MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **84** (2020) 739-751

ISSN 0340 - 6253

Characterization of the Forgotten Topological Index and the Hyper–Zagreb Index for the Unicyclic Graphs

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(Received March 25, 2020)

Abstract

Let G be a molecular graph with $V(G)$ and $E(G)$ be the vertex set and edge set, respectively. Various investigations show that many degree and distance based topological indices are used to exhibit strong intrinsic connection between the molecular structures and the physico-chemical properties of the chemical compounds. In this paper, we focus on two degree-based topological indices, namely, the forgotten topological index and the hyper-Zagreb Index expressed as $F(G) = \sum_{u \in V(G)} d(u)^3$ and $HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2$, respectively, where $d(u)$ and $d(v)$ are the degrees of the vertices u and v, respectively, in the graph G. We show that the unicyclic graphs can take any even positive integer except 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 26, 28, 30, 34, 36, 38, 42, 46, 50, 50, 54, 58, 62, 66, 70, 74, 78, 86 and 94 for the forgotten index. A comparable result for the hyper-Zagreb index is also presented.

1 Introduction

The Quantitative Structure Property Relationship (QSPR) explains the relation between the structure and the physico-chemical properties of the chemical compounds. This is achieved through the help of various molecular descriptors. Molecular descriptor is a numerical value by examining the structure of the chemical compound [1]. One among them is the topological descriptor (index) which is a graph invariant enumerated from the molecular graph of a chemical compound. It is observed that the topological indices

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such as PI index, Harmonic index and Zagreb indices are very close to various chemical and biological properties such as boiling point, surface tension etc. thereby reducing the number of experiments and cost [4, 5].

The study of inverse problem in combinatorial chemistry attracted a variety of researchers since the last decade of the 20th century [6, 7].

Recently, Yutras et al. [10] settled the inverse problem for the first and the second Zagreb indices and presented analogous results for the forgotten index (F) and the hyper-Zagreb index (HM). They left the problem of finding the possible values of the forgotten index and the hyper-Zagreb index of trees and unicyclic graphs open. However, they had given the hint that the forgotten index may assume any even integer greater than 198. Further, they added that the hyper-Zagreb index could achieve any positive even integer above 170.

The open problem about trees is settled recently. It is proved in [2] that the forgotten index of trees can be any even positive integer except 4, 6, 8, 12, 16, 20, 22, 24, 28, 32, 36, 40, 48, 52, 56, 60, 64, 72, 80 and 88. Further, it is also proved in [2] that the hyper-Zagreb index of trees can be any even positive integer except 4, 6, 8, 10, 12, 14, 16, 20, 22, 24, 26, 28, 30, 32, 36, 38, 40, 42, 44, 46, 48, 52, 54, 56, 58, 60, 62, 64, 68, 70, 72, 74, 76, 78, 80, 86, 88, 90, 92, 94, 96, 104, 106, 108, 110, 112, 122, 124, 126, 128, 138, 142, 144 and 158.

In this paper, we settle the inverse problem regarding the unicyclic graphs associated with the forgotten index (F-index) and the hyper-Zagreb index (HM-index).

2 Preliminaries

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $u \in V(G)$, let $d(u)$ denote its degree. For $u, v \in V(G)$, let uv denote an edge $uv \in E(G)$. In this study we consider only simple connected undirected graphs. A graph is unicyclic if it has exactly one cycle in it. For every unicyclic graph G, $|V(G)| = |E(G)|$. In Chemistry, a compound with single ring (cycle) is known as a monocyclic compound. The cycloalkanes, pentazole, azetidine, pyridine, benzene, octasulfur, etc. are some monocyclic compounds.

