STUDIA UBB CHEMIA, LVIII, 2, 2013 (p. 71 – 86)
(RECOMMENDED CITATION)

MAXIMAL HARARY INDEX OF UNICYCLIC GRAPHS WITH A GIVEN MATCHING NUMBER

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ABSTRACT. The Harary index is defined as the sum of reciprocals of distances between all the vertex pairs of a connected graph. In this paper we present upper bounds on Harary index of unicyclic graphs with a given matching number and characterize the extremal graphs for which the upper bounds on Harary index are attained.

Key Words: *Graph, Reciprocal distance, Harary Index, upper bound*

INTRODUCTION

The Harary index of a graph, denoted by *H*(*G*), has been introduced in 1993, independently by Ivanciuc *et al*.[1] and by Plavšić *et al*.[2] Even earlier, the QSAR group in Timisoara, Romania, particularly Ciubotariu [3], have used this index to express the decay of interactions between atoms in molecules as the distances between them increased. It has been so named in the honor of Professor Frank Harary, on the occasion of his 70[th] birthday. The Harary index is defined as

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)}$$

where the summation runs over all unordered pairs of vertices of the graph *G* and $d_G(u,v)$ denotes the topological distance between any two vertices *u* and *v* of *G* (i.e., the number of edges in a shortest path connecting *u* and *v*). Mathematical properties and applications of *H* are reported in refs. [4-14].

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Chemical applications of this index, in correlating with thermodynamic properties or octane number of alkanes, or in discriminating alkane isomers, are presented in refs. [5,15-18]. Some new interesting properties of other distance-based graph invariants can be seen in refs. [19-21].

Let $\gamma(G,k)$ be the number of vertex pairs of *G* lying to each other at the distance *k*. Then, from refs.[8,12] we have:

$$H(G) = \sum_{k\geq 1} \frac{1}{k} \gamma(G,k). \tag{1}$$

All graphs herein considered are finite and simple ones. Let *G* = (*V;E*) be a graph with the vertex set *V* (*G*) and edge set *E*(*G*). A connected graph *G* is called a unicyclic graph if $|V(G)| = |E(G)|$. Two edges e_1 and e_2 are called independent if they do not have a common vertex. A matching of *G* is a subset of *E*(*G*) with some pairwise independent edges. For a graph *G*, the *matching number* $\beta(G)$ is the maximum cardinality among the independent sets of edges in *G*. For a matching *M* of a graph *G*, if a vertex $v \in V(G)$ is incident to an edge of *M*, then *v* is said *M*-saturated. For a graph *G*, *D*(*G*) denotes the diameter of *G*, or the maximum topological distance between any two vertices in *G*. In the following, we denote by P_n, C_n and S_n the path graph, the cycle graph and the star graph with *n* vertices, respectively. For other notations and terminology in the Graph Theory, the readers may consult refs. [22,23].

Let $\bigcup(n,m)$ be the set of connected unicyclic graphs, of order *n* and having the matching number *m*. Recently, Ilić *et al.* [24] have determined the tree with the maximal Harary index among all the trees of order *n* and having the matching number *m*. Du and Zhou [25] determined the extremal graph of $\bigcup(n,m)$ with the minimal Wiener index. Inspired by the above results, the graphs of $\bigcup(n,m)$, having the maximal Harary index and their characterization, will be presented in the following.

SOME LEMMAS

As preliminaries, let us introduce some basic lemmas. For a graph *G*, with $v \in V(G)$, one defines [12]

$$Q_G(v) = \sum_{u \in V(G)} \frac{d_G(u,v)}{d_G(u,v)+1}.$$

For convenience, we will write $Q_G(v)$ as $Q_{V(G)}(v)$. Note that the function $f(x)=\dfrac{x}{x+1}$ is strictly increasing for $x>1$.

Let $U_{n,m}$ be a unicyclic graph obtained by attaching $n-2m+1$ pendent edges and $m-2$ pendent paths, of length 2, to one vertex of the triangle C_3, as shown in Figure 1. By equality (1), we can obtain

$$H(U_{n,m})=n+\frac{1}{2}[\binom{n-m+1}{2}-1+m-2]+\frac{1}{3}[(n-2m+3)(m-2)+(m-2)(m-3)]+\frac{1}{4}\binom{m-2}{2}$$

$$=n+\frac{1}{2}\frac{(n-m)^2+n+m-6}{2}+\frac{1}{3}(n-m)(m-2)+\frac{1}{4}\binom{m-2}{2}$$

$$=\frac{1}{24}(6n^2-4mn+m^2+14n+7m-18). \qquad (*)$$

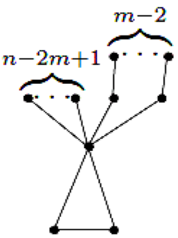

Fig.1 The graph $U(n,m)$

For a vertex *v* of *G*, the *eccentricity ecc*(*v*) is defined as the maximum distance from *v* to any other vertex in *G*.

