

THE TOP TEN VALUES OF HARMONIC INDEX IN CHEMICAL TREES

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ABSTRACT. Let G be an n -vertex graph with degree sequence d_1, d_2, \dots, d_n . The harmonic index $H(G)$ is defined as $n/I(G)$, where $I(G) = \sum_{i=1}^n (1/d_i)$. In this paper the top ten values of harmonic index in the set of all chemical trees of order n are determined.

Keywords: Harmonic index, chemical tree.

INTRODUCTION

We use West [1] for terminology and notation not defined here and consider finite simple connected graphs only. Suppose G is such a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$. If we sort vertices of G in such a way that $\deg(v_1) \leq \deg(v_2) \leq \dots \leq \deg(v_n)$ then the sequence (d_1, d_2, \dots, d_n) is called a degree sequence for G , where $d_i = \deg(v_i)$, $1 \leq i \leq n$.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. A big number of different invariants have been employed to date in chemistry for solving some chemical problems. Here we are interested to the harmonic index defined as $H(B) = n/I(B)$, where $I(B) = \sum_{i=1}^n (1/d_i)$, for a graph B . This topological index was introduced by Narumi [2].

A chemical tree is a tree in which every vertex has degree at most 4. We denote by $\mathcal{g}(n)$, the set of all n -vertex chemical trees. It is easy to see that if A and B are two elements of $\mathcal{g}(n)$ with the same degree sequence then $H(A) = H(B)$. This is motivation for defining an equivalence relation \sim on $\mathcal{g}(n)$ by $A \sim B$ if and only if A and B have the same degree sequence. Suppose $\mathcal{C}(n)$ denotes the set of all equivalence classes of \sim on $\mathcal{C}(n)$ and $T_1, T_2 \in \mathcal{C}(n)$. Define $T_1 \preceq T_2$ if and only if for each element $A \in T_1$ and $B \in T_2$, we have $H(A) \leq H(B)$.

The aim of this paper is to compute the first 10 maximum value of harmonic index. We encourage the reader to consult [3–8] for basic computational techniques on the problem.

MAIN RESULTS

In this section, we are analyzing chemical trees with k^{th} , $1 \leq k \leq 10$, maximum values for the harmonic index. In order to formulate our results, we need introduce some graph notations used in this paper. Define:

$$T_{i,H}(n) = \{M \in CT(n) \mid \forall T \in CT(n); H(T) \leq H(M)\},$$

and for each i , $1 \leq i \leq r = |CT(n)|$, we have:

$$T_{i,H}(n) = \{M \in CT(n) - T_1 \cup \dots \cup T_{i-1} \mid \forall T \in CT(n) - T_1 \cup \dots \cup T_{i-1}; H(T) \leq H(M)\},$$

where r is the number of n -vertex chemical trees. The elements of $T_{i,H}(n)$ are called i^{th} maximum class of chemical trees with respect to H index.

Lemma 1. Let T_n be an n -vertex chemical tree and T_n' is an n -vertex chemical tree obtained from T_n by deleting a pendant vertex and appending a pendant vertex to another pendant vertex of T_n . Then $I(T_n') \leq I(T_n)$.

Proof. Suppose uv is a pendant edge of T_n , $\deg(v) = 1$, $\deg(u) \geq 2$ and w is a pendant vertex of T_n such that T_n' is obtained by deleting uv and appending it to w . Then $\deg_{T_n}(w) = 1 = \deg_{T_n'}(w) - 1$, $\deg_{T_n}(u) = \deg_{T_n'}(u) + 1$ and for another vertex x different

from u and w , $\deg_{T_n}(x) = \deg_{T_n'}(x)$. On the other hand, $I(T_n) = \sum_{x \neq u, w} \frac{1}{d_x} + \frac{1}{d_u} + \frac{1}{d_w} =$

$$\sum_{x \neq u, w} \frac{1}{d_x} + \frac{1}{d_u} + 1 \quad \text{and} \quad I(T_n') = \sum_{x \neq u, w} \frac{1}{d_x} + \frac{1}{d_u - 1} + \frac{1}{d_w + 1} =$$

$$\sum_{x \neq u, w} \frac{1}{d_x} + \frac{1}{d_u - 1} + \frac{1}{2}. \text{ Thus } \frac{1}{d_u - 1} + \frac{1}{2} \leq \frac{1}{d_u} + 1 \text{ which is equivalent to } \frac{1}{d_u(d_u - 1)} \leq \frac{1}{2},$$

proving the lemma. ◀

Corollary 2. Let T be an n -vertex chemical tree then $I(T) \geq 1 + n/2$ with equality if and only if T is a path of length n . The second-minimum value of I index is $4/3 + n/2$ and it is attained if and only if T is isomorphic to P_n^* , where P_n^* is a tree with exactly three pendant vertices.

