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Benzenoid Systems with Extremal Vertex–Degree–Based Topological Indices

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Abstract

In the current chemical literature, a large number of vertex–degree–based topological indices TI are considered, defined as the sum over all edges of the molecular graph of some function $\Psi(x, y)$, where x and y are the degrees of the end-vertices of the respective edge. In order to find the minimal value of TI over benzenoid systems with h hexagons, we characterize convex benzenoid systems W such that $n_i(W) = n_i(S_h)$, where n_i is the number of internal vertices and S_h is the spiral benzenoid system. If such W does exist, then W has minimal TI-value. Otherwise, the spiral S_h has minimal TI-value.

1 Introduction

In the current chemical literature, a large number of graph–based structure descriptors ("topological indices") have been put forward, that all depend only on the degrees (= number of first neighbors) of the vertices of the underlying molecular graph. Most of these are equal to the sum over all edges of some conveniently chosen function $\Psi(x, y)$, where x and y are the degrees of the end-vertices of the respective edge. For instance, $\Psi(x,y) = x\,y$ pertains to the second Zagreb index [4,17,20], $\Psi(x,y) = \frac{1}{\sqrt{x\,y}}$ to the Randić connectivity index [14,21,23], whereas $\frac{2\sqrt{x\,y}}{x+y}$, $\frac{1}{\sqrt{x+y}}$, $\frac{(x\,y)^3}{(x+y-2)^3}$, and $\frac{2}{i+j}$ pertain, respectively, to the recently conceived geometric–arithmetic [5,25,28], sum-connectivity [9,24,30], augmented Zagreb [10,19,26], and harmonic [6,27,29] indices. More details on vertex–degree–based topological indices and on their comparative study can be found in [7,8,11,12,16] and the references cited therein.

Let $\{\Psi_{ij}\}$ be a set of real numbers for every $1 \leq i \leq j \leq n-1$. Then a general expression for vertex–degree–based topological indices is

$$TI = TI(G) = \sum_{1\leq i\leq j\leq n-1} m_{ij}\,\Psi_{ij}$$

where G is a (molecular) graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j.

In previous studies [1,2,15], we have examined the variation of TI over the set of benzenoid systems. (For the definition of benzenoid systems and details of their theory see [13]. Recall that in mathematical literature, benzenoid systems are usually referred to as "hexagonal systems".)

We denote by $\mathcal{HS}_h$ the set of benzenoid systems with h hexagons. Since any benzenoid system S has only vertices of degree 2 and 3, the general expression for its vertex–degree–based topological indices reads

$$TI(S) = m_{22}\,\Psi_{22} + m_{23}\,\Psi_{23} + m_{33}\,\Psi_{33}\;. \tag{1}$$

In [22], the number of inlets of a benzenoid system S was introduced as

$$r(S) = f(S) + B(S) + C(S) + F(S)$$

where $f(S)$, $B(S)$, $C(S)$, and $F(S)$ are the number of fissures, bays, coves and fjords in S, respectively [3,13], and the following relations were shown for a benzenoid system S with n vertices and h hexagons

$$\left.\begin{array}{rcl} m_{22} &=& n-2h-r+2 \\ m_{23} &=& 2r \\ m_{33} &=& 3h-r-3 \end{array}\right\}. \tag{2}$$

If n_i is the number of internal vertices of a benzenoid system, then from (2) and the well-known relation

$$n = 4h + 2 - n_i$$

we deduce from (1) that for every $S, U \in \mathcal{HS}_h$

$$TI(S) - TI(U) = q\left[r(S) - r(U)\right] + \Psi_{22}\left[n_i(U) - n_i(S)\right] \tag{3}$$

where $q = 2\Psi_{23} - \Psi_{22} - \Psi_{33}$. Furthermore, it was shown in [2] that for every benzenoid system S

$$r(S) = 2(h-1) - b(S) - n_i(S)$$

where $b(S)$ is the number of bay regions of S. It follows from (3) that

$$TI(S) - TI(U) = q\left[b(U) - b(S)\right] + \left[\Psi_{22} + q\right]\left[n_i(U) - n_i(S)\right] \tag{4}$$

for every $S, U \in \mathcal{HS}_h$.