Lemma 2.1. *Let G be a connected graph of order n* > 4, *with a pendent vertex v adjacent to the vertex u, and let w be a neighbor of u different from v. Then*

$$H(G)-H(G-v)\le\frac{n}{3}+\frac{1}{6}+\frac{1}{6}d_G(v) \qquad (2)$$

with the equality holding if and only if ecc(*u*) = 2. *Moreover, if* $d_G(u)=2$, *then*

$$H(G)-H(G-\{u,v\})\le\frac{7n}{12}+\frac{1}{2}+\frac{1}{4}d_G(w) \qquad (3)$$

with the equality holding if and only if ecc(*w*) = 2.

Proof. Considering that *v* is a pendent vertex of *G*, we have

$$\begin{aligned} H(G)-H(G-v) &= n-1-Q_{G-v}(u) \\ &\le n-1-[\frac{1}{2}(d_G(u)-1)+\frac{2}{3}(n-1-d_G(u))] \\ &= \frac{n}{3}+\frac{1}{6}+\frac{1}{6}d_G(u) \end{aligned}$$

with the equality holding if and only if *ecc*(*u*) = 2.

When $d_G(u)=2$, we have

$$\begin{aligned} H(G)-H(G-\{u,v\}) &= H(G)-H(G-v)+H(G-v)-H(G-\{u,v\}) \\ &= n-1-Q_{G-v}(u)+n-2-Q_{G-\{u,v\}}(w) \\ &\le n-1-[\frac{1}{2}+\frac{2}{3}(d_G(w)-1)+\frac{3}{4}(n-2-d_G(w))] \\ &\quad +n-2-[\frac{1}{2}(d_G(w)-1)+\frac{2}{3}(n-2-d_G(w))] \\ &= \frac{7n}{12}+\frac{1}{2}+\frac{1}{4}d_G(w) \end{aligned}$$

with the equality holding if and only if *ecc*(*w*) = 2.

Lemma 2.2. [26] *Let* $G\in\bigcup(2m,m)$, $m\ge 3$ *and T be a branch of G with the root r. If* $u\in V(T)$ *is a pendent vertex closest to the root r, with* $d_G(u,r)\ge 2$ *¸ then u is adjacent to a vertex of degree two.*

Lemma 2.3. [27] *Let* $G\in\bigcup(n,m)$, *with n > 2m and* $G\ne C_n$. *Then, there is a maximum matching M and a pendent vertex v of G such that v is not M-saturated.*

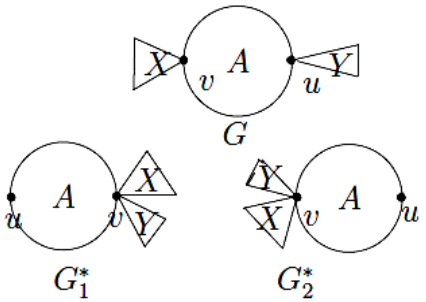

Fig. 2 The graphs G, G_1^* and G_2^* in Lemma 2.4

Lemma 2.4. [10,13] *Let A, X and Y be three connected graphs with disjoint vertex sets. Suppose that u, v are two vertices of A,* v_0 *is a vertex of X and* u_0 *is a vertex of Y . Let G be the graph obtained from A, X and Y by identifying v with* v_0 *and u with* u_0*, respectively. Let* G_1^* *be the graph obtained from A, X and Y by identifying three vertices v,* v_0 *and* u_0*, and let* G_2^* *be the graph obtained from A, X and Y by identifying three vertices u,* v_0 *and* u_0 *(Figure 2). Then we have:*

$$H(G_1^*) > H(G) \text{ or } H(G_2^*) > H(G).$$

From Lemma 2.4, the following corollary is immediate.

