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Note

Modified Zagreb M_2 Index – Comparison with the Randić Connectivity Index for Benzenoid Systems

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Two theorems have been derived for benzenoid systems with the following implications: (i) for any arbitrarily large m (*e.g.*, m = 1000000) there is a number n and a set with m benzenoid systems with n vertices so that every pair of them posseses the same Randić connectivity index, but no two graphs exist with the same modified Zagreb M_2 index, and (ii) for any arbitrarily large m (*e.g.*, m = 10000000) there is a number n and a set with m benzenoid systems with n vertices so that (a) every pair of graphs posseses a different Randić connectivity index, (b) every pair of graphs has a different modified Zagreb M_2 index, and (c) Randić connectivity indices order these graphs in the reverse order with respect to modified Zagreb M_2 indices. We have shown with these two theorems that the modified Zagreb M_2 index differs fundamentally from the Randić connectivity index.

INTRODUCTION

The modified Zagreb M_2 index has been proposed recently.[1] The original Zagreb M_2 index, together with the related M_1 index, was introduced in 1972 (Ref. 2) and elaborated in 1975.[3] In recent years, mathematical properties of Zagreb indices have also been studied.[4,5] Both of these indices have been continuously used in QSPR and QSAR.[6–8] They are also included in a number of programs for the routine computation of molecular descriptors, such as POLLY,[9] DRAGON,[10] TAM,[11] *etc*.

The Randić connectivity index was introduced in 1975 (Ref. 12) and it soon became the most used topological index in all kinds of structure-property-activity studies.[6–8]

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. The Randić connectivity index complies with chemical intuition.

Here, we will show that the discriminatory power of the modified Zagreb M_2 index surpasses that of the Randić connectivity index for certain arbitrarily large classes of benzenoid systems.

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ORIGINAL AND MODIFIED ZAGREB M_2 INDICES AND THE RANDIĆ CONNECTIVITY INDEX

The original Zagreb M_2 of a graph G is given by:[2]

$$M_2(\mathrm{G}) = \sum_{\text{edges}} d(i)d(j)\,. \qquad (1)$$

The modified version of (1) is defined as:[1]

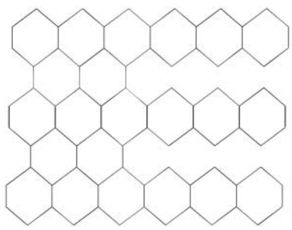
$$^*M_2(\mathrm{G}) = \sum_{\text{edges}} [d(i)d(j)]^{-1}\,. \qquad (2)$$

The Randić connectivity index χ of G is similar to the Zagreb indices:[12]

$$\chi(\mathrm{G}) = \sum_{\text{edges}} [d(i)d(j)]^{-1/2}\,. \qquad (3)$$

MODIFIED M_2 INDEX AND THE RANDIĆ CONNECITIVITY INDEX OF BENZENOID SYSTEMS

Let a,b,c be natural numbers so that $a \geq b + 2$ and $c \geq 2$. Denote by $\mathrm{S}(a,b,c)$ a benzenoid system[13] 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.



S(6,2,3)

Let S be an arbitrary benzenoid system and let $n(\mathrm{S})$ be the number of vertices of that system, $h(\mathrm{S})$ the number of hexagons of the system and $r(\mathrm{S})$ the number of inlets of the system (an inlet is each path of a length of at least two on the boundary of the benzenoid system G so that its terminal vertices have degree 2 in G and its non-terminal vertices have degree 3 in G). Denote by $m_{22}(\mathrm{S})$ the number of edges connecting the vertices of degree 2, denote by $m_{23}(\mathrm{S})$ the number of edges that connect one vertex of degree 2 and one vertex of degree 3, and denote by $m_{33}(\mathrm{S})$ the number of edges that connect degree 3 vertices. This notation is taken from Rada *et al.*[14]

We shall use the following Lemma and Theorem as given by Rada *et al.*[14]

LEMMA 1. Let S be a benzenoid system. Then

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

THEOREM 2. Let S be a benzenoid system. Then

$$\chi(\mathrm{S}) = \frac{n(\mathrm{S})}{2} - \frac{5-2\sqrt{6}}{6}\,r(\mathrm{S})\,.$$

We shall also need the following Lemmas:

LEMMA 3. Let S be a benzenoid system. Then

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

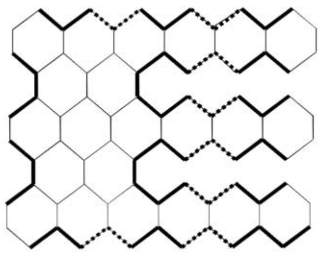
PROOF. We have

$$\begin{aligned} &^*M_2(\mathrm{S}) = \frac{1}{4}m_{22}(\mathrm{S}) + \frac{1}{6}m_{23}(\mathrm{S}) + \frac{1}{9}m_{33}(\mathrm{S}) = \\ &\frac{1}{4}\big(n(\mathrm{S})-2h(\mathrm{S})-r(\mathrm{S})+2\big) + \frac{1}{6}\cdot 2r(\mathrm{S}) + \frac{1}{9}\big(3h(\mathrm{S})-r(\mathrm{S})-3\big) = \\ &\frac{1}{4}n(S) - \frac{1}{6}h(S) - \frac{1}{36}r(S) + \frac{1}{6}\,. \end{aligned}$$

