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A New Comparison between the Modified Zagreb M_2^* Index and the Randić Index for Benzenoid Systems

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Abstract

For any arbitrarily large $m(e.g., m = 1000000)$ natural number, a set of m benzenoid systems with the same number vertices have been found so that every pair of them possesses the same Randić index, but no two of them exist with the same modified Zagreb M_2^* index, on the other hand, another set of m benzenoid systems with the same number vertices have also been discovered so that every pair of them have the same the modified Zagreb M_2^* index, but any two of them don't possess the same Randić index.

1 Introduction

Both Zagreb index and Randić index are very important chemical indices, and have been closely correlated with many chemical properties. The two indices have been continuously applied in QSPR and QSAR and then received considerable attention from chemist and mathematicians. The modified Zagreb M_2^* index was introduced to amend the feature that the original Zagreb M_2 index gives greater weights to inner bonds and smaller weights to outer bonds. This opposes the chemists' intuition that outer bonds should have greater weights than inner bonds because outer bonds are associated with a larger part of the molecular surface and are consequently expected to make a greater contribution to physical, chemical and biological properties.

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In 1975 Randić index was introduced by Randić in the study of branching properties of alkanes. With the intention of extending the applicability of the Randić index, it soon became one of most used topological indices in all kinds of structure property activity studies.

The modified Zagreb index is defined as:

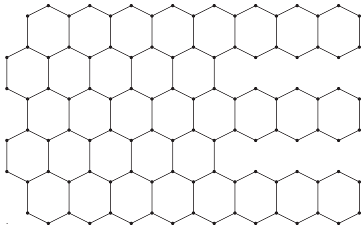
$$M_2^*(G) = \sum_{\text{edges}} (d(i)d(j))^{-1}$$

and the Randić index of G is similar to the modified Zagreb index:

$$R(G) = \sum_{\text{edges}} (d(i)d(j))^{-\frac{1}{2}}$$

A comparison between the two indices for benzenoid systems was executed in the paper[15]. But there existed a small mistaken in it, i.e., the number of vertices for benzenoid system in the paper [15] isn't $6ac$ but $(4a + 2)c$, then it meant that all conclusions were obtained after the comparison was made between two benzenoid systems with different number of vertices in it. Thus the following question is also brought naturally. For any arbitrarily large $m(e.g., m = 1000000)$ natural number, whether it exists a set of m benzenoid systems with the same number vertices so that every pair of them possesses the same Randić index, but no two of them exist with the same modified Zagreb M_2^* index? In this paper, the interesting question has been solved, on the other hand, another set of m benzenoid systems with the same number vertices have also been discovered so that every pair of them have the same the modified Zagreb M_2^* index, but any two of them don't possess the same Randić index.

First we introduce some concepts and notations. Let a, b, c be natural numbers so that $a \geq b + 1$ and $c \geq 1$. Denote by $B(a, b, c)$ a benzenoid system so that there are $2c + 1$ rows, each odd row consisting of a hexagons and each even row consisting of b hexagons arranged as in the following system.



Let B be an arbitrary benzenoid system and let $n(B)$ be the number of vertices of that system,we define an inlet is each path of a length of at least two on the boundary of the benzenoid system B so that its terminal vertices have degree 2 and its non-terminal vertices have degree 3 in B, let $h(B)$ the number of hexagons of the system and $r(S)$ the number of inlets of the benzenoid systems. Denote by $m_{22}(B)$ the number of edges connecting the vertices of degree 2, denote by $m_{23}(B)$ the number of edges that connect one vertex of degree 2 and one vertex of degree 3, and denote by $m_{33}(B)$ the number of edges that connect degree 3 vertices.

2 Modified M_2^* Index and The Randić Index of Benzenoid Systems

Now we introduce three Lemmas that will be used in our following proof.