The forgotten topological index [3] or simply the forgotten index of a graph G, $F(G)$, is

$$F(G) = \sum_{u \in V(G)} d(u)^3.$$

The hyper-Zagreb index [8] of a graph G, $HM(G)$, is

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

To prove the nonexistence of unicyclic graphs with F-indices and hyper-Zagreb indices mentioned in Table 1 and Table 8, respectively, we analyze the set of all non isomorphic unicyclic graphs with C_3 of all orders from $n = 3$ to $n = 9$. For this, we use the proof technique presented in [10]. We find graphs smaller in terms of their order and size. From them, we construct graphs through a process of the subdivision of their edges or adjoining of edges. The subdivision of an edge is an operation of introducing a vertex in the place of an edge and making the new vertex adjacent to the end vertices of the erstwhile deleted edge. Through each subdivision the graph gains a new vertex of degree two and a new edge. Adjoining of an edge is an operation of introducing a vertex and making it adjacent to exactly one vertex of the existing graph. Through each adjoining the graph gains a vertex and an edge. Further, degree of the vertex to which the edge is adjoined is increased by one.

Let us now have a glitter on different transformations and ideas that are utilized in the journey of writing this paper. It is not difficult to see that the forgotten index and the hyper-Zagreb index can take only even positive integers. Further we adapt the following observation from [10].

Observation 2.1. *Let uv be an edge of a graph G. The subdivision of the edge uv generates a modified graph, say, G^* with the forgotten index given by,*

$$F(G^*) = F(G) + 8. \tag{1}$$

We have one more observation to achieve the goal of this paper.

Observation 2.2. *Let v be a vertex edge of a graph G with $d(v) = s$. Let u be the new vertex that is introduced. If u is made adjacent to v, then the forgotten index of the modified graph G^* is*

$$F(G^*) = F(G) + 3s(s + 1) + 2. \tag{2}$$

The above two observations are key points in solving the open problems related to the unicyclic graphs. For a graph G, the graph G^* is called a transformed graph. The process of constructing G^* from G is known as transformation [10]. This transformation is very important since it gives the smallest increase in the indices of our discussion with the increase in order or/and size of the graphs.

3 Results and Discussions

In this section, we discuss two theorems characterizing the forgotten index and hyper-Zagreb index of unicyclic graphs.

Theorem 3.1. *The forgotten topological index of unicyclic graphs can be any even positive integer except 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 26, 28, 30, 34, 36, 38, 42, 46, 50, 50, 54, 58, 62, 66, 70, 74, 78, 86 and 94.*

Proof. We prove this theorem through two claims. Firstly, we manifest the idea of inverse problem for F-indices, that is, to show the existence of unicyclic graphs with F-indices greater than 94 for any even positive integer. Secondly, we show that the set of unicyclic graphs with F-indices less than 94 is an empty set for all even positive integers given in Table 1.

G_0		8	16									
G_2	2	10	18	26	34	42	50	58	66	74		
G_4	4	12	20	28	36							
G_6	6	14	22	30	38	46	54	62	70	78	86	94

Table 1. F-indices for which unicyclic graphs do not exist

To establish the first claim, we start with a collection of four unicyclic graphs denoted by G_0, G_2, G_4 and G_6 as given in Figure 1 (a)-(d) with F-indices 24, 82, 44, 102 congruent to 0, 2, 4 and 6 (mod 8), respectively. These are the four unicyclic graphs with the smallest F-indices congruent to 0, 2, 4 and 6 (mod 8).

Now, we begin with G_0. It is nothing but the cycle C_n with the smallest F-index. It is also the unicyclic graph with the smallest F-index. By Observation 2.1, subdivisions of edges create cycles with F-indices 32, 40, 48, ... In general, in this way, we get all unicyclic graphs with F-indices of the form $24+4k$, where k is the number of subdivisions.

Similarly, if we apply the transformations as given above, on the graphs G_2, G_4 and G_6, we can construct unicyclic graphs with F-indices of the form 82+8k, 44+8k and 102+8k from the unicyclic graphs G_2, G_4 and G_6, respectively, where k is the number of subdivisions made in the respective graphs.

