfrak{g}}$. The class $\mathbb{U}^{I}_{\eta,\mathfrak{g}}$ is the graph generated from the $\mathfrak{g}-$order cycle $C_{\mathfrak{g}}$ by joining one pendant vertex at a single vertex $\alpha \in V(C_{\mathfrak{g}})$ and two pendant vertices at one unique vertex $\beta \in V(C_{\mathfrak{g}})$. The class $\mathbb{U}^{II}_{\eta,\mathfrak{g}}$ is the graph generated from the $\mathfrak{g}-$order cycle $C_{\mathfrak{g}}$ by joining three pendent vertices at a single vertex $\alpha \in V(C_{\mathfrak{g}})$. The class $\mathbb{U}^{III}_{\eta,\mathfrak{g}}$ is the graph generated from the

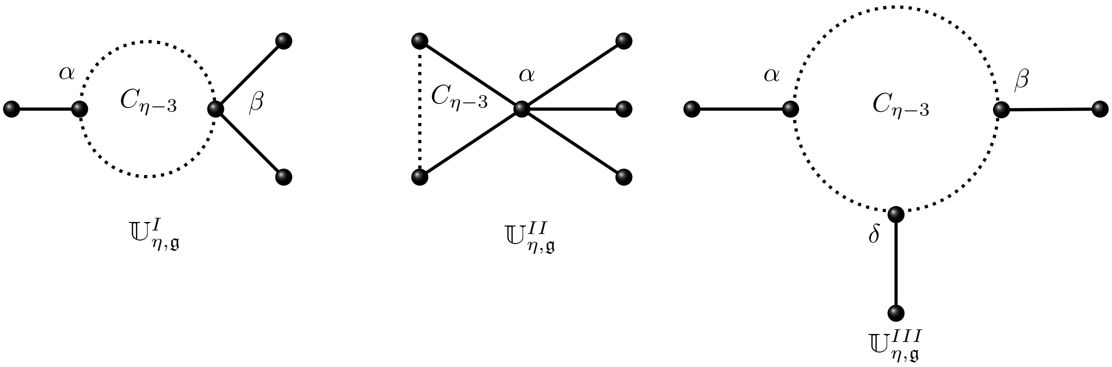


Figure 4: $\mathbb{U}^{I}_{\eta,\mathfrak{g}}$, $\mathbb{U}^{II}_{\eta,\mathfrak{g}}$, and $\mathbb{U}^{III}_{\eta,\mathfrak{g}}$ represent the general forms of the graphs.

$\mathfrak{g}-$order cycle $C_{\mathfrak{g}}$ by joining three pendent vertices at three distinct vertices $\alpha, \beta, \delta \in V(C_{\mathfrak{g}})$. From Table 2, $p = 3$ has $HA(Z) < \eta - 0.481111$, where $HA(G_3^1) = 0.481111$ (see Table 3).

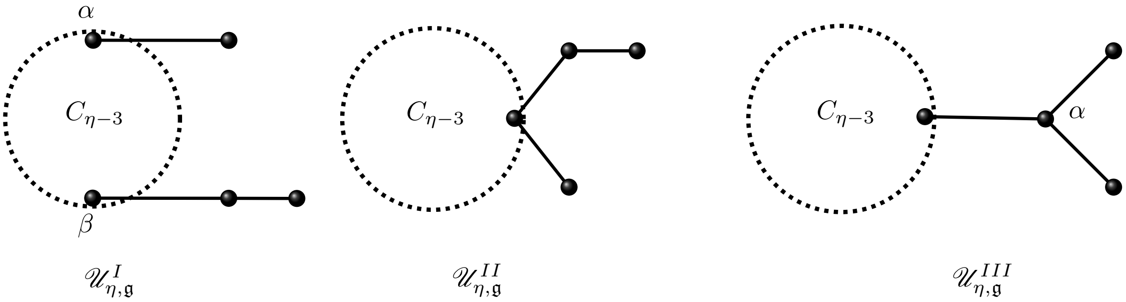


Figure 5: $\mathscr{U}^{I}_{\eta,\mathfrak{g}}$, $\mathscr{U}^{II}_{\eta,\mathfrak{g}}$ and $\mathscr{U}^{III}_{\eta,\mathfrak{g}}$ are the general forms of graphs.