Lemma 2.1[14] Let B be a benzenoid system. Then

$$\begin{aligned} m_{22}(B) &= n(B) - 2h(B) - r(B) + 2 \\ m_{23}(B) &= 2r(B) \\ m_{33}(B) &= 3h(B) - r(B) - 3 \end{aligned}$$

Lemma 2.2[14] Let B be a benzenoid system. Then

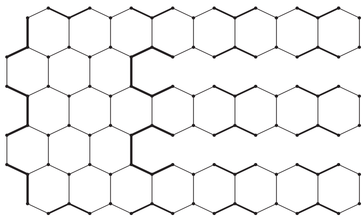
$$R(B) = \frac{1}{2}n(B) - \frac{5 - 2\sqrt{6}}{6}r(B)$$

Lemma 2.3[15] Let B be a benzenoid system. Then

$$M_2^*(B) = \frac{1}{4}n(B) - \frac{1}{6}h(B) - \frac{1}{36}r(B) + \frac{1}{6}$$

Lemma 2.4 Let $a, b, c \in N$ so that $a \geq b+1, c \geq 1$ and let $B(a, b, c)$ be a system. Then

$$\begin{aligned} n(B(a,b,c)) &= 4(a+1)(c+1)-2 \\ h(B(a,b,c)) &= a(c+1)+bc \\ r(B(a,b,c)) &= 2a(c+1)-2bc-1 \end{aligned}$$



Proof From the above sketch, we obtain immediately the second statement. In the following we will prove other two statements, it can be easily seen that for each $a, b, c \in N$, so that $a \geq b+1, c \geq 1$. Then

$$\begin{aligned} n(B(a,b,c)) &= (4a+2+2)c+4a+2 \\ &= 4(a+1)(c+1)-2 \\ r(B(a,b,c)) &= 2(a-1)+2(a-b-1)c+2c+1 \\ &= 2a-2+2ac-2bc-2c+2c+1 \\ &= 2a(c+1)-2bc-1 \end{aligned}$$

Theorem 2.5 Let m be any natural number. There is a set of m benzenoid systems with the same number of vertices such that each of them has the same Randić index, but no two of them have the same modified M_2^* index.

Proof The following set of benzenoid systems F is constructed,

$$F = \left\{ B\left(\frac{4(m+1)!}{x+1} - 1, \frac{(m+1)!}{x} - 1, x \right) : x \in \{1, 2, \cdots, m\} \right\}.$$

Obviously, we know easily that there are m graphs in F. For $x \in \{1, 2, \cdots, m\}$, we have

$$\frac{4(m+1)!}{x+1} - \frac{(m+1)!}{x} \geq 1$$

$$n\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) =$$

$$4(x+1) \cdot \left(\frac{4(m+1)!}{x+1}-1+1\right)-2$$

$$= 16(m+1)!-2$$

$$h\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) =$$

$$(x+1)\cdot\left(\frac{4(m+1)!}{x+1}-1\right) + x\cdot\left(\frac{(m+1)!}{x}-1\right)$$

$$= 5(m+1)!-2x-1$$

$$r\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) =$$

$$2(x+1)\cdot\left(\frac{4(m+1)!}{x+1}-1\right) - 2x\cdot\left(\frac{(m+1)!}{x}-1\right)-1$$

$$= 6(m+1)!-3$$

So, for each $x \in \{1, 2, \cdots, m\}$, we have

$$R\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) =$$

$$\frac{1}{2}\cdot n\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) -$$

$$\frac{5-2\sqrt{6}}{6}\cdot r\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right)$$

$$= (3+2\sqrt{6})\cdot(m+1)! + \frac{1}{2}\cdot(3-2\sqrt{6})$$

$$M_2^*\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) =$$

$$\frac{1}{4}\cdot n\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) -$$

$$\frac{1}{6}\cdot h\left(B\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}-1,x\right)\right) -$$

$$\frac{1}{36} \cdot r\left(B\left(\frac{4(m+1)!}{x+1}-1, \frac{(m+1)!}{x}-1, x\right)\right) \quad + \quad \frac{1}{6}$$
$$= 3(m+1)! \quad - \quad \frac{1}{12}+\frac{1}{3}x$$

Thus, for two different natural numbers $x_1, x_2 \in \{1, 2, \cdots, m\}$,

$$R\left(B\left(\frac{4(m+1)!}{x_1+1}-1, \frac{(m+1)!}{x_1}-1, x_1\right)\right) =$$
$$R\left(B\left(\frac{4(m+1)!}{x_2+1}-1, \frac{(m+1)!}{x_2}-1, x_2\right)\right)$$
$$M_2^*\left(B\left(\frac{4(m+1)!}{x_1+1}-1, \frac{(m+1)!}{x_1}-1, x_1\right)\right) \neq$$
$$M_2^*\left(B\left(\frac{4(m+1)!}{x_2+1}-1, \frac{(m+1)!}{x_2}-1, x_2\right)\right)$$

Theorem 2.6 Let m be any natural number and $m \geq 2$. There is a set of m benzenoid systems with the same number of vertices such that each of them has the same modified M_2^* index, but no two of them have the same Randić index.