On the other hand, Harary and Harborth [18] showed that for every $S \in \mathcal{HS}_h$

$$0 \le n_i(S) \le 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil \tag{5}$$

where the upper bound is attained in the spiral benzenoid system S_h (see Fig. 1).

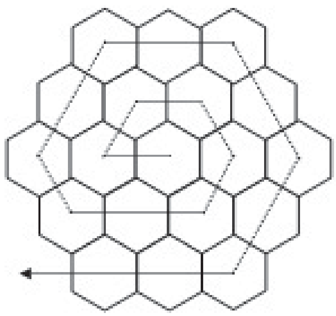

Fig. 1. A spiral benzenoid system

Consequently, if W is a convex benzenoid system (i.e., $b(W) = 0$, see [2]), such that

$$n_i(W) = 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil \tag{6}$$

then it follows from (4) that for every $S \in \mathcal{HS}_h$

$$TI(S) - TI(W) = q\left[-b(S)\right] + \left[\Psi_{22} + q\right]\left[\left(2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil\right) - n_i(S)\right].$$

In particular, if $-\Psi_{22} \leq q \leq 0$, then we conclude from (5) that

$$TI(S) - TI(W) \geq 0 \ .$$

In other words, we deduce the following result [1]:

Theorem 1.1. *Let W be a convex benzenoid system with h hexagons which satisfies Eq. (6). If $-\Psi_{22} \leq q \leq 0$, then W has minimal TI-value among all benzenoid systems with h hexagons.*

Examples of convex benzenoid systems with h hexagons satisfying Eq. (6) were given in [2], for several values of h. The idea was to transform a spiral benzenoid system into a convex benzenoid system with equal number of internal vertices. Mistakenly it was inferred in [2] that this method works for every positive integer h. We will now show that this is not true. More precisely, in Theorem 2.1 we determine necessary and sufficient conditions for the existence of convex benzenoid systems with maximal number of internal vertices. As a byproduct, in Theorem 2.2 we show that given a positive integer h, the existence of convex benzenoid systems with maximal number of internal vertices imply the existence of a solution to the Diophantine equation

$$21x^2 + 3y^2 + z^2 = 28 \left[\left\lceil \sqrt{12h-3} \right\rceil^2 - (12h-3) \right] . \tag{7}$$

In Example 2.3, we find values of h for which equation (7) has no solution, concluding in this way that it is not always possible to construct convex benzenoid systems with h hexagons that satisfy the condition (6). However, for these values of h, we later show in Theorem 3.1 that the spiral benzenoid system S_h has minimal TI-value among all benzenoid systems with h hexagons, provided the condition $\frac{-\Psi_{22}}{2} \leq q \leq 0$ is satisfied. By direct checking we demonstrate that this condition on q is obeyed by most of the well-known degree–based topological indices.

2 Convex benzenoid systems with maximal number of internal vertices

The structure of a convex benzenoid system W can be specified as

$$W = H\left(a_1, a_2, a_3, a_4, a_5, a_6\right)$$

for positive integers $a_1, a_2, a_3, a_4, a_5, a_6$ (cf. Fig. 2).

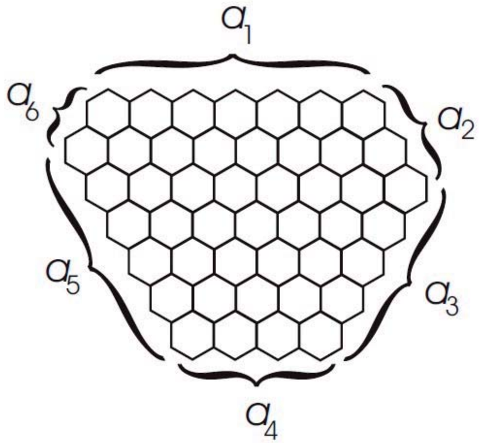

Fig. 2. A convex benzenoid system

It has been demonstrated [2] that W is completely determined by the parameters a_1, a_2, a_3, a_4, since it must be

$$a_5 = a_1 + a_2 - a_4 \qquad \text{and} \qquad a_6 = a_3 + a_4 - a_1 \ . \tag{8}$$