Case 2. $p = 2$.
Here, either the graph Z may be classified into one of the three graphs, which are presented in Figure 5 or $Z \in \mathbb{U}^{\Phi}_{\eta,\eta-3}$. Consequently, we have

$$HA(G_3^1) = \eta - 0.481111 > HA\left(G_4^i\right),$$

for every $i \in \{2, 3, 4\}$, as desired.

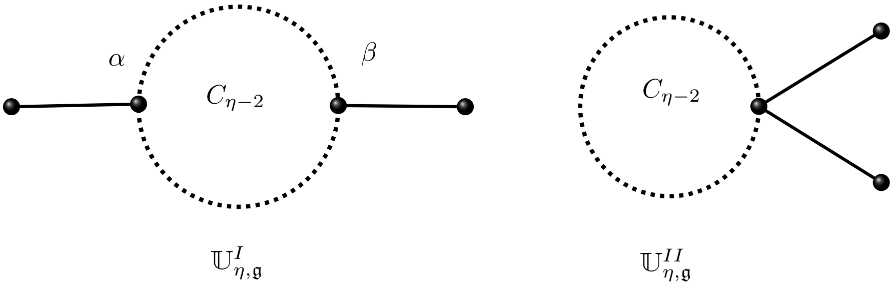


Figure 6: $\mathbb{U}^{I}_{\eta,\mathfrak{g}}$ and $\mathbb{U}^{II}_{\eta,\mathfrak{g}}$ are the general forms of graphs.

Table 2: Classification of the graphs G_2^i along with their corresponding conditions and HA index values.

Class	**Graphs**	**Conditions**	e_{12}	e_{13}	e_{14}	e_{15}	e_{22}	e_{23}	e_{24}	e_{25}	e_{33}	e_{34}	**HA**
$\mathbb{U}^{I}_{\eta,\mathfrak{g}}$	G_2^1	$\alpha\beta \in E(G)$	0	1	2	0	$\eta - 6$	1	1	0	0	1	$\eta - 1.141519$
	G_2^2	$\alpha\beta \notin E(G)$	0	1	2	0	$\eta - 7$	2	2	0	0	0	$\eta - 1.272222$
$\mathbb{U}^{II}_{\eta,\mathfrak{g}}$	G_2^3	unique graph exists	0	0	0	3	$\eta - 5$	0	0	2	0	0	$\eta - 1.700680$
	G_2^4	All three vertices (α, β, δ) are pairwise adjacent, $\eta = 6$	0	3	0	0	0	0	0	0	3	0	5.25
$\mathbb{U}^{III}_{\eta,\mathfrak{g}}$	G_2^5	Among three vertices (α, β, δ) two pairwise adjacent	0	3	0	0	$\eta - 7$	2	0	0	2	0	$\eta - 0.83$
	G_2^6	Among three vertices (α, β, δ) one pairwise adjacent	0	3	0	0	$\eta - 8$	4	0	0	1	0	$\eta - 3.84$
	G_2^7	No three vertices (α, β, δ) are pairwise adjacent	0	3	0	0	$\eta - 9$	6	0	0	0	0	$\eta - 0.99$

Table 3: Classification of the graphs G_3^i along with their corresponding conditions and HA index values.

Class	**Graphs**	**Conditions**	e_{12}	e_{13}	e_{14}	e_{22}	e_{23}	e_{24}	e_{33}	**HA**
$\mathscr{U}^{I}_{\eta,\mathfrak{g}}$	G_3^1	$u = 2, v = 1,$ $\alpha\beta \in E(G)$	1	1	0	$\eta - 6$	3	0	1	$\eta - 0.481111$
	G_3^2	$u = 2, v = 1,$ $\alpha\beta \notin E(G)$	1	1	0	$\eta - 7$	5	0	0	$\eta - 0.935185$
$\mathscr{U}^{II}_{\eta,\mathfrak{g}}$	G_3^3	$u = 2, v = 1$	1	0	1	$\eta - 5$	0	3	0	$\eta - 0.804444$
$\mathscr{U}^{III}_{\eta,\mathfrak{g}}$	G_3^4	$v = 1,$ α is adjacent to 2 pendent vertices	0	2	0	$\eta - 5$	2	0	1	$\eta - 0.58$

Hence, $HA(Z) \leq \eta - 0.481111$ with equality is achieved if and only if $Z = G_3^1 \in \mathbb{U}^{\Phi}_{\eta,\eta-3}$(see Figure 1).