As 24, 82, 44 and 102 are congruent to 0, 2, 4 and 6 (mod 8), respectively, we establish the fact that there exist unicyclic graphs with F-indices for every even positive integer greater than 94 for sure. That is, there exist unicyclic graphs with F-index of the form 24+8k, 44+8k, 84+8k and 102+8k, for $k = 0, 1, 2, \ldots$

(a). G_0 **(b).** G_2 **(c).** G_4 **(d).** G_6

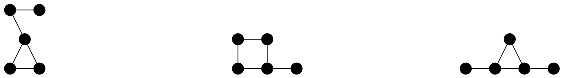
Figure 1. Basic Graphs for the F-index

The proof is complete only after the establishment of the second claim. We know that C_3, i. e., G_0 is the only unicyclic graph on three vertices. Its F-index is 24. Hence, it is also the unicyclic with the smallest F-index. So it is vacuously proved that there are no unicyclic graphs with F-index for even integers from 2 to 22.

Now, we consider the unicyclic graphs of four vertices. The cycle C_4 has the F-index 32. But 32 is congruent to 0 (mod 8). There is only one more unicyclic graph on four vertices. It is the graph G_4. It is nothing but the 3-pan graph. The graph G_4 is obtained from G_0, through the process of adjoining of an edge to one of the vertices of G_0. From the Observation 2.2, we can see that if we adjoin an edge to a vertex of degree 2, then the F-index is increased by 20 which is congruent to 4 (mod 8). Therefore, the graph G_4 has F-index 44. The cycle C_5 is the unicyclic graph with the smallest F-index among all unicyclic graphs of five vertices. The F-index of C_5 is 40. Hence, we can conclude that there are no unicyclic graphs with F-index for all even positive integers less than 44 except 24, 32 and 40. Therefore, we consolidate that, there are unicyclic graphs with F-indices of the form 24+8k and 44+8k, for $k = 0, 1, 2, \ldots$.

Now, we prove that there are no unicyclic graphs with F-indices 50, 58, 66 and 74, and 46, 54, 62, 70, 78, 86 and 94.

For this, at first we analyze all unicyclic graphs on five vertices. There are only five unicyclic graphs on five vertices. They are the graphs C_5, G_2 (Figure 1(b)), and the graphs in Figure 2.



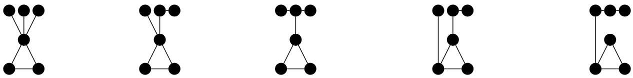
(a). G_α (b). G_β (c). G_γ

Figure 2. Unicyclic graphs on five vertices other than G_2 and C_5

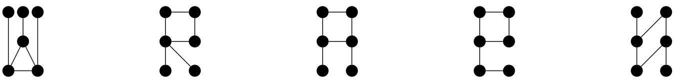
The graphs G_α and G_β in Figure 2 have the F-indices 52. They are obtained from the subdivision of G_4. The graph G_γ has F-index 64 which is 24+40. Hence, this is also not useful to us. The cycle C_5 has the F-index 40 which is 24+16. This is also a case that we had discussed. We are now left with the graph G_2. It is obtained from G_4, through the process of adjoining of an edge to the vertex of degree 3. From the Observation 2.2, the F-index is increased by 38 which is congruent to 6 (mod 8). Therefore, the graph G_2 has F-index 82 congruent to 2 (mod 8). Any other unicyclic graph with F-index less than 82, if it exists is obtained by the subdivision of either G_0 or G_4. That is, there are no other unicyclic graphs with F-index less than 82 which is not of the form 24+8k or 44+8k, for $k = 0, 1, 2, \ldots$.

Hence, we conclude that there are no unicyclic graphs with the F-indices 46, 50, 54, 58, 62, 66, 70, 74 and 78. Further, from G_2, we can generate unicyclic graph with F-index 90.

Hence, we are left with the positive integers 86 and 94 only (Table 1). We now consider unicyclic graphs on six vertices.



(a). G_a (b). G_b (c). G_c (d). G_d (e). G_e



(f). G_f (g). G_g (h). G_h (i). G_i (j). G_j

Figure 3. Unicyclic graphs on six vertices other than C_6, the 5-pan graph and G_6

There are only 13 unicyclic graphs on six vertices. They are the ten graphs $G_a \ldots G_j$ given Figure 3, C_6, the 5-pan graph and G_6 given in Figure 1. The F-indices of all the 13 unicyclic graphs on six vertices are given in Table 2.