Corollary 2.1. *Let G be a connected graph with* $u, v \in V(G)$*. Denote by G(s;t) the graph obtained by attaching s >* 1 *pendent vertices to vertex u and t >* 1 *pendent vertices to vertex v. Then, we have*

$$H(G(1, s+t-1)) > H(G) \text{ or } H(G(s+t-1, 1)) > H(G).$$

Lemma 2.5. [13] *Let G be a (connected) graph with a cut vertex w such that* G_1 *and* G_2 *are two connected subgraphs of G having w as the only common vertex and* $G_1 \cup G_2 = G$*. Let* $|V(G_i)| = n_i$ *for* $i = 1,2$*. Then*

$$H(G) = H(G_1) + H(G_2) + \sum_{u \in V(G_1)\setminus\{w\}} \sum_{v \in V(G_2)\setminus\{w\}} \frac{1}{d_{G_1}(u,w) + d_{G_2}(w,v)}.$$

Let $C_k(1^{n-k})$ be a graph obtained by attaching $n-k$ pendent edges to a vertex of C_k. Based on equality (1), we can claim that $H(C_k(1^1)) > H(C_{k+1})$, for $k \geq 5$. Denote by $C_k^*(n-k-1,1)$ a unicyclic graph obtained by attaching one pendent vertex and $n-k-1$ pendent vertices, respectively, to two adjacent vertices of a cycle C_k.

Lemma 2.6. *Let* $k \geq 5$ *and* $C_k^*(n-k-1,1)$ *be a unicyclic graph defined as above. Then*

$$H(C_k^*(n-k-1,1)) > H(C_{k+1}^*(n-k-2,1)).$$

Proof. To prove this lemma, we first prove that

$$H(C_k(1^{n-k})) > H(C_{k+1}(1^{n-k-2})).$$

Note that $C_k(1^{n-k})$ is obtained by identifying the unique vertex of degree 3 in $C_k(1^1)$ with the center of star S_{n-k-1}, where the new vertex is labeled as w_1

and $C_{k+1}(1^{n-k-2})$ is obtained by identifying one vertex C_{k+1} with the center of the star S_{n-k-1}, where the new vertex is labeled as w_2. Set $A = H(C_k(1^{n-k})) - H(C_{k+1}(1^{n-k-2}))$. So, by Lemma 2.5, we have

$$H(C_k(1^{n-k-1})) = H(S_{n-k-1}) + H(C_k(1^1)) + (n-k-2) \sum_{v \in V(C_k(1^1)) \setminus \{w_1\}} \frac{1}{1 + d_{C_k(1^1)}(w_1, v)},$$

$$H(C_{k+1}(1^{n-k-2})) = H(S_{n-k-1}) + H(C_{k+1}) + (n-k-2) \sum_{v \in V(C_{k+1}) \setminus \{w_2\}} \frac{1}{1 + d_{C_{k+1}}(w_2, v)}.$$

Thus, considering that $H(C_k(1^1)) > H(C_{k+1})$, for $k \geq 5$, from above we get

$$A > (n-k-2)\Big(\sum_{v \in V(C_k(1^1)) \setminus \{w_1\}} \frac{1}{1 + d_{C_k(1^1)}(w_1, v)} - \sum_{v \in V(C_{k+1}) \setminus \{w_2\}} \frac{1}{1 + d_{C_{k+1}}(w_2, v)} \Big)$$

$$= (n-k-2)\Big(\frac{1}{2} - \frac{1}{1 + \left\lceil \frac{k}{2} \right\rceil}\Big) > 0$$

as expected.

Assume that the unique vertex of degree 3 in $C_k^*(n-k-1,1)$ is u_1 and the unique vertex of degree 3 in $C_{k+1}^*(n-k-2,1)$ is u_2. Suppose that $V(C_k(1^{n-k-1})) = V(C_k^*(n-k-1,1)) \setminus \{v_1\}$ and $V(C_k(1^{n-k-1})) = V(C_k^*(n-k-1,1)) \setminus \{v_1\}$, where v_1 is adjacent to u_1 in $C_k^*(n-k-1,1)$ and v_2 is adjacent to u_2 in $C_{k+1}^*(n-k-2,1)$. Let $B = H(C_k^*(n-k-1,1)) - H(C_{k+1}^*(n-k-2,1))$. Similarly, by Lemma 2.5, we arrive at

$$H(C_k^*(n-k-1,1)) = 1 + H(C_k(1^{n-k-1})) + \sum_{v \in V(C_k(1^{n-k-1})) \setminus \{u_1\}} \frac{1}{1 + d_{C_k(1^{n-k-1})}(u_1, v)},$$

$$H(C_{k+1}^*(n-k-2,1)) = 1 + H(C_{k+1}(1^{n-k-2})) + \sum_{v \in V(C_{k+1}(1^{n-k-2})) \setminus \{u_2\}} \frac{1}{1 + d_{C_{k+1}(1^{n-k-2})}(u_2, v)}.$$

From above, we get

$$B > \sum_{v \in V(C_k(1^{n-k-1})) \setminus \{u_1\}} \frac{1}{1 + d_{C_k(1^{n-k-1})}(u_1, v)} - \sum_{v \in V(C_{k+1}(1^{n-k-2})) \setminus \{u_2\}} \frac{1}{1 + d_{C_{k+1}(1^{n-k-2}) \setminus \{u_2\}}(u_2, v)}$$

as $H(C_{k+1}(1^{n-k-2})) > H(C_{k+1}(1^{n-k-2}))$

$= \frac{1}{3} - \frac{1}{1+\left\lceil \frac{k}{2} \right\rceil} > 0$, thus ending the proof of this lemma.