(iii) Given that $\mathfrak{g} = \eta - 2$, the graph Z can be categorized into one of the two classes of graphs, which are presented in Figure 6.

Table 4: Classification of the graphs G_4^i along with their corresponding conditions and HA index values.

Class	**Graphs**	**Conditions**	e_{12}	e_{13}	e_{14}	e_{22}	e_{23}	e_{24}	e_{33}	**HA**
$\mathbb{U}^{I}_{\eta,\mathfrak{g}}$	G_4^1	$u = 1, v = 1, \alpha\beta \in E(G)$	0	2	0	$\eta - 5$	2	0	1	$\eta - 0.58$
	G_4^2	$u = 1, v = 1, \alpha\beta \notin E(G)$	0	2	0	$\eta - 6$	4	0	0	$\eta - 0.66$
$\mathbb{U}^{II}_{\eta,\mathfrak{g}}$	G_4^3	$u = 1, v = 1$	0	0	2	$\eta - 4$	0	2	0	$\eta - 0.942222$

Consequently, we have

$$HA(G_4^1) = \eta - 0.58 > HA\left(G_4^i\right),$$

for every $i \in \{2, 3\}$, as desired (Table 4).

Hence, $HA(Z) \leq \eta - 0.58$ with equality is achieved if and only if $Z = G_4^1 \in \mathbb{U}^{\Phi}_{\eta,\eta-2}$ (see Figure 1).

■

The following result is derived from Theorem 2.6.

Corollary 2.7. *Assume $U^*_{\eta,\mathfrak{g}}$ and $U'_{\eta,\mathfrak{g}}$ are the graphs specified earlier.*

i) If $\eta = 5$, then
$HA(\mathbb{U}^{\Phi}_{5,3}) < HA(U^*_{5,4}) < HA(U^*_{5,3}) < HA(C_5)$.

ii) If $\eta = 6$, then
$HA(\mathbb{U}^{\Phi}_{6,4}) < HA(\mathbb{U}^{\Phi}_{6,3}) < HA(U^*_{6,5}) < HA(U^*_{6,3}) = HA(U^*_{6,4}) < HA(C_6)$.

iii) If $\eta \geq 7$, then
$HA(U'_{\eta,\eta-4}) = \cdots = HA(U'_{\eta,3}) < HA(U^*_{\eta,\eta-1}) < HA(U^*_{\eta,3}) = \cdots = HA(U^*_{\eta,\eta-2}) < HA(C_\eta)$.

The only graph with the maximum harmonic-arithmetic index is C_η. From Theorem 2.2, Theorem 2.6, and Corollary 2.7, we may infer that the unique graphs with the second-maximum harmonic-arithmetic index for graphs in U_η are $U^*_{\eta,\mathfrak{g}}(3 \leq \mathfrak{g} \leq \eta - 2)$, and the unique graphs with the third and fourth maximum harmonic-arithmetic index for graphs in U_η are $U^*_{\eta,\eta-1}$ and $U'_{\eta,i}(3 \leq i \leq \eta - 4)$. Additionally, among all graphs in U_5, $\mathbb{U}^{\Phi}_{5,3}$ is the unique graph that is the fourth-maximum harmonic-arithmetic index; among all graphs in U_6, $HA(\mathbb{U}^{\Phi}_{6,3})$ is the unique graph with the fourth-maximum harmonic-arithmetic index, and therefore among all the graphs

in U_η, $U'_{\eta,\mathfrak{g}}(3 \leq \mathfrak{g} \leq \eta-4)$ are the unique graphs with the fourth-maximum harmonic-arithmetic index, if $\eta \geq 7$.
It is important to remember that a chemical graph is one in which each vertex has at most four degrees. A chemical unicyclic graph is a unicyclic graph in which the maximal vertex degree is not greater than four.

Remark 1. In Corollary 2.4, Theorem 2.2, and Theorem 2.6, if the term *"unicyclic graphs"* is replaced by *"chemical unicyclic graphs"*, the corresponding statements remain valid.