Theorem 2.1. *Let h be a positive integer. The following conditions are equivalent:*

1. *There exists a convex benzenoid system W with h hexagons satisfying Eq. (6).*

2. There exist a set of positive integers a_1, a_2, a_3, a_4 *which are solutions of the system of equations*

$$\left.\begin{aligned} h &= a_1\,a_3 + a_1\,a_4 + a_2\,a_3 + a_2\,a_4 - a_2 - a_3 \\ &- \tfrac{1}{2}\,a_1\,(a_1+1) - \tfrac{1}{2}\,a_4\,(a_4+1) + 1 \\ \left\lceil \sqrt{12h-3} \right\rceil &= a_1 + 2a_2 + 2a_3 + a_4 - 3\ . \end{aligned}\right\} \tag{9}$$

Proof. 1. $\Rightarrow$ 2. Assume that W is a convex benzenoid system with h hexagons, satisfying Eq. (6). Let $a_1, a_2, a_3, a_4, a_5, a_6$ be positive integers such that $W = H\,(a_1, a_2, a_3, a_4, a_5, a_6)$.

We know from [2, Theorem 2] that

$$\left.\begin{aligned} h &= a_1\,a_3 + a_1\,a_4 + a_2\,a_3 + a_2\,a_4 - a_2 - a_3 \\ &- \tfrac{1}{2}\,a_1\,(a_1+1) - \tfrac{1}{2}\,a_4\,(a_4+1) + 1 \\ n_i\,(W) &= 2\,(a_1\,a_3 + a_1\,a_4 + a_2\,a_3 + a_2 a_4) - a_1\,(a_1+2) \\ &- a_4\,(a_4+2) - 4\,(a_2+a_3) + 6\ . \end{aligned}\right\} \tag{10}$$

Substituting these expressions for h and $n_i(W)$ back into Eq. (6) yields

$$\left\lceil \sqrt{12h-3} \right\rceil = a_1 + 2a_2 + 2a_3 + a_4 - 3\ .$$

2. $\Rightarrow$ 1. Conversely, if the set of positive integers a_1, a_2, a_3, a_4 is a solution of the system of equations (9), consider the convex benzenoid $Z = H\,(a_1, a_2, a_3, a_4, a_5, a_6)$, where a_5 and a_6 are given by Eqs. (8). Again, by [2, Theorem 2], we have expressions for h and $n_i(Z)$ as in (10). Consequently,

$$2h + 1 - n_i(Z) = a_1 + 2a_2 + 2a_3 + a_4 - 3 = \left\lceil \sqrt{12h-3} \right\rceil\ .$$

Solving for $n_i(Z)$ in this relation, we deduce that

$$n_i(Z) = 2h + 1 - \left\lceil \sqrt{12h-3} \right\rceil\ .$$

□

We now show that not for every positive integer h there is a solution for the system of equations (9). This is a consequence of our next result.

Theorem 2.2. *Let h be a positive integer. If the set of positive integers $\{a_1, a_2, a_3, a_4\}$ is a solution of the system of equations (9), then there exists a solution to the Diophantine equation*

$$21x^2 + 3y^2 + z^2 = 28H \tag{11}$$

where $H = \left\lceil\sqrt{12h-3}\right\rceil^2 - (12h-3)$.