Lemma 3. Let T_n be an n -vertex chemical tree containing vertices u, z such that $\deg_T(u) = 2$ and $\deg_T(z) = 2$ or 3 . Suppose T_1 and T_2 are maximal subtrees of T_n containing u as a pendant vertex and $z \in V(T_2)$, Figure 1. If T_n^* is the chemical tree constructed from T_1 and T_2 by identifying u and z then $I(T_n) \leq I(T_n^*)$, Figure 2.

Proof. It is easy to see that $\deg_{T_n}(u) = 2$, $\deg_{T_n^*}(u) = 1$, $\deg_{T_n^*}(z) = \deg_{T_n}(z) + 1$ and for another arbitrary vertex x , $\deg_{T_n}(x) = \deg_{T_n^*}(x)$.

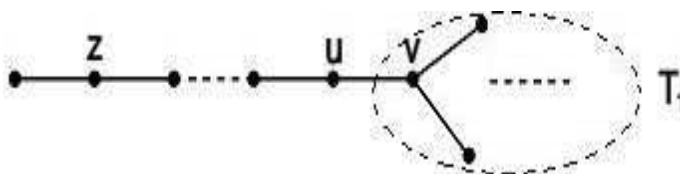


Figure 1. The Chemical Tree T_n Containing a Subtree T_1 .

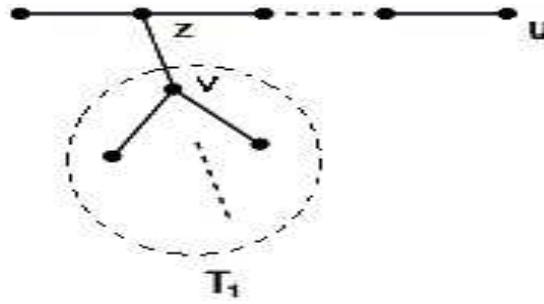


Figure 2. The Chemical Tree T_n^* Constructed from T_1 and T_2 .

Therefore, $I(T_n) = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{d_u} + \frac{1}{d_z} = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{2} + \frac{1}{d_z}$ and
 $I(T_n^*) = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{1} + \frac{1}{d_z + 1}$. Since $\frac{1}{2} + \frac{1}{d_z} < \frac{1}{1} + \frac{1}{d_z + 1}$, $\frac{1}{d_z} - \frac{1}{d_z + 1} < \frac{1}{2}$ and so
 $\frac{1}{d_z(d_z + 1)} < \frac{1}{2}$, proving the lemma. ◀

Lemma 4. Let T_n be an n -vertex chemical tree containing vertices u and z of degree 3. We also assume that T_1, T_2 and T_3 are maximal subtrees of T_n with u as a pendant and $z \in T_3$. If T_n'' is the chemical tree constructed from T_1 and T_2 by identifying u and z then $I(T_n) \leq I(T_n'')$.

Proof. By our assumption $\deg_{T_n}(u) = 3, \deg_{T_n''}(u) = 2, \deg_{T_n}(z) = 3$ and $\deg_{T_n''}(z) = 4$. Thus,

$$I(T_n) = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{d_u} + \frac{1}{d_z} = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{3} + \frac{1}{3},$$

$$I(T_n'') = \sum_{x \neq z, u} \frac{1}{d_x} + \frac{1}{2} + \frac{1}{4},$$

which implies that $I(T_n) \leq I(T_n'')$. ◀

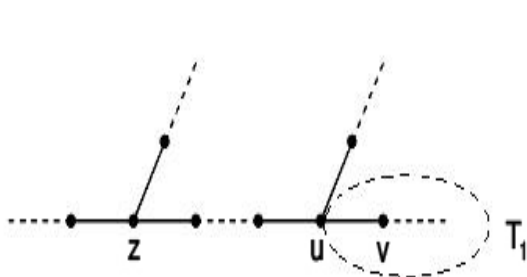


Figure 3. The Chemical Tree T_n .