MAIN RESULTS

In this section, the graph of $\bigcup(n,m)$, with the maximal Harary index, will be determined. Before presenting the main results, we first will deal with some special cases of this problem.

When *n* = 3, there is only one unicyclic graph, which is just the triangle C_3, with the matching number 1. There is nothing to prove, in this case. Clearly, only C_3 belongs to $\bigcup(n,1)$. Next, we only need to consider the set $\bigcup(n,m)$, with $n \geq 4$ and $m \geq 2$. If *n* = 4, there are exactly two unicyclic graphs, C_4 and $C_3(1^1)$, which belong to $\bigcup(4,2)$, with $H(C_4) = H(C_3(1^1))$. When *n* = 5, we can easily check that (see ref.[11]) only two graphs C_n and $C_3(1^2)$ have the maximal Harary index in $\bigcup(5,2)$. From ref. [17] we find that the unique graph $C_3(1^{n-3})$ has the maximal Harary index in $\bigcup(n,2)$, with $n \geq 6$.

Now we consider the case *n* = 6. Two graphs, $G_6^{(1)}$ and $G_6^{(2)}$ are shown in Fig. 2. It is not difficult to check that there are only five graphs: $U_{6,3}$, $C_5(1^1)$, $G_6^{(1)}$, $G_6^{(2)}$ and C_6, in $\bigcup(6,3)$, and

$$H(C_5(1^1)) = 6 + \frac{1}{2}\times 7 + \frac{1}{3}\times 2 = 10\frac{1}{6}$$
$$> H(U_{6,3}) = H(C_6) = H(G_6^{(1)}) = H(G_6^{(2)})$$
$$= 6 + \frac{1}{2}\times 6 + \frac{1}{3}\times 3 = 10.$$

Thus $C_5(1^1)$ has the maximal Harary index in $\bigcup(6,3)$. In the following we assume that $n \geq 7$ and $m \geq 3$.

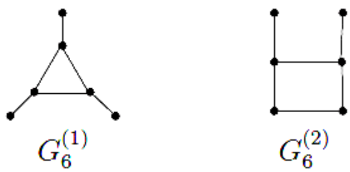

Fig. 3 The graphs $G_6^{(1)}$ and $G_6^{(2)}$

Let $\bigcup^{(1)}(m)$ be the set of graphs from $\bigcup(6,3)$ having a pendent vertex whose neighbor is of degree two. Also, let $\bigcup^{(2)}(m) = \bigcup(m) \setminus \bigcup^{(1)}(m)$. Denote by $C_5(1,1,1)$ the graph obtained by attaching three pendent vertices to three consecutive vertices in C_5.

Lemma 3.1. *Let* $G \in \bigcup^{(2)}(m)$, *with* $m \geq 4$. *Then, we have*

$$H(G) \leq \frac{1}{24}(17m^2 + 35m - 18)$$

with the equality holding if and only if $G \cong C_5(1,1,1)$.

Proof. If $G \cong C_5(1,1,1)$, the equality holds immediately. So it suffices to prove that

$H(G) < \frac{1}{24}(17m^2 + 35m - 18)$, when $G \neq C_5(1,1,1)$.

For any graph $G \in \bigcup^{(2)}(m) \setminus \{C_5(1,1,1)\}$, by Lemma 2.2, we find that *G* is the cycle C_{2m} or a graph obtained by attaching some pendent vertices to some vertices of C_k with $m \leq k \leq 2m-1$. Combining the structure of $U_{n,m}$ with *n* = 2*m* and formula (*), we can easily find

$$\frac{17m^2 + 35m - 18}{24} = 2m + \frac{1}{2}\frac{m^2 + 3m - 6}{2} + \frac{1}{3}m(m-2) + \frac{1}{4}\binom{m-2}{2}$$

Moreover, for $m \geq 4$,

$$\gamma(C_{2m},2) = 2m < \frac{m^2 + 3m - 6}{2}, \ \gamma(C_{2m},3) = 2m < m(m-2) \text{ and}$$

$$\gamma(C_{2m},4) \geq m, \ \ldots, \gamma(C_{2m},m) = m.$$

Therefore, from (1), we have $H(C_{2m}) < \frac{17m^2 + 35m - 18}{24}$.