G_a	G_b	G_c	G_d	G_e	G_f	G_g	G_h	G_i	G_j	C_6	5-pan graph	G_6
144	90	72	72	60	84	90	72	60	72	48	60	102

Table 2. F-indices of unicyclic graphs on six vertices

All these graphs except G_6 have their F-indices of the from $24+8k$, $44+8k$ or $82+8k$ for $k = 0, 1, 2, \ldots$. The graph G_6 has the F-index 102. The graph G_6 is obtained from G_2, through the process of adjoining of an edge. From the Observation 2.2, we can see that if we adjoin an edge to a vertex of degree 2, then the F-index is increased by 20 which is congruent to 4 (mod 8). Both 86 and 94 are congruent to 6 (mod 8). The F-index of G_2 is smallest integer congruent to 2 (mod 8) among all the graphs of order up to 5. Hence, the adjoining of an edge to a vertex of degree of G_2 generates the graph G_6 with F-index 102 which is congruent to 6 (mod 8). This implies that there are no unicyclic graphs that have the F-indices 86 and 94. We, therefore, complete the arguments of the second claim and thereby the proof of the theorem itself. ■

In the case of the forgotten index, the change in the index effected either by the subdivision or by the adjoining is for exactly one vertex at a time. On the contrary, the hyper-Zagreb index is changed by the change in the degree of a vertex to which an edge is adjoined and all the vertices in its neighborhood. Hence, we have so many cases to analyze. This analysis is crucial in the proof of the next theorem.

Theorem 3.2. *The hyper-Zagreb indices of unicyclic graphs can be any even positive integer greater than 46 except 50, 52, 54, 56, 58, 60, 62, 66, 68, 70, 72, 74, 76, 78, 84, 86, 88, 90, 92, 94, 102, 104, 106, 108, 110, 120, 122, 124, 126, 140, 142 and 172.*

Proof. The hyper-Zagreb index of a graph is based on the degrees of end vertices of each of the edges of a graph. As this theorem is about the unicyclic graphs, several facts about the unicyclic graphs would help us.

All the unicyclic graphs with girth greater than three whose hyper-Zagreb indices are less than 172 can be obtained from some basic operations such as subdivision of edges and adjoining of edges on the the unicyclic graphs with C_3. Hence, the proof is achieved through the fundamental analysis of the unicyclic graphs with C_3.

We now see the effect of subdivision and adjoining as far as hyper-Zagreb index is concerned.

Subdivision of an edge: We consider an edge at a time for the subdivision. Let us consider a graph G. Let G^* be the transformed graph after the subdivision of an edge. For even a tree with any two of its vertices having degree 4, the hyper-Zagreb index will exceed 200. Hence, we analyze the variations in the hyper-Zagreb indices of a graph after the single subdivision of an edge whose end vertices are of degrees from 1 to 4. In the Table 3, the first row and the first column represent the various degrees and the entries inside the table give corresponding rise in the hyper-Zagreb index of the graph.

degree	**1**	**2**	**3**	**4**
1	14	16	18	20
2	16	16	16	16
3	18	16	14	12
4	20	16	12	8

Table 3. Change in hyper-Zagreb indices after the subdivision of an edge

Adjoining of an edge: Here too, we consider an edge at a time for the adjoining. Let u a vertex of the graph G and let its neighbors be u_1, u_2 ... Tables 4, 5 and 6 represent various scenarios of the degree of the vertex u and the change (IC) in the hyper-Zagreb Index of the graph G is in the last row.

u_1	1	2	1	2	3	1	2	3	4	1	2	3	4	5
u_2	2	2	3	3	3	4	4	4	4	5	5	5	5	5
IC	32	34	34	36	38	36	38	40	42	38	40	42	44	46

Table 4. Degree of the vertex u is 2

u_1	1	1	2	1	1	1	2	2	3	1	1	1	1	2	2	2	3	3	4
u_2	1	2	2	1	2	3	2	3	3	1	2	3	4	2	3	4	3	4	4
u_3	2	2	2	3	3	3	3	3	3	4	4	4	4	4	4	4	4	4	4
IC	54	56	58	56	58	60	60	62	64	58	60	62	64	62	64	66	66	68	70