3 Smallest HA index of connected graphs $G_{n,\delta}$ with minimum degree δ

This article examines connected, loopless, simple, and finite graphs. For a determined graph G, consider the vertex c to have $d(c)$ as the degree. Consider $\delta(G)$ to be the minimum degree of G and $\Delta(G)$ to be the maximum degree of G. Divnić [27] found the minimum value of a connected graph with minimum degree. The neighbors of x are denoted as $N(c)$ (i.e., the adjacent vertices of c), and $d(c) = |N(c)|$ denotes the degree of vertex c in graph G. Let c be the pendant vertex in G if $d_c = 1$. The edge that intersects with c is defined as a pendant edge. The support vertex is the neighbor of a pendant vertex. A trivial graph is a graph with order 1. P_n and C_n are the denotations for the n-order path graph and cycle graph, respectively. In graph G, the length of the shortest path between c and h is represented as $d(c,h)$. $D(G)$ is the diameter of G, which is the length of the longest shortest path between any two vertices in the graph. The pendant path of the graph is represented by p. Let η_x represent the number of vertices in the graph G that have a degree of x. The weight of an edge $(e = ch)$ in G is $w_G(e) = \dfrac{4d_cd_h}{(d_c+d_h)^2}$.

Theorem 3.1. *([16]). If T_η be a tree with η vertices and $\eta-1$ edges, then*

$$4\left(1-\frac{1}{\eta}\right)^2 \leq HA(T_\eta) \leq (\eta-3)+\frac{16}{9},$$

where the lower bound is achieved if and only if T_η is a star graph S_η and the upper bound is achieved if and only if T_η is a path graph P_η.

3.1 The problem is modeled as a linear programming problem:

Here, we define the smallest HA index of graphs, $G_{n,\delta}$ with girth δ. We shall list a few linear equality and inequality conditions that each graph in $G(\delta,\eta)$ must meet. The number of edges connecting vertices of degrees ω and κ is denoted by $u_{\omega,\kappa}$. The problem P can be mathematically explained by identifying

$$\min\left\{ HA(G) = \textstyle\sum_{\delta\leq\omega\leq\kappa\leq\eta-1} \dfrac{4\omega\kappa}{(\omega+\kappa)^2}u_{\omega,\kappa} \,\middle|\, G \in G(\delta,\eta)\right\} \text{ is}$$

$$\min \sum_{\delta\leq\omega\leq\kappa\leq\eta-1} \frac{2\sqrt{\omega\kappa}}{\omega+\kappa}u_{\omega,\kappa},$$

subject to

$$\begin{aligned}
&2u_{\delta,\delta}+u_{\delta,\delta+1}+u_{\delta,\delta+2}+\cdots+u_{\delta,\eta-1}=\delta\eta_{\delta},\\
&u_{\delta,\delta+1}+2u_{\delta+1,\delta+1}+u_{\delta+1,\delta+2}+\cdots+u_{\delta+1,\eta-1}=(\delta+1)\eta_{\delta+1},\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&u_{\delta,\eta-1}+u_{\delta+1,\eta-1}+u_{\delta+2,\eta-1}+\cdots+2u_{\eta-1,\eta-1}=(\eta-1)\eta_{\eta-1},
\end{aligned}\tag{a}$$

$$\eta_{\delta}+\eta_{\delta+1}+\eta_{\delta+2}+\cdots+\eta_{\eta-1}=\eta,\tag{b}$$

$$u_{\omega,\kappa}\geq 0,\quad \delta\leq\omega\leq\kappa\leq\eta-1,\quad \eta_{\omega}\geq 0,\quad \delta\leq\omega\leq\eta-1.\tag{c}$$

The variables $u_{\omega,\kappa}$ and η_{ω} are integers. (a) - (c) specify a linear programming optimization problem.

Theorem 3.2. *If $G\in G(\delta,\eta)$, then $\delta\geq\lceil\delta_0\rceil$, where $\delta_0=p_0(\eta-1)$. The distinct positive root of the equation $p^2+4p-1=0$ is $p_0\approx 0.23606$, then*

$$HA(G)\geq\frac{\delta\eta}{2},$$

equality is achieved if and only if G is a regular graph of degree δ, if δ or η is even.