Proof. Substituting

$$a_2 = \frac{1}{2}\left\lceil\sqrt{12h-3}\right\rceil - a_3 - \frac{1}{2}a_4 - \frac{1}{2}a_1 + \frac{3}{2} \tag{12}$$

in the first equation of (9), we obtain

$$\begin{aligned} h &= \frac{3}{2}a_3 + \frac{3}{2}a_4 - \frac{1}{2}\left\lceil\sqrt{12h-3}\right\rceil - \frac{1}{2}a_1^2 - a_3^2 - a_4^2 + \frac{1}{2}a_1 a_3 + \frac{1}{2}a_1 a_4 - \frac{3}{2}a_3 a_4 \\ &+ \frac{1}{2}a_3\left\lceil\sqrt{12h-3}\right\rceil + \frac{1}{2}a_4\left\lceil\sqrt{12h-3}\right\rceil - \frac{1}{2}. \end{aligned}$$

Next, by solving for a_4 in this equation, it follows that

$$a_4 = \frac{1}{4}a_1 - \frac{3}{4}a_3 + \frac{1}{4}\left\lceil\sqrt{12h-3}\right\rceil + \frac{3}{4} \pm \frac{1}{4}\sqrt{P(a_1, a_3)} \tag{13}$$

where

$$\begin{aligned} P(a_1, a_3) &= -7a_1^2 + 2a_1 a_3 + 2a_1\left\lceil\sqrt{12h-3}\right\rceil + 6a_1 - 7a_3^2 + 2a_3\left\lceil\sqrt{12h-3}\right\rceil \\ &+ 6a_3 + \left\lceil\sqrt{12h-3}\right\rceil^2 - 2\left\lceil\sqrt{12h-3}\right\rceil - 16h + 1. \end{aligned}$$

Since $\sqrt{P(a_1, a_3)} \in \mathbb{Z}$, we may assume that $P(a_1, a_3) = x^2$ for some $x \in \mathbb{N}$. Solving for a_1 we get

$$a_1 = \frac{1}{7}a_3 + \frac{1}{7}\left\lceil\sqrt{12h-3}\right\rceil + \frac{3}{7} \pm \frac{1}{7}\sqrt{Q(a_3)} \tag{14}$$

where

$$\begin{aligned} Q(a_3) &= -7x^2 - 48a_3^2 + 16a_3\left\lceil\sqrt{12h-3}\right\rceil + 48a_3 + 8\left\lceil\sqrt{12h-3}\right\rceil^2 \\ &- 8\left\lceil\sqrt{12h-3}\right\rceil - 112h + 16. \end{aligned}$$

Since $\sqrt{Q(a_3)} \in \mathbb{Z}$, there exists an integer $y \in \mathbb{N}$ such that $Q(a_3) = y^2$. Now we solve for a_3 to obtain

$$a_3 = \frac{1}{6}\left\lceil\sqrt{12h-3}\right\rceil + \frac{1}{2} \pm \frac{1}{12}\sqrt{R} \tag{15}$$

where

$$R = -21x^2 - 3y^2 + 28\left(\left\lceil\sqrt{12h-3}\right\rceil^2 - (12h-3)\right). \qquad (16)$$

Similarly $\sqrt{R} \in \mathbb{Z}$ and so $R = z^2$ for $z \in \mathbb{N}$. Hence

$$z^2 = -21x^2 - 3y^2 + 28\left(\left\lceil\sqrt{12h-3}\right\rceil^2 - (12h-3)\right)$$

and we are done. □

Theorem 2.2 gives a method to find values of h for which there are no convex benzenoid systems which satisfy Eq. (6).

