Molecular trees with extremal Harmonic indices

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The Harmonic index of a graph G is defined as the sum of the weights $\frac{2}{d(u)+d(v)}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we determine molecular trees with minimum, second-minimum, third-minimum, maximum, second-maximum and third-maximum Harmonic indices.

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1. Introduction

Molecular descriptors play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. Among them, topological indices have a prominent place. Nowadays, there exist a legion of topological indices that found some applications in chemistry [1].

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$, proposed by Randić [2] in 1975, is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ denotes the degree of a vertex u in G. Randić [2] noticed that this index was well correlated with several physico-chemical properties of alkanes: boiling point, enthalpy of formation, surface area and solubility in water, etc. Eventually, this index became one of the most successful topological indices, and scores of its pharmacological and chemical applications have been reported. For mathematical properties of this topological index see [3, 4].

The Harmonic index $H(G)$ [5] is a closely related variant of the Randić index. This index is defined as

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

Favaron et al. [6] considered the relation between the Harmonic index and the eigenvalues of graphs. In [7], the author established some relationships between the Harmonic index and several other topological indices. See [8, 9] for more mathematical properties of this index.

A connected graph with maximum degree at most four is said to be a molecular graph. Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in chemistry. A tree in which the maximum degree does not exceed four is said to be a molecular tree. Hence a molecular tree is also a molecular graph.

In this paper, we first present sharp lower and upper bounds of the Harmonic index of molecular graphs with $n \geq 5$ vertices and m edges, where $n-1 \leq m \leq 2n$. Then we determine molecular trees with minimum, second-minimum, third-minimum, maximum, second-maximum and third-maximum Harmonic indices.

2. Main results

In this section, we prove the main results of this paper. First, we present sharp lower and upper bounds of the Harmonic index of molecular graphs with $n \geq 5$ vertices and m edges, where $n-1 \leq m \leq 2n$.

Let G be such a molecular graph. Denote by x_{ij} the number of edges of G that connect vertices of degree i and j with $1 \leq i \leq j \leq 4$. Then

$$H(G) = \sum_{1 \leq i \leq j \leq 4} \frac{2}{i+j} x_{ij}. \tag{1}$$

Note that $x_{11} = 0$ since G is connected and $n \geq 5$. Gutman et al. [10] obtained

$$x_{14} = \frac{4n-2m}{3} - \frac{4}{3}x_{12} - \frac{10}{9}x_{13} - \frac{2}{3}x_{22} - \frac{4}{9}x_{23} - \frac{1}{3}x_{24} - \frac{2}{9}x_{33} - \frac{1}{9}x_{34}$$

and

$$x_{44}=\frac{5m-4n}{3}+\frac{1}{3}x_{12}+\frac{1}{9}x_{13}-\frac{1}{3}x_{22}-\frac{5}{9}x_{23}-\frac{2}{3}x_{24}-\frac{7}{9}x_{33}-\frac{8}{9}x_{34}.$$

Combining with (1), we have

$$H(G)=\frac{1}{5}n+\frac{3}{20}m+\frac{13}{60}x_{12}+\frac{1}{12}x_{13}+\frac{3}{20}x_{22}+\frac{1}{12}x_{23}+\frac{1}{30}x_{24}+\frac{1}{20}x_{33}+\frac{2}{105}x_{34} \quad (2)$$

with positive coefficients for $x_{12}, x_{13}, x_{22}, x_{23}, x_{24}, x_{33}$, x_{34}. Similarly, Gutman et al. [10] also obtained

$$x_{12}=2n-2m-\frac{2}{3}x_{13}-\frac{1}{2}x_{14}+\frac{1}{3}x_{23}+\frac{1}{2}x_{24}+\frac{2}{3}x_{33}+\frac{5}{6}x_{34}+x_{44}$$

and

$$x_{22}=3m-2n-\frac{1}{3}x_{13}-\frac{1}{2}x_{14}-\frac{4}{3}x_{23}-\frac{3}{2}x_{24}-\frac{5}{3}x_{33}-\frac{11}{6}x_{34}-2x_{44}.$$

Substituting these into (1), we see that

$$H(G)=\frac{1}{3}n+\frac{1}{6}m-\frac{1}{9}x_{13}-\frac{11}{60}x_{14}-\frac{2}{45}x_{23}-\frac{1}{12}x_{24}-\frac{1}{18}x_{33}-\frac{19}{252}x_{34}-\frac{1}{12}x_{44}$$

with negative coefficients for $x_{13}, x_{14}, x_{23}, x_{24}, x_{33}, x_{34}$, x_{44}. Hence we have the following theorem.