Proof. We will find the smallest graph among (η,δ); thus, the problem to be considered

$$\min\sum_{\delta\leq\omega\leq\kappa\leq\eta-1}\frac{4\omega\kappa}{(\omega+\kappa)^2}u_{\omega,\kappa},$$

according to (a) - (c). This is a linear programming problem. The fundamental variables are $u_{\delta,\delta}$ and $\eta_{\omega},\delta\leq\omega\leq\eta-1$. This implies that we will use η_{ω} and $u_{\delta,\delta}$ to solve equalities (a) and (b). We have

$$\eta_{\omega}=\frac{u_{\delta,\omega}+u_{\delta+1,\omega}+\cdots+2u_{\omega,\omega}+\cdots+u_{\omega,\eta-1}}{\omega},\quad \delta+1\leq\omega\leq\eta-1.\tag{d}$$

From (b), we get

$$\eta_{\delta}=\eta-\sum_{\omega=\delta+1}^{\eta-1}\eta_{\omega}=\eta-\sum_{\omega=\delta+1}^{\eta-1}\frac{1}{\omega}u_{\delta,\omega}-\sum_{\delta\leq\omega\leq\kappa\leq\eta-1}\left(\frac{1}{\omega}+\frac{1}{\kappa}\right)u_{\omega,\kappa}.\tag{e}$$

From the first equation of (a), we get

$$u_{\delta,\delta}=\frac{1}{2}\delta\eta_{\delta}-\frac{1}{2}\sum_{\omega=\delta+1}^{\eta-1}u_{\delta,\omega}.\tag{f}$$

After substitution of η_{δ} from (e) into (f), we have

$$u_{\delta,\delta}=\frac{\delta\eta}{2}-\frac{1}{2}\sum_{\omega=\delta+1}^{\eta-1}\left(1+\frac{\delta}{\omega}\right)u_{\delta,\omega}-\frac{1}{2}\sum_{\delta+1\leq\omega\leq\kappa\leq\eta-1}\left(\frac{\delta}{\omega}+\frac{\delta}{\kappa}\right)u_{\omega,\kappa}.$$

Then

$$\begin{aligned}
HA(G) &= \sum_{\delta\le\omega\le\kappa\le\eta-1} \frac{4\omega\kappa}{(\omega+\kappa)^2} u_{\omega,\kappa} \\
&= \sum_{\delta+1\le\omega\le\kappa\le\eta-1} \frac{4\omega\kappa}{(\omega+\kappa)^2} \left[u_{\delta,\delta} + u_{\delta,\omega} + u_{\omega,\kappa}\right] \\
&= \frac{4\delta\delta}{(\delta+\delta)^2} \left(\frac{\delta\eta}{2} - \frac{1}{2} \sum_{\omega=\delta+1}^{\eta-1} \left(1 + \frac{\delta}{\omega}\right) u_{\delta,\omega} - \frac{1}{2} \sum_{\delta+1\le\omega\le\kappa\le\eta-1} \left(\frac{\delta}{\omega} + \frac{\delta}{\kappa}\right) u_{\omega,\kappa} \right) \\
&\quad + \sum_{\omega=\delta+1}^{\eta-1} \frac{4\delta\omega}{(\delta+\omega)^2} u_{\delta,\omega} + \sum_{\delta+1\le\omega\le\kappa\le\eta-1} \frac{4\omega\kappa}{(\omega+\kappa)^2} u_{\omega,\kappa} \\
&= \frac{\delta\eta}{2} + \sum_{\omega=\delta+1}^{\eta-1} \left(\frac{4\delta\omega}{(\delta+\omega)^2} - \frac{\delta}{2}\left(\frac{1}{\delta} + \frac{1}{\omega}\right)\right) u_{\delta,\omega} \\
&\quad + \sum_{\delta+1\le\omega\le\kappa\le\eta-1} \left(\frac{4\omega\kappa}{(\omega+\kappa)^2} - \frac{\delta}{2}\left(\frac{1}{\omega} + \frac{1}{\kappa}\right)\right) u_{\omega,\kappa}.
\end{aligned}$$

Define

$$a_{\omega,\kappa} = \frac{4\omega\kappa}{(\omega+\kappa)^2} - \frac{\delta}{2}\left(\frac{1}{\omega} + \frac{1}{\kappa}\right),$$

for $\delta \le \omega \le \kappa \le \eta - 1$. We will demonstrate that $a_{\omega,\kappa} \ge 0$ for $\delta \le \omega \le \kappa \le \eta - 1$. We hold

$$a_{\omega,\omega} = 1 - \frac{\delta}{\omega} \ge 1 - \frac{\delta}{\delta} = 0,$$

for $\delta \le \omega \le \eta - 1$. Since

$$\frac{\partial a_{\omega,\kappa}}{\partial\omega} = \frac{4\kappa(\kappa-\omega)}{(\omega+\kappa)^3} + \frac{\delta}{2\omega^2} > 0,$$