Proof The following set of benzenoid systems $F^{'}$ is constructed,

$$F^{'} = \left\{B^{'}\left(\frac{4(m+1)!}{x+1}-1, \frac{(m+1)!}{x}+2, x\right) : x \in \{1, 2, \cdots, m\}\right\}.$$

Obviously, we know easily that there are m graphs in $F^{'}$. For $x \in \{1, 2, \cdots, m\}$, then

$$\frac{4(m+1)!}{x+1} - \frac{(m+1)!}{x} \quad = \quad \frac{3x-1}{x(x+1)} \cdot (m+1)!$$
$$\geq \quad (3m-1) \cdot (m-1)! > 4$$

Let $f(x) = \frac{3x-1}{x(x+1)}$, when $x > 1$, $f^{'}(x) = -\frac{(3x+1)(x-1)}{x^2(x+1)^2} < 0$. Then $f(x)$ is monotonously decreasing in x, so the above two inequalities hold and we have

$$\frac{4(m+1)!}{x+1} - 1 > (\frac{(m+1)!}{x} + 2) + 1$$

$$n\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) =$$

$$4(x+1) \cdot \left(\frac{4(m+1)!}{x+1}-1+1\right)-2$$

$$= 16(m+1)!-2$$

$$h\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) =$$

$$(x+1)\cdot\left(\frac{4(m+1)!}{x+1}-1\right) + x\cdot\left(\frac{(m+1)!}{x}+2\right)$$

$$= 5(m+1)!+x-1$$

$$r\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) =$$

$$2(x+1)\cdot\left(\frac{4(m+1)!}{x+1}-1\right) - 2x\cdot\left(\frac{(m+1)!}{x}+2\right)-1$$

$$= 6(m+1)!-6x-3$$

So, for each $x \in \{1,2,\cdots,m\}$, we have

$$M_2^*\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) =$$

$$\frac{1}{4}\cdot n\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) -$$

$$\frac{1}{6}\cdot h\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) -$$

$$\frac{1}{36}\cdot r\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) + \frac{1}{6}$$

$$= 3(m+1)! - \frac{1}{12}$$

$$R\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) =$$

$$\frac{1}{2}\cdot n\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right) -$$

$$\frac{5-2\sqrt{6}}{6}\cdot r\left(B'\left(\frac{4(m+1)!}{x+1}-1,\frac{(m+1)!}{x}+2,x\right)\right)$$

$$= (3+2\sqrt{6})\cdot(m+1)! + \frac{3-2\sqrt{6}}{2} \quad + \quad (5-2\sqrt{6})x$$

Thus, for two different natural numbers $x_1, x_2 \in \{1, 2, \cdots, m\}$,

$$M_2^*\left(B'\left(\frac{4(m+1)!}{x_1+1}-1, \frac{(m+1)!}{x_1}+2, x_1\right)\right) =$$

$$M_2^*\left(B'\left(\frac{4(m+1)!}{x_2+1}-1, \frac{(m+1)!}{x_2}+2, x_2\right)\right)$$

$$R\left(B'\left(\frac{4(m+1)!}{x_1+1}-1, \frac{(m+1)!}{x_1}+2, x_1\right)\right) \neq$$

$$R\left(B'\left(\frac{4(m+1)!}{x_2+1}-1, \frac{(m+1)!}{x_2}+2, x_2\right)\right)$$

From the above proofs of Theorem 2.5 and Theorem 2.6, it is known easily that a set of m benzenoid systems with the same number vertices possessing the result of Theorem 2.5 is transformed to another benzenoid systems satisfying Theorem 2.6 if we add three hexagons being adjacent with the b-th hexagon in each even row of benzenoid system defined in this paper.

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