Table 5. Degree of the vertex u is 3

u_1	1	1	1	2	1	1	1	2	3	1	1	1	1	2	2	2	3	3	4
u_2	1	1	2	2	1	1	1	3	3	1	2	3	4	2	3	4	3	4	4
u_3	1	2	2	2	1	2	2	3	3	4	4	4	4	4	4	4	4	4	4
u_4	2	2	2	2	3	3	3	3	3	4	4	4	4	4	4	4	4	4	4
IC	82	84	86	88	84	86	60	62	64	58	60	62	64	62	64	66	66	68	70

Table 6. Degree of the vertex u is 4

Any unicyclic graph with at least one of its vertices of degree four that is adjacent to at least one vertex of degree four has the hyper-Zagreb index more than 172. Hence, we need not consider unicyclic graphs whose degree conditions do not exceed than that are given in Table 6.

We prove the theorem in two stages. In the initial stage we show that there exist unicyclic graphs with hyper-Zagreb indices greater than 142 for any even positive integer except 172. In the second stage we show that there are no unicyclic graphs with the hyper-Zagreb indices with positive integers less than 48 and the integers given in Table 8.

We consider a collection of eight unicyclic graphs Q_0, Q_2, Q_4, Q_6, Q_8, Q_{10}, Q_{12} and Q_{14} given in Figure 4(a)-4(h). The hyper-Zagreb indices of these graphs are given Table 7. These indices are congruent to 0, 2, 4, 6, 8, 10, 12 and 14 (mod 16), respectively.

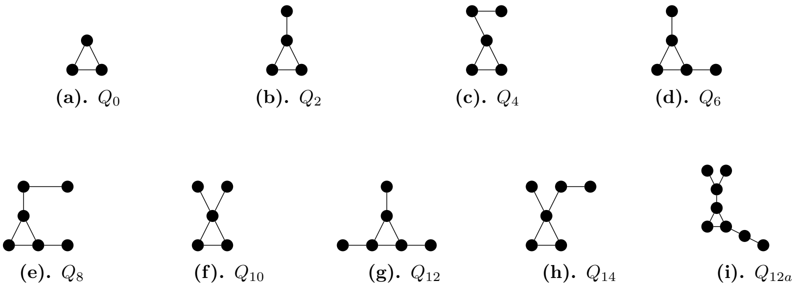


Figure 4. Basic Graphs for the HM-index

Graph	Q_0	Q_2	Q_4	Q_6	Q_8	Q_{10}	Q_{12}	Q_{14}
HM-index	48	82	100	118	136	138	156	158

Table 7. Hyper-Zagreb indices of the basic graphs $Q_0 \ldots Q_{14}$

We note that if we subdivide an edge of the cycle in a unicyclic graph where one of the vertices of the edge is of degree 2, the new graph formed is a unicyclic graph with its hyper-Zagreb index increased by 16 than that of the original graph. (See Table 3.) The graph Q_{12a} has hyper-Zagreb index 188.

As each of the graphs Q_0, Q_2, Q_4, Q_6, Q_8, Q_{10}, Q_{12a} and Q_{14} has at least one vertex of degree two in their cycles, by subdividing an edge incident to a vertex of degree two, we can construct unicyclic graphs with hyper-Zagreb indices 48+16k, 82+16k, 100+16k, 118+16k, 138+16k, 136+16k, 188+16k and 158+16k, respectively, for $k = 0, 1, 2, \ldots$ where k is the number of subdivisions.

With this we conclude the first stage. That is, there exist unicyclic graphs with hyper-Zagreb indices for all even integers greater than 142 except 172.

The next stage is to prove there are no unicyclic graphs with the hyper-Zagreb indices less than 48 and for the integers that are given in Table 8.