for $\kappa \ge \omega$, we have $a_{\omega,\kappa} > a_{\delta,\kappa}, \delta \le \omega \le \kappa \le \eta - 1$. Further,

$$\begin{aligned}
a_{\delta,\kappa} &= \frac{4\delta\kappa}{(\delta+\kappa)^2} - \frac{\delta}{2}\left(\frac{1}{\delta} + \frac{1}{\kappa}\right) = 1 - \frac{(\delta-\kappa)^2}{(\delta+\kappa)^2} - \frac{1}{2} - \frac{\delta}{2\kappa} \\
&= \frac{\kappa-\delta}{2\kappa} - \frac{(\delta-\kappa)^2}{(\delta+\kappa)^2} = (\kappa-\delta)\left(\frac{1}{2\kappa} - \frac{(\kappa-\delta)}{(\delta+\kappa)^2}\right) \\
&= \frac{(\kappa-\delta)}{2\kappa(\delta+\kappa)^2}\left[\delta^2 - \kappa^2 + 4\delta\kappa\right] = \frac{(\kappa-\delta)}{2\kappa(\delta+\kappa)^2} \tilde{a}_{\delta,\kappa},
\end{aligned}$$

where $\tilde{a}_{\delta,\kappa} = \delta^2 - \kappa^2 + 4\delta\kappa$. Since

$$\frac{\partial^2 \tilde{a}_{\delta,\kappa}}{\partial\kappa^2} = -2 < 0,$$

for $\delta \le \kappa \le \eta - 1$, we determine that $\tilde{a}_{\delta,\kappa}$ is a concave function. Additionally, if $\tilde{a}_{\delta,\eta-1} = \delta^2 - (\eta-1)^2 + 4\delta(\eta-1) \ge 0$, then $\tilde{a}_{\delta,\kappa} \ge 0$ and $\tilde{a}_{\delta,\delta} = 4\delta^2 > 0$. Then,

$$\begin{aligned}
&\delta^2 - (\eta-1)^2 + 4\delta(\eta-1) \ge 0, \\
\Rightarrow\ &\frac{\delta^2}{4\delta(\eta-1)} - \frac{(\eta-1)^2}{4\delta(\eta-1)} + 1 \ge 0, \\
\Rightarrow\ &\frac{p}{4} - \frac{1}{4p} + 1 \ge 0,
\end{aligned}$$

thus $p = \dfrac{\delta}{\eta - 1}$. It is simple to determine that the equation $p^2 + 4p - 1 = 0$ has a unique positive root that is $p_0 \approx 0.23606$, and for $p \geq p_0$, $p^2 + 4p - 1 \geq 0$. This indicates that for $\delta \geq p_0(\eta - 1)$, $\tilde{a}_{\delta,\eta-1} \geq 0$ (and $a_{\delta,\eta-1} \geq 0$).

As all $a_{\omega,\kappa} \geq 0$ for $\delta \leq \omega \leq \kappa \leq \eta - 1$, we deduce that if we set $u_{\omega,\kappa} = 0$ for all $\delta \leq \omega \leq \kappa \leq \eta - 1$, with the exception of $u_{\delta,\delta}$, the harmonic-arithmetic index would reach its smallest value $\dfrac{\delta\eta}{2}$. Consequently, we have demonstrated that

$$HA(G) \geq \frac{\delta\eta}{2}.$$

On graphs for $u_{\delta,\delta} = \dfrac{\delta\eta}{2}, \eta_\delta = \eta$, and with all other $u_{\omega,\kappa} = 0$ and $\eta_\omega = 0$, the harmonic-arithmetic index would reach its smallest value $\dfrac{\delta\eta}{2}$ if δ or η is even. ■

4 Conclusion

In this work, Theorems 2.2 and 2.6 explore the tasks of finding graphs that achieve the first and second maximum values of the HA index in the class of all unicyclic graphs (chemical unicyclic graphs) of specific order and with a defined girth. Using these theorems in Corollaries 2.4 and 2.7, we have solved the problem of finding graphs with the first four maximum values of the HA index in the class of all unicyclic graphs of a specific order. We also present the relevant graphs that reach the specified boundaries.

The extremal graphs and lower bound for $\delta \geq \lceil \delta_0 \rceil$ are found. Determining extremal graphs seems more difficult in this case. We demonstrate that the extremal graphs when δ or η are even are regular graphs of degree δ.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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