Now, let us consider the case when *G* is a graph obtained by attaching some pendent vertices to some vertices of C_k, with $m \leq k \leq 2m-1$. To prove this lemma, we need to look at the following three cases.

Case 1: *k* = *m*. In this case, we can easily find that *G* is a graph obtained by attaching

a pendent vertex to each vertex of C_m. If *m* = 4, we can easily check that $H(G) < H(C_5(1,1 1))$. When $m \geq 5$, we have $\gamma(G,2) = 3m < \frac{m^2+3m-6}{2}$, $\gamma(G,3) = 3m + \gamma(C_m,3) \leq m(m-2)$, $\gamma(G,4) = m + 2\gamma(C_m,4),\cdots,$
$\gamma(G,\left\lfloor \frac{m}{2} \right\rfloor + 2) = \gamma(C_m,\left\lfloor \frac{m}{2} \right\rfloor) = \left\lfloor \frac{m}{2} \right\rfloor > 1.$

Therefore, according to (1), we have $H(G) < \frac{17m^2+35m-18}{24}$.

Case 2. $m+1 \leq k \leq 2m-2$. For this case, by Corollary 2.1, we claim that any graph *G* of this type can be changed into a graph $C_k(n-k-1,1) = C_k(1,n-k-1)$.

Considering the equality (1), $H(C_k(2m-k-1,1))$ reaches its maximum value when the two vertices of degrees 3 and $2m-k+1$ are adjacent. We denote by C_k^* the type of graph with the maximal Harary index. When *m* = 4, since $G \neq C_5(1,1,1)$, we have $G \cong C_6^*$. A simple calculation shows that $H(C_6^*) = \frac{97}{6} < \frac{197}{12} = H(C_5(1,1,1))$. In the following, we assume that $m \geq 5$. By Lemma 2.6, we claim that the maximum value of $H(C_k^*)$ is attained at *k* = *m* + 1. Moreover,

$$\begin{aligned}
\gamma(C_{m+1}^*,2) &= m+1+2(m-1)+\binom{m-2}{2} \\
&= 3m-1+\frac{(m-2)(m-3)}{2} \\
&\leq \frac{m^2+3m-6}{2}, \\
\gamma(C_{m+1}^*,3) &= \gamma(C_{m+1},3)+2(m-1)+(m-2) \\
&= \begin{cases} 3m-1 & \text{if } m=5 \\ 4m-3 & \text{if } m \geq 6 \end{cases} \\
&< m^2-2m, \\
D(C_{m+1}^*) &= \left\lfloor \frac{m+1}{2} \right\rfloor + 1 \geq 4.
\end{aligned}$$

Combining the above arguments with the equality (1), we have

$$H(G) < H(C^*_{m+1}) < \frac{17m^2+35m-18}{24}.$$

Case 3. $k = 2m-1$. In this case, we claim that $G \cong C_{2m-1}(1^1)$. If *m* = 4, it is easy to see that $H(C_7(1^1)) = 16 < \frac{197}{12} = H(C_5(1,1,1))$. For $k \geq 5$, we can find that $\gamma(C_{2m-1}(1^1),2) = 2m+1 < \frac{m^2+3m-6}{2}$,

$\gamma(C_{2m-1}(1^1),3) = 2m+1 < m(m-2)$ and $D(C_{2m-1}(1^1)) = m \geq 5$.

Similarly to the above two cases, we have $H(C_{2m-1}(1^1)) < \frac{17m^2+35m-18}{24}$.

Thus we completed the proof of this lemma.

Lemma 3.2. *Let* $G \in \bigcup(2m,m)$ *and v be any vertex in V* (*G*)*. Then* $d_G(v) \leq m+1$.

Proof. There exists a graph $G \in \bigcup(2m,m)$ with a vertex $v \in V(G)$, of degree $s \geq m+2$. Assume that $v_1, v_2, \cdots, v_s$ are all the neighbors of *v* in *G*. Now there are $2m-s \leq m-2$ edges remained in $G \in \bigcup(2m,m)$.

Therefore, $\beta(G) \leq m-2+1 = m-1$. This is a contradiction to the fact that $G \in \bigcup(2m,m)$, thus proving this lemma.

Lemma 3.3. *Let* $G \in \bigcup(8,4)$. *Then* $H(G) \leq \frac{197}{12}$, *with the equality holding if* $G \cong U_{8,4}$ *or* $G \cong C_5(1,1,1)$.