Example 2.3. Let h be a positive integer and H as in the hypothesis of Theorem 2.2. If $28H - 21x^2 - 3y^2$ is not the square of an integer for every $(x, y) \in \mathbb{N} \times \mathbb{N}$ satisfying

$$0 \le x \le \sqrt{\frac{28H}{21}} \qquad \text{and} \qquad 0 \le y \le \sqrt{\frac{28H - 21x^2}{3}}$$

then there are no convex benzenoid systems with h hexagons satisfying Eq. (6). Using a computer is easy to check that the first values of h are the following:

121	163	211	235	265	292	325	355	391	424
463	499	541	580	625	667	706	715	760	802
811	859	904	913	955	964	1012	1021	1066	1075
1126	1135	1183	1192	1246	1255	1306	1315	1372	1381

(17)

On the other hand, for those values of h where the Diophantine equation (11) has a solution, we were able to find convex benzenoid systems with maximal number of vertices, using the proof of Theorem 2.2 as follows: starting from a solution x, y, z of Eq. (11), we compute R, a_3, a_1, a_4, and a_2, in that order, from relations (16), (15), (14), (13), and (12), respectively. Then a_5 and a_6 are computed using Eq. (8). It turns out that $W = H(a_1, a_2, a_3, a_4, a_5, a_6)$ is a convex benzenoid system satisfying Eq. (6). For instance,

for $h = 120$ we get $H(7, 6, 8, 6, 7, 7)$

for $h = 5306$ we get $H(39, 43, 42, 47, 35, 50)$

for $h = 10000$ we get $H(63, 60, 54, 59, 64, 50)$.

3 Benzenoid systems with minimal TI-value

We now return to the study of vertex–degree–based topological indices of benzenoid systems. If the system of equations (9) has a solution for a positive integer h, then there exists a convex benzenoid system W such that Eq. (6) holds, which by Theorem 1.1 implies that W has a minimal TI-value when $-\Psi_{22} \leq q \leq 0$. So a question arises naturally: if Eq. (9) has no solution for certain h, which is the minimal TI-value in the set of all benzenoid systems with h hexagons?

Answer to this question is provided by the following:

Theorem 3.1. *Let h be a positive integer and assume that the system of equations (9) has no solution. If $\frac{-\Psi_{22}}{2} \leq q \leq 0$, then the spiral benzenoid system S_h has minimal TI-value over the set of all benzenoid systems with h hexagons.*

Proof. Since Eq. (9) has no solution, $b(S_h) = 1$. Let S be a benzenoid system with h hexagons. From (4),

$$TI(S) - TI(S_h) = q\,[1 - b(S)] + [\Psi_{22} + q]\,[n_i(S_h) - n_i(S)]\,. \tag{18}$$

We consider two cases. If $b(S) = 0$, then $n_i(S_h) - n_i(S) \geq 1$ since (9) has no solution. Consequently from (18) and the fact that $\frac{-\Psi_{22}}{2} \leq q \leq 0$ we deduce

$$\begin{aligned} TI(S) - TI(S_h) &= q + [\Psi_{22} + q]\,[n_i(S_h) - n_i(S)] \\ &\geq q + [\Psi_{22} + q] = 2q + \Psi_{22} \geq 0\ . \end{aligned}$$

Otherwise $b(S) \geq 1$, which implies $1 - b(S) \leq 0$. Since $n_i\,(S_h) - n_i\,(S) \geq 0$ by (5) then again by (18) and $\frac{-\Psi_{22}}{2} \leq q \leq 0$ it follows that

$$TI\,(S) - TI(S_h) = q\,[1 - b(S)] + [\Psi_{22} + q]\,[n_i(S_h) - n_i(S)] \geq 0\ .$$

Thus S_h has minimal TI-value among all benzenoid systems with h hexagons. □

Example 3.2. For every value of h given listed (17) in in Example 2.3, the spiral benzenoid system S_h has minimal TI-value over $\mathcal{HS}_h$.

Remark 3.3.

1°. The condition $\frac{-\Psi_{22}}{2} \le q \le 0$ holds for most of the well-known topological indices, as can be seen from the following table:

	ij	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{2}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{(ij)^3}{(i+j-2)^3}$
q	-1	-.0168	-.0404	-.0333	-.0138	-3.3906
$-\frac{\Psi_{22}}{2}$	-2	-.25	-.5	-.25	-.25	-4

2°. Theorems 2.1 and 3.1 from Ref. [1] hold only if h is a solution of the system of equations (9).

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