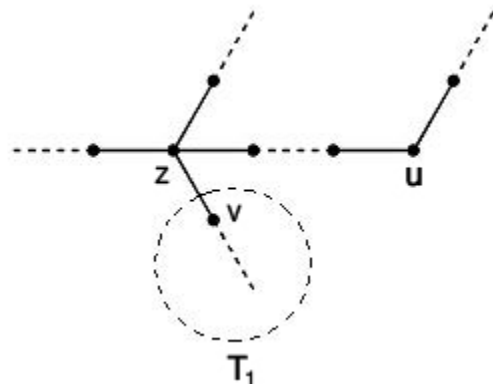


Figure 4. The Chemical Tree T_n'' .

Remark 5. Suppose T is a chemical tree with maximum I index and $r(i), i \leq 4$, denotes the number of vertices of degree i . Then by Lemmas 3 and 4, $r(2) + r(3) = 0, 1$.

In what follows $\mathcal{G}(n)$ denotes the set of all n -vertex chemical trees.

Corollary 6. An n -vertex chemical tree T has the maximum value of I index in $\mathcal{G}(n)$, if T has the maximum number of pendants in $\mathcal{G}(n)$ and non-pendant vertices satisfying $r(2) + r(3) \leq 1$.

In Table 1, the number of pendants, the number of vertices of degree 2, the number of vertices of degree 3 and the number of vertices of degree 4 are computed for the maximal chemical trees with respect to I index, when the number of vertices are at most 16. In Table 2, the n -vertex chemical trees with respect to I index, $4 \leq n \leq 13$, are depicted.

Table 1. The Number of Vertices of Each Degree in n -Vertex Chemical Trees, $4 \leq n \leq 16$.

| # Vertices of Degree 2 | # Vertices of Degree 3 | # Vertices of Degree 4 | # Pendants | N |
|------------------------|------------------------|------------------------|------------|---------------------|
| 0 | 1 | 0 | 3 | $4=3 \times 1 + 1$ |
| 0 | 0 | 1 | 4 | $5=3 \times 1 + 2$ |
| 1 | 0 | 1 | 4 | $6=3 \times 1 + 3$ |
| 0 | 1 | 1 | 5 | $7=3 \times 2 + 1$ |
| 0 | 0 | 2 | 6 | $8=3 \times 2 + 2$ |
| 1 | 0 | 2 | 6 | $9=3 \times 2 + 3$ |
| 0 | 1 | 2 | 7 | $10=3 \times 3 + 1$ |
| 0 | 0 | 3 | 8 | $11=3 \times 3 + 2$ |
| 1 | 0 | 3 | 8 | $11=3 \times 3 + 3$ |
| 0 | 1 | 3 | 9 | $13=3 \times 4 + 1$ |
| 0 | 0 | 4 | 10 | $14=3 \times 4 + 2$ |
| 1 | 0 | 4 | 10 | $15=3 \times 4 + 3$ |
| 0 | 1 | 4 | 11 | $16=3 \times 5 + 1$ |

Table 2. The Maximal Chemical Trees with respect to I Index, $4 \leq n \leq 13$.

| | | | |
|------|--|------|--|
| n=4 | | n=5 | |
| n=6 | | n=7 | |
| n=8 | | n=9 | |
| n=10 | | n=11 | |
| n=12 | | n=13 | |

From Table 2, it is natural to ask whether or not the maximal tree with respect to I index is unique. In the following example we respond negatively to this question.

Example 7. Consider the graphs A and B depicted in Figures 5 and 6, respectively. By simple calculations, one can see that A and B are non-isomorphic graphs with the same I index. This shows that the maximum of I index can be occurred in more than 2 chemical trees.

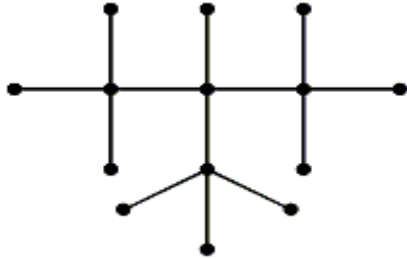


Figure 5. The Graph A.

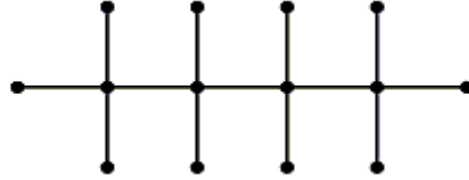


Figure 6. The Graph B.