Q_2	Q_4	Q_6	Q_8	Q_{10}	Q_{12}	Q_{14}
50	52	54	56	58	60	62
66	68	70	72	74	76	78
	84	86	88	90	92	94
		102	104	106	108	110
			120	122	124	126
					140	142
					172	

Table 8. Hyper-Zagreb indices for which unicyclic graphs do not exist

The hyper-Zagreb index of cycle C_{10} is 160. It is the unicyclic graph with the smallest hyper-Zagreb index among all the unicyclic graphs with vertices 10 or more. Hence, in this stage, the analysis is limited to unicylic graphs of order 3 to 9.

For the reasons given in the beginning of the proof, to complete the analysis of this stage, it is enough to check the hyper-Zagreb indices of all non-isomorphic unicyclic graphs with C_3 of order $n \leq 9$. See Table 9 for the number of all non-isomorphic unicyclic graphs with C_3 and the number of all non-isomorphic unicyclic graphs, order $n \leq 9$ [9].

Order of the graph	3	4	5	6	7	8	9
Unicyclic graphs with C_3	1	1	3	7	18	44	117
All unicyclic graphs	1	2	5	13	33	89	240

Table 9. Number of all non-isomorphic unicyclic graphs of order $n \leq 9$

Now we begin the analysis. Consider the graph Q_0. It is nothing but C_3. Incidentally, it is also the unicyclic graph with the smallest hyper-Zagreb index. The hyper-Zagreb index of Q_0 is 48. Thus, vacuously, there are no unicyclic graphs with hyper-Zagreb indices from 2 to 46.

Further, by the subdivision of the edges of Q_0 we can construct unicyclic graphs with hyper-Zagreb indices of the form $48{+}16k$ for $k = 0, 1, 2, \dots$ in general. In particular, the cycles C_4, C_5, C_6, C_7 and C_8 are the unicyclic graphs with hyper-Zagreb indices 64, 80, 96, 112, 128, 144, and 160, respectively.

There are only two unicyclic graphs on 4 vertices. They are C_4 and Q_2. As C_4 has the hyper-Zagreb index 64, we consider the other unicyclic graph Q_2. The graph Q_2 is nothing but the 3-pan graph which is obtained by the adjoining operation. The hyper-

Zagreb index of Q_2 is 82. (See column 3 of Table 4.) We had already found out that C_5 has the hyper-Zagreb index 80. We thus conclude that there are no unicyclic graphs with hyper-Zagreb indices from 2 to 78 except for 48 and 64. As done early, by subdividing the edges in the cycle of Q_2, we get the unicyclic graphs (n-pan graphs) with hyper-Zagreb indices of the form $82+16k$ for $k = 0, 1, 2, \ldots$ in general. In particular, we get unicyclic graphs with hyper-Zagreb indices 98, 114, 130, 146 and 162. But we can not get unicyclic graphs with the hyper-Zagreb index 84 through 94.

There are only five unicyclic graphs of order 5. They are C_5, the 4-pan graph, Q_4, Q_6 and Q_{10}. Their hyper-Zagreb indices are 80, 98, 100, 118 and 138, respectively. The 4-pan graph, Q_4, Q_6 and Q_{10} are obtained from Q_2 either by the subdivision of or by the adjoining of a single edge. Since the cycle in Q_4 has a vertex of degree 2, using subdivision, we can generate unicyclic graphs of hyper-Zagreb indices 116, 132, 148, 164 $\ldots$. In additions to this, since Q_4 has a vertex of degree 2, say u, having neighboring vertices with degree 2 and 3, by adjoining an edge to the vertex u, we get a unicyclic graph of hyper-Zagreb index 136. Then by subdivisions we can generate a graph with hyper-Zagreb indices 152, 168 $\ldots$. Since Q_6 has a vertex in the cycle of degree 2, we can construct unicyclic graphs with hyper-Zagreb indices 134, 150, 166, $\ldots$.

Every unicyclic graph of order 4 and above can be constructed from unicyclic graphs of lower order either by the subdivision or by the adjoining operations. With the exhaustive list of the rise in the hyper-Zagreb indices given in the Tables 3, 4, 5 and 6, we can see that there are no unicyclic graphs whose hyper-Zagreb indices are 84, 86, 88, 90, 92, 94, 102, 104, 106, 108, 110, 120, 122, 124, 126, 140 or 142.