Proof. If $G \in \bigcup^{(2)}(4)$, by Lemma 3.1, we have $H(G) \leq \frac{197}{12}$ with the equality holding if and only if *G* = *C*$_5$(1*;* 1*;* 1). If $G \in \bigcup^{(1)}(4)$, with a pendent vertex $v \in V(G)$ and *u* as the neighbor of *v,* of degree two, then $G - \{u,v\} \in \bigcup(6,3)$. By Lemmas 2.1 and 3.2, we have

$$H(G) \leq H(G-\{u,v\}) + \frac{31}{6} + \frac{1}{4}d_G(w)$$

$$\leq H(G-\{u,v\}) + \frac{31}{6} + \frac{5}{4}$$

with the equality holding if and only if *ecc*(*w*) = 2 and $d_G(w)=5$.

Considering the structures of $U_{6,3}$, $C_5(1^1)$, $G_6^{(1)}$, $G_6^{(2)}$ and C_6 (there is only $U_{6,3}$ with the maximum degree 4), we claim that the above equality holds if and only if $G \cong U_{8,4}$. The lemma follows immediately.

In the following, we give a lemma as a starting point for our main results. In this lemma, the graph of $\bigcup(10,5)$, with the maximum Harary index, will be completely characterized.

Lemma 3.4. *Let* $G \in \bigcup(10,5)$. *Then,* $H(G) \le \frac{97}{4}$ *with the equality holding if and only if* $G \cong U_{10,5}$.

Proof. By Lemma 3.1, we have $H(G) \le \frac{97}{4}$ if $G \in \bigcup^{(2)}(5)$. For any graph

$G \in \bigcup^{(1)}(5)$, from Lemmas 2.1, 3.2 and 3.3, we have

$$H(G) \le H(G-\{u,v\}) + \frac{38}{6} + \frac{1}{4} d_G(w)$$
$$\le \frac{197}{12} + \frac{38}{6} + \frac{3}{2} = \frac{97}{4}$$

with the equality holding if and only $G-\{u,v\} \cong U_{8,4}$ or $G \cong C_5(1,1,1)$, *ecc*(*w*) = 2 and $d_G(w)=6$, that is, $G \cong U_{10,5}$.

Theorem 3.1. *Let* $G \in \bigcup(2m,m)$ *with* $m \ge 5$. *Then we have*

$$H(G) < \frac{17m^2+35m-18}{24} \tag{4}$$

with the equality holding in (4) if and only if $G \cong U_{2m,m}$.

Proof. We prove this theorem by induction on *m*. For *m* = 5, from Lemma 3.4, this lemma follows immediately.

Assume that the result is true for any graphs in $\bigcup(2m-2,m-1)$, with $m \ge 6$.

If $G \in \bigcup^{(2)}(m)$, then by Lemma 3.1, we have $H(G) < \frac{17m^2+35m-18}{24}$. If $G \in \bigcup^{(1)}(m)$, with a pendent vertex $v \in V(G)$ and *u* as the neighbor of *v*, of degree two, we can conclude that $G-\{u,v\} \in \bigcup(2m-2, m-1)$. By Lemma 2.1 and the induction hypothesis, it follows that

$$H(G) \le H(G-\{u,v\}) + \frac{7m+3}{6} + \frac{1}{4}d_G(w)$$
$$\le \frac{17(m-1)^2+35(m-1)-18}{24} + \frac{7m+3}{6} + \frac{m+1}{4} = \frac{17m^2+35m-18}{24}$$

with the equalities holding if and only if $G-\{u,v\} \cong U_{2m-2,m-1}$, *ecc*(*w*) = 2 and $d_G(w) = m+1$; thus, *G* is just $U_{2m,m}$ and the theorem is completely proved.

Theorem 3.2. *Let* $G \in \bigcup(n,m)$ *with* $3 \le m \le \frac{n}{2}$ *and* $n \ge 7$ *. Then we have*

$$H(G) < \frac{6n^2-4mn+m^2+14n+7m-18}{24} \tag{5}$$

with the equality holding in (5) if and only if $G \cong U_{7,3}$ *or* $C_5(1^2)$ *for* $(n,m) = (7,3)$*;* $G \cong U_{8,4}$ *or* $C_5(1,1,1)$ *for* $(n,m) = (8,4)$*;* $G \cong U_{n,m}$ *otherwise.*

Proof. First we define a function

$$f(n,m) = \frac{6n^2-4mn+m^2+14n+7m-18}{24},$$

where n, m are all positive integers. In view of formula (*) we obtain

$$f(n,m) = n + \frac{1}{2}\frac{(n-m)^2+n+m-6}{2} + \frac{1}{3}(n-m)(m-2) + \frac{1}{4}\binom{m-2}{2}.$$

For the cycle C_n, we have $n = 2m+1$ or $n = 2m$. Based on equality (1), using a procedure as that followed in the proof of Lemma 3.1, we can get $H(C_n) < f(n,m)$.