Suppose $\mathcal{g}(n)$ denotes the set of all n -vertex chemical trees, $n = 3k + t$, $1 \leq t \leq 3$, $n \geq 3$ and $T \in \mathcal{g}(n)$ is an n -vertex chemical tree having maximum I index. One can easily see that $r(1) = 2k + 2 - \lfloor 1/t \rfloor$ and $r(2) + r(3) = 1$. If $t = 3$ then $r(2) = 1$, $r(3) = 0$, and if $t = 1$ then $r(2) = 0$ and $r(3) = 1$. Therefore, $r(4) = n - r(1) - r(2) - r(3) = n - (2k + 2 - \lfloor 1/t \rfloor) - (r(2) + r(3)) = 3k + r - 2k - 2 + \lfloor 1/t \rfloor - 1 = k + t - 3 + \lfloor 1/t \rfloor$.

Remark 8. Suppose $T \in \mathcal{g}(n)$, $n = 3k + t$, $1 \leq t \leq 3$, and $n \geq 3$. Then the maximum of I index is occurred if $r(1) = 2k + 2 - \lfloor 1/t \rfloor$, $r(2) + r(3) = 1$ and $r(4) = k + t - 3 + \lfloor 1/t \rfloor$. In this case, the value of I index is computed by $I(T) = 2k + 2 - \lfloor 1/t \rfloor + \frac{1}{4}(k + r - 3 + \lfloor 1/t \rfloor) + r(2)/2 + r(3)/3$. Moreover, if $n = 3k + 3$ then $r(2) = 1$, $r(3) = 0$ and if $n = 3k + 1$ then $r(2) = 0$ and $r(3) = 1$.

Corollary 9. Suppose T is an n -vertex chemical tree having maximal I index in $\mathcal{g}(n)$, $n \geq 4$. Construct the chemical tree S from T by deleting a pendant connected to vertex v of degree 4 in T and connecting to a vertex of degree 2. If there is not a vertex of degree 2 then we connect it to a pendant. Then the chemical tree S attain the second maximum value of I index.

Example 10. In this example two chemical trees C and D are constructed such that the number of pendants of C is greater than D , but $I(D) < I(C)$. These are depicted in Figures 7 and 8. It is easy to calculate $I(D) = 17 + 1/4 < 17 + 1/6 = I(C)$.

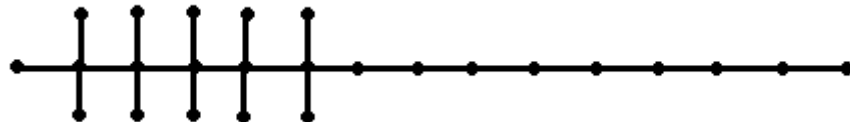


Figure 7. The Graph C.

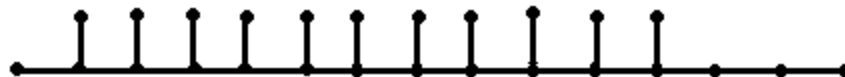


Figure 8. The Graph D.

We now compute the first ten values of harmonic index in the class of all chemical trees. At first, it is an easy fact that the path P_n and the chemical tree P_n^* have the maximum and second maximum harmonic index, respectively.

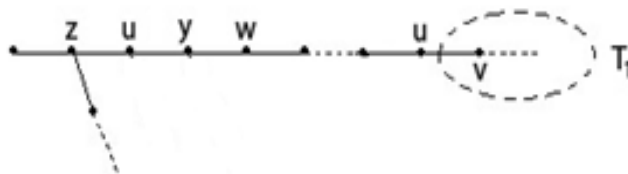


Figure 9. The Graph P_n^* .

To find the third maximum value of harmonic index, we consider two classes X_n and Y_n of chemical trees with exactly four pendant vertices in which X_n has exactly two vertices of degree 3 and remaining vertices of degree 2, and Y_n has exactly one vertex of degree 4 and remaining vertices has degree 2.

Remark 11. The third and fourth maximum values of harmonic index in the class of chemical trees will attain in X_n and Y_n , respectively.

We are now ready to compute the fifth and sixth values of harmonic index in the class of chemical trees. We consider n -vertex chemical trees with five pendant vertices. These are in the form of graphs which are depicted in Figures 10 or 11. These values for the fifth and sixth maximum values of n -vertex chemical trees, $n \geq 8$, are $2n/(n+4)$ and $12n/(6n+25)$, respectively.