The graphs Q_{12} and Q_{14} of order 6, have hyper-Zagreb indices 156 and 158, respectively. The graph Q_{14} has a vertex of degree two. Hence, we can generate unicyclic graphs with hyper-Zagreb indices 174, 190 $\ldots$. However, the graph Q_{12} does not have a vertex of degree two. Hence, from Q_{12}, we can not generate a unicyclic graph with the hyper-Zagreb index 172.

There are exactly 24 unicyclic graphs with C_3 with their hyper-Zagreb index less than 172. Nine of them are displayed in Figure 4 and their hyper-Zagreb indices are given in Table 7. The remaining 15 unicyclic graphs and their hyper-Zagreb indices are displayed in Figure 5.

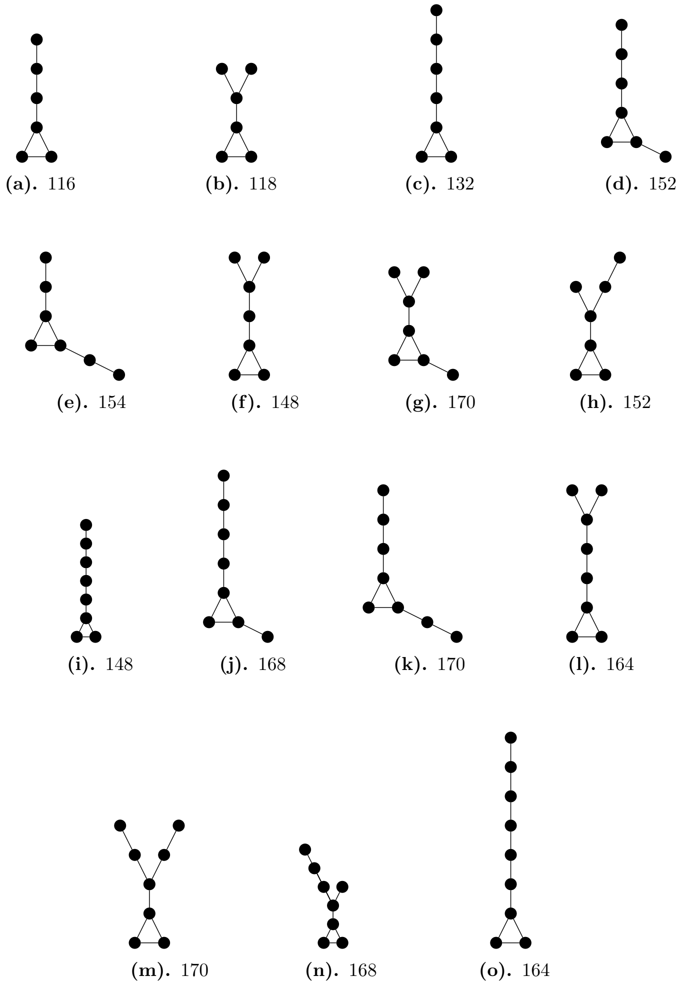


Figure 5. Unicyclic Graphs with C_3 with HM-index less than 172

It is to be noted that graph Q_{12} is the only unicyclic graph with the hyper-Zagreb index 156.

In the beginning of the proof we had discussed on the contributions of unicyclic graphs with C_3 and their impacts of other unicyclic graphs with larger girths. Further, with the help of the degree conditions presented Tables 3, 4, 5 and 6, we can establish that there there are no unicyclic graphs from which a unicyclic graph with hyper-Zagreb index 172 can be generated.

The unicyclic graph with the smallest hyper-Zagreb index of order nine is with the degree sequence $\{3, 2, 2, 2, 2, 2, 2, 2, 1\}$ given in Figure 5(o). We can see that all the even positive integers of our concern are less than 174 as given in Table 8. Since among all the nine-vertex unicyclic graphs of girth three, the smallest hyper-Zagreb index is 164, it is immediate from the definition of the hyper-Zagreb index that no unicyclic graph of orders $n \geq 9$ can have hyper-Zagreb index smaller than 174. Hence, we complete this stage and the proof this theorem. ■

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