For any graph $G \in \bigcup(n,m)$, with $n > 2m$ different from C_n, by Lemma 2.3, there must be a pendent vertex *v* of *G* and a maximum matching *M* such that *v* is not *M*-saturated in *G*. Clearly, $G - v \in \bigcup(n-1, m)$. Let *u* be the unique neighbor of *v* in *G*. As proved in ref. [25] $d_G(u) \le n-m+1$.

Now we prove this result by induction on *n*. According to the value of *m*, we divide the discussion into the following three cases.

Case 1: *m* = 3. For *n* = 7, $G-v\in\bigcup(6,3)$. If $G-v\cong C_5(1^1)$, we have $d_G(u)\le 4$. Then, by Lemma 2.1, it follows that

$$H(G)\le H(C_5(1^1))+\frac{5}{2}+\frac{1}{6}d_G(u)\le\frac{61}{6}+\frac{5}{2}+\frac{2}{3}=\frac{40}{3}$$

with the equalities holding if and only if $d_G(u)=4$ and *ecc*(*u*) = 2, that is, $G\cong C_5(1^2)$. If $G-v\neq C_5(1^1)$, by Lemma 2.1, we have

$$H(G)\le H(G-v)+\frac{5}{2}+\frac{1}{6}d_G(u)\le 10+\frac{5}{2}+\frac{5}{6}=\frac{40}{3}$$

with the equalities holding if and only if $G\cong U_{6,3}$, C_6, $G_6^{(1)}$, *or* $G_6^{(2)}$ (Fig. 2), $d_G(u)=5$ and *ecc*(*u*) = 2, which implies $G\cong U_{7,3}$. Thus, we claim that $H(G)\le\frac{40}{3}$. When $G\in\bigcup(n,m)$, with $(n,m)=(7,3)$, the equality is holding if and only if $G\cong C_5(1^2)$*; or* $U_{7,3}$.

When *n* = 8, we get $G-v\in\bigcup(7,3)$. By Lemma 2.1,

$$H(G)\le H(G-v)+\frac{17}{6}+\frac{1}{6}d_G(u)\le\frac{40}{3}+\frac{17}{6}+1=f(8,3)$$

with the equalities holding if and only if $G-v\cong U_{7,3}$, $d_G(u)=6$ and *ecc*(*u*) = 2, i.e., $G\cong U_{8,3}$. Assume that the result holds for all graph $G\in\bigcup(n-1,3)$ with $n\ge 9$. By Lemma 2.1 and induction hypothesis, we have

$$H(G)\le H(G-v)+\frac{2n+1}{6}+\frac{1}{6}d_G(u)\le f(n-1,m)+\frac{2n+1}{6}+\frac{n-2}{6}=f(n,3)$$

with the equalities holding if and only if $G-v\cong U_{n-1,3}$, $d_G(u)=n-2$ and *ecc*(*u*) = 2, equivalently, $G\cong U_{n,3}$.

Case 2: *m* = 4. For *n* = 8, the result follows from Lemma 3.3. In case $n=9$, $G-v\in\bigcup(8,4)$. Based on Lemma 2.1, by analogy to the Case 1, we have $H(G)\le\frac{197}{12}+\frac{19}{6}+1=f(9,4)$

with the equality holding if and only if $G \cong U_{9,4}$. Suppose that the result holds for any graph $G - v \in \bigcup(n-1,4)$, with $n \geq 10$; from Lemma 2.1 and induction hypothesis, we have

$$H(G) \leq H(G-v) + \frac{2n+1}{6} + \frac{1}{6}d_G(u) \leq f(n-1,4) + \frac{2n+1}{6} + \frac{n-3}{6} = f(n,4)$$

with the equalities holding if and only if $G - v \cong U_{n-1,4}$, $d_G(u) = n-3$ and *ecc*(*u*) = 2, equivalently, $G \cong U_{n,4}$.

Case 3: $m \geq 5$. When $n = 2m$, the result holds from Lemma 3.4. Assume the result is true for any graph $G \in \bigcup(n-1,4)$ with $\geq 2m$. By a similar procedure, we obtain

$$H(G) \leq H(G-v) + \frac{2n+1}{6} + \frac{1}{6}d_G(u) \leq f(n-1,4) + \frac{2n+1}{6} + \frac{n-m+1}{6} = f(n,m)$$

with the equalities holding if and only if $G - v \cong U_{n-1,m}$, $d_G(u) = n-m+1$ and *ecc*(*u*) = 2, that is, $G \cong U_{n,m}$. Thus, the proof of this theorem is completed.