Theorem 1. *Let G be a molecular graph with $n \geq 5$ vertices and m edges, where $n-1 \leq m \leq 2n$. Then $\frac{1}{5}n+\frac{3}{20}m \leq H(G) \leq \frac{1}{3}n+\frac{1}{6}m$. The lower bound is attained if and only if G has only vertices of degree one and four, and the upper bound is attained if and only if G has only vertices of degree one and two (i.e., G is either a path or a cycle).*

Deng et al. [9] determined trees on n vertices with maximum, second-maximum and third-maximum Harmonic indices for $n \geq 7$. Since all such trees are molecular trees, we obtain the following result.

Theorem 2. *Among molecular trees with n vertices,*
(*i*) *for $n \geq 4$, the tree without vertices of degree three and four (i.e., the path) is the unique tree with maximum Harmonic index $\frac{n}{2}-\frac{1}{6}$;*
(*ii*) *for $n \geq 7$, the trees with a single vertex of degree three, adjacent to three vertices of degree two, and without vertices of degree four are the unique trees with second-maximum Harmonic index $\frac{n}{2}-\frac{3}{10}$;*
(*iii*) *for $n \geq 7$, the trees with a single vertex of degree three, adjacent to one vertex of degree one and two vertices of degree two, and without vertices of degree four are the unique trees with third-maximum Harmonic index $\frac{n}{2}-\frac{11}{30}$.*

In the following argument, we determine molecular trees with minimum, second-minimum and third-minimum Harmonic indices.

Let T be a molecular tree with n vertices. Denote by n_i the number of vertices of T having degree i, $i=1,2,3,4$. Then we deduce that $2n_2 = x_{12}+2x_{22}+x_{23}+x_{24}$ and $3n_3 = x_{13}+x_{23}+2x_{33}+x_{34}$. Let $\Delta = H(T)-\left(\frac{7}{20}n-\frac{3}{20}\right)$. Then by (2), we have

$$\begin{aligned}\Delta &= \frac{13}{60}x_{12}+\frac{1}{12}x_{13}+\frac{3}{20}x_{22}+\frac{1}{12}x_{23}+\frac{1}{30}x_{24}+\frac{1}{20}x_{33}+\frac{2}{105}x_{34}\\ &= 0.21667x_{12}+0.08333x_{13}+0.15x_{22}+0.08333x_{23}+0.03333x_{24}+0.05x_{33}+0.01905x_{34},\end{aligned}$$

because $m=n-1$. Since the remainder of the division of n by three is determined only by n_2 and n_3, and is independent of n_1 and n_4 (see [11]), we now consider the value of n_2+n_3.

First suppose $n_2+n_3=3.$ If $n_2=3$ and $n_3=0,$ then $\Delta\geq 0.03333\times 6=0.19998>0.17.$ If $n_2=2$ and $n_3=1,$ then $\Delta\geq 0.03333\times 4+0.01905\times 3=0.19047>0.17.$ If $n_2=1$ and $n_3=2,$ then $\Delta\geq 0.03333\times 2+0.01905\times 6=0.18096>0.17.$ If $n_2=0$ and $n_3=3,$ then $\Delta\geq 0.01905\times 9=0.17145>0.17.$ In summary, if $n_2+n_3=3,$ then $\Delta>0.17.$

If $n_2+n_3>3,$ then by the same argument as above, we conclude that $\Delta>0.17.$

For the case that $n_2+n_3<3,$ the graphically feasible combinations of $x_{12},x_{13},x_{22},x_{23},x_{24},x_{33},x_{34}$ for which $\Delta<0.17$ are listed in Table 1, where $n\equiv k\ (\mathrm{mod}\,3).$ There are nine such combinations.