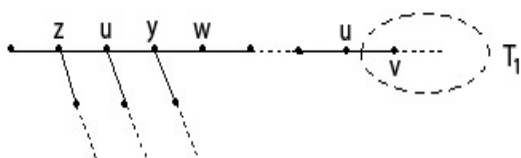


Figure 10.

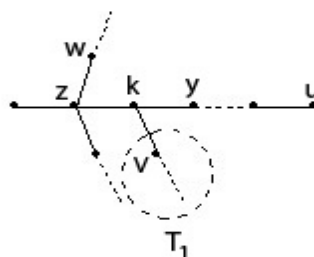


Figure 11.

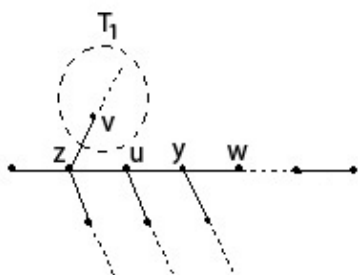


Figure 12.

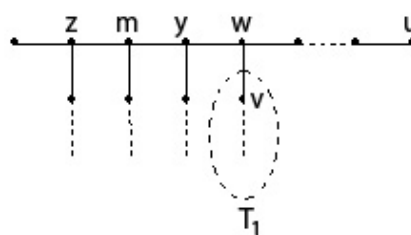


Figure 13.

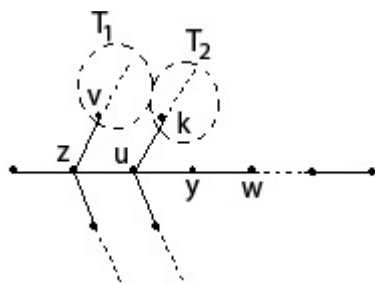


Figure 14.

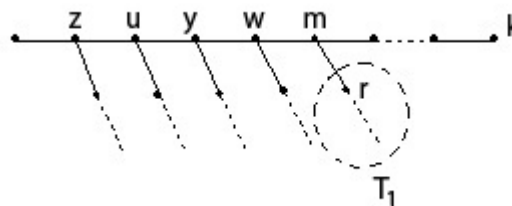


Figure 15.

Apply again our algorithm to compute the seventh, eighth and ninth maximum values in the class of all n -vertex chemical trees. These chemical trees have exactly six pendants and can be drawn as Figures 12–14. The tenth maximum value can be occurred in chemical trees having seven pendants. This chemical tree is depicted in Figure 15.

We record our main result in the following theorem:

Theorem 12. For each δ , $1 \leq \delta \leq 10$, $T_{\delta, H}(n) = \{A_{\delta, n}\}$, where chemical trees $A_{\delta, n}$ are depicted in Table 3.

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Table 3. The k^{th} Maximum of Harmonic Index of Chemical Trees, $3 \leq k \leq 10$.

| Names | K | #Vertices | H Index | The k^{th} Maximum of Harmonic Index |
|-------------|----------|-------------|---------------|---|
| $A_{3,5}$ | $k = 3$ | $n = 5$ | $20/17$ | |
| $A_{3,n}$ | $k = 3$ | $n \geq 6$ | $6n/(3n+10)$ | |
| $A_{4,n}$ | $k = 4$ | $n \geq 6$ | $4n/(2n+7)$ | |
| $A_{5,7}$ | $k = 5$ | $n = 7$ | $84/67$ | |
| $A_{5,n}$ | $k = 5$ | $n \geq 8$ | $2n/(n+4)$ | |
| $A_{6,n}$ | $k = 6$ | $n \geq 8$ | $12n/(6n+25)$ | |
| $A_{7,8}$ | $k = 7$ | $n = 8$ | $16/13$ | |
| $A_{7,9}$ | $k = 7$ | $n = 9$ | $108/83$ | |
| $A_{7,n}$ | $k = 7$ | $n \geq 10$ | $6n/(3n+14)$ | |
| $A_{8,9}$ | $k = 8$ | $n = 9$ | $9/7$ | |
| $A_{8,n}$ | $k = 8$ | $n \geq 10$ | $12n/(6n+29)$ | |
| $A_{9,n}$ | $k = 9$ | $n \geq 10$ | $2n/(n+5)$ | |
| $A_{10,10}$ | $k = 10$ | $n = 10$ | $60/47$ | |
| $A_{10,11}$ | $k = 10$ | $n = 11$ | $4/3$ | |
| $A_{10,n}$ | $k = 10$ | $n \geq 12$ | $6n/(3n+16)$ | |