The cyclomatic number η of *G* is defined as $\eta(G) = |E(G)| - |V(G)| + \omega(G)$, where $\omega(G)$ is the number of connected components of *G*. Denote by $G(n,\eta,m)$ the set of connected graphs of order *n* and by *m* the matching number. Clearly, when $\eta = 0$, $G(n,\eta,m)$ denotes the set of trees of order *n,* of the matching number *m*; if $\eta = 1$, then $G(n,\eta,m) = \bigcup(n,m)$. Considering the main results in this paper (for $\eta = 1$) and those in ref. [24] (for $\eta = 0$), we naturally ask the following problem:

Problem 3.1. *Can we determine the graph of* $G(n,\eta,m)$ *with the maximal Harary index being an integer* $\eta \geq 2$*?*

Even more difficult is to determine the graph of $G(n,\eta,m)$ with the minimal Harary index, even for the case $\eta = 0$. Therefore, we will end this paper with the following interesting problem:

Problem 3.2. *Which graph of* $G(n,\eta,m)$ *has the minimal Harary index for a given integer* $\eta \geq 0$*?*

ACKNOWLEDGEMENT

K. X. is supported by NUAA Research Funding, No. NN2012080 and NNSF of China (No. 11201227). K. Ch. D. and H. H. acknowledge, respectively, for the support of Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea and Qing Lan Project of Jiangsu Province, PR China.

REFERENCES

1. O. Ivanciuc, T. S. Balaban, and A. T. Balaban, *J. Math. Chem.* **1993**, *12*, 309.
2. D. Plavšić, S. Nikolić, N. Trinajstić, ad Z. Mihalić, *J. Math. Chem.* **1993**, *12*, 235.
3. D. Ciubotariu, PhD thesis, 1987, Timisoara, Romania; D. Ciubotariu, M. Medeleanu, V. Vlaia, T. Olariu, C. Ciubotariu, D. Dragos, and C. Seiman, *Molecules*, **2004**, *9*, 1053.
4. K.C. Das, B. Zhou, and N. Trinajstic, *J. Math. Chem.* **2009**, *46*, 1369.
5. M.V. Diudea, *J. Chem. Inf. Comput.* Sci. **1997**, 37, 292.
6. E. Estrada, L. Rodriguez, *MATCH Commun. Math. Comput. Chem.* **1997**, *35*, 157.
7. L. Feng and A. Ilic, *Appl. Math. Lett.* **2010**, *23*, 943.
8. I. Gutman, *Indian J. Chem.* **1997**, *36 A*, 128.
9. B. Lucić, A. Miličević, S. Nikolić, and N. Trinajstić, *Croat. Chem. Acta* **2002**, *75*, 847.
10. K. Xu, *Discrete Appl. Math.* **2012**, *160*, 321.
11. K. Xu and K. C. Das, *Bull. Malys. Math. Sci. Soc.***2013**, 36, 373.
12. K. Xu and K. C. Das, *Discrete Appl. Math.* **2011**, *159*, 1631.
13. K. Xu and N. Trinajstić, *Utilitas Math.* **2011**, *84*, 153.
14. B. Zhou, X. Cai, and N. Trinajstić, *J. Math. Chem.* **2008**, *44*, 611.
15. M.V. Diudea, *MATCH Commun. Math. Comput. Chem.* **1995**, *32*, 85.
16. M.V. Diudea and C. M. Pop, *Indian J. Chem.* **1996**, *35A*, 257.
17. M.V. Diudea, O. Ivanciuc, S. Nikolić, and N. Trinajstić, *MATCH Commun. Math. Comput. Chem.* **1997**, *35*, 41.
18. M.V. Diudea and I. Gutman, *Croat. Chem. Acta,* **1998**, *71*, 21.
19. H. Deng, *Math. Comput. Model.* **2012**, *55*, 634.
20. M.H. Khalifeh, H. Yousefi-Azari, and A.R. Ashrafi, *Comput. Math. Appl.* **2008**, *56*, 1402.

21. A. Hamzeh, S. Hossein-Zadeh, and A. R. Ashrafi, *Appl. Math. Lett.* **2011**, *24*, 1099.
22. J.A. Bondy and U.S.R. Murty, *Graph Theory with Applications*, Macillan Press, New York, 1976.
23. M.V. Diudea, I. Gutman, and L. Jäntschi, *Molecular Topology*, NOVA, New York, 2002.
24. A. Ilić, G. Yu, and L. Feng, *Utilitas Math.*, in press.
25. Z. Du and B. Zhou, *MATCH Commun. Math. Comput. Chem.* **2010**, *63*, 101.
26. A. Chang and F. Tian, *Lin. Algebra Appl.* **2003,** *370*, 237.
27. A. Yu and F. Tian, *MATCH Commum. Math. Comput. Chem.* **2004**,*51*, 97.