From the data shown in Table 1, we immediately have the following result.

Theorem 3. (i) *If* $n\equiv 2\ (\mathrm{mod}\,3),$ *then among molecular trees with* n *vertices,*

(a) *for* $n\geq 5,$ *the trees with only degrees one and four are the unique trees with minimum Harmonic index* $\frac{7n}{20}-\frac{3}{20};$

Table 1. Graphically feasible combinations of $x_{12},x_{13},x_{22},x_{23},x_{24},x_{33},x_{34}$ *for which* $\Delta<0.17.$

n_2	n_3	Non-zero x_{ij}	Δ	k
0	0		0	2
1	1	$x_{24}=2,x_{34}=3$	0.12381	2
1	1	$x_{23}=x_{24}=1,x_{34}=2$	0.15476	2
0	1	$x_{34}=3$	0.05715	1
0	1	$x_{13}=1,x_{34}=2$	0.12143	1
2	0	$x_{24}=4$	0.13332	1
1	0	$x_{24}=2$	0.06666	0
0	2	$x_{34}=6$	0.11430	0
0	2	$x_{33}=1,x_{34}=4$	0.12620	0

(b) *for* $n\geq 17,$ *the trees with a single vertex of degree two, adjacent to two vertices of degree four, and a single vertex of degree three, adjacent to three vertices of degree four are the unique trees with second-minimum Harmonic index* $\frac{7n}{20}-\frac{11}{420};$

(c) *for* $n\geq 17,$ *the trees with a single vertex of degree two, adjacent to one vertex of degree four and the vertex of degree three, and a single vertex of degree three, adjacent to two vertices of degree four and the vertex of degree two are the unique trees with third-minimum Harmonic index* $\frac{7n}{20}+\frac{1}{210}.$

(ii) *If* $n\equiv 1\ (\mathrm{mod}\,3),$ *then among molecular trees with* n *vertices for* $n\geq 13,$

(a) *the trees with a single vertex of degree three, adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with minimum Harmonic index* $\frac{7n}{20}-\frac{13}{140};$

(b) *the trees with a single vertex of degree three, adjacent to one vertex of degree one and two vertices of degree four, and without vertices of degree two* are the *unique trees with second-minimum Harmonic index* $\frac{7n}{20}-\frac{1}{35};$

(c) *the trees with two vertices of degree two, each adjacent to two vertices of degree four, and without vertices of degree three are the unique trees with the third-minimum Harmonic index* $\frac{7n}{20}-\frac{1}{60}.$

(iii) *If* $n\equiv 0\ (\mathrm{mod}\,3),$ *then among molecular trees with* n *vertices,*

(a) *for* $n\geq 9,$ *the trees with a single vertex of degree two, adjacent to two vertices of degree four, and without vertices of degree three are the unique trees with minimum Harmonic index* $\frac{7n}{20}-\frac{1}{12};$

(b) *for* $n\geq 21,$ *the trees with two vertices of degree three, each adjacent to three vertices of degree four, and without vertices of degree two are the unique trees with second-minimum Harmonic index* $\frac{7n}{20}-\frac{1}{28};$

(c) *for* $n\geq 21,$ *the trees with two adjacent vertices of* *degree three, each adjacent to two vertices of degree four, and without vertices of degree two are the unique trees with third-minimum Harmonic index* $\frac{7n}{20}-\frac{1}{42}$.

3. Concluding remarks

In recent years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. The problem of computing topological indices of nanostructures was first introduced by Diudea et al. [12]. Since then, there are lots of papers dealing with computing topological indices of various nanostructures, see [13-18] and the references cited therein for more information. In [19], the authors computed the Harmonic index of nanocones and triangular benzenoid graphs. It would be interesting to compute this index for other nanostructures.

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