LEMMA 4. Let $a,b,c \in N$ so that $a \geq b + 2$, $c \geq 2$ and let $\mathrm{S}(a,b,c)$ be a benzenoid system. Then

$$\begin{aligned} n(\mathrm{S}(a,b,c)) &= 6ac \\ h(\mathrm{S}) &= ac + b(c-1) \\ r(\mathrm{S}) &= 2ac - 2b(c-1) - 2c\,. \end{aligned}$$

PROOF. The first two statements are obvious. Let us prove the third one. From the following sketch



it can be easily seen that for each $a,b,c \in N$ so that $a \geq b + 2$, $c \geq 2$, we have

$$\begin{aligned} &r(\mathrm{S}(a,b,c)) = 2(a-1) + [2(a-b-2) + 2]\cdot(c-1) = \\ &2ac - 2bc - 2b - 2c = \\ &2ac - 2b(c-1) - 2c\,. \end{aligned}$$

THEOREM 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 connectivity index and no two of them have the same modified M_2 index.

PROOF. Let us observe the following set of benzenoid systems

$$\mathrm{F} = \left\{ \mathrm{S}\left(\frac{6(m+1)\,!}{x}, \frac{(m+1)\,!}{x-1} - 1, x\right) : x \in \left\{2,3,\dots,m+1\right\}\right\}.$$

Obviously, there are m graphs in F. For each $x \in \{2,3,\dots,m+1\}$, we have

$$\frac{6(m+1)\,!}{x} \geq \frac{(m+1)\,!}{x-1} + 2\,.$$

Also, for each $x \in \{2,3,...,m+1\}$, we have

$$n\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= 6\cdot\frac{6(m+1)!}{x}\cdot x = 36\cdot(m+1)!$$

$$h\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= \frac{6(m+1)!}{x}\cdot x+\left(\frac{(m+1)!}{x-1}-1\right)\cdot(x-1)= 7\cdot(m+1)!+1-x\,;$$

$$r\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= 2\cdot\frac{6(m+1)!}{x}\cdot x-2\cdot\left(\frac{(m+1)!}{x-1}-1\right)(x-1)-2x= 10\cdot(m+1)!-2\,.$$

Now, for each $x \in \{2,...,m+1\}$, we have

$$\chi\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= \frac{n\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)}{2}- \frac{5-2\sqrt{6}}{6}\,r\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= \frac{36\cdot(m+1)!}{2}-\frac{5-2\sqrt{6}}{6}\cdot(10(m+1)!-2)$$

and

$$*M_2\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)= \frac{1}{4}n\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)- \frac{1}{6}h\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)- \frac{1}{36}r\left(S\left(\frac{6(m+1)!}{x},\frac{(m+1)!}{x-1}-1,x\right)\right)=$$

$$\frac{1}{4}\cdot 36\cdot(m+1)!-\frac{1}{6}(7\cdot(m+1)!+1-x)- \frac{1}{36}(10(m+1)!-2)+\frac{1}{6}= \frac{68}{9}\cdot(m+1)!+\frac{1}{18}+\frac{1}{6}x\,.$$

Thus, indeed, for two different numbers $x_1, x_2 \in \{2,..., m+1\}$, we have

$$\chi\left(S\left(\frac{6(m+1)!}{x_1},\frac{(m+1)!}{x_1-1}-1,x_1\right)\right)= \chi\left(S\left(\frac{6(m+1)!}{x_2},\frac{(m+1)!}{x_2-1}-1,x_2\right)\right);$$

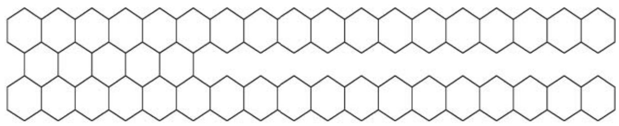
$$*M_2\left(\chi\left(S\left(\frac{6(m+1)!}{x_1},\frac{(m+1)!}{x_1-1}-1,x_1\right)\right)\right)\neq *M_2\left(\chi\left(S\left(\frac{6(m+1)!}{x_2},\frac{(m+1)!}{x_2-1}-1,x_2\right)\right)\right)$$

and the claim is proved.

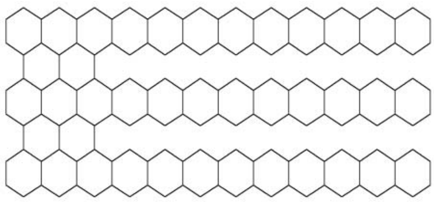
The application of Theorem 5 is demonstrated by the following example.

EXAMPLE. Take $m = 2$. Then, F consists of the following two graphs:

S(18,5,2)



S(12,2,3)



From Theorem 5, it follows that

$$\chi(S(18,5,2)) = \chi(S(12,2,3)) = \frac{36\cdot(2+1)!}{2}-\frac{5-2\sqrt{6}}{6}\,(10(2+1)!-2)\,.$$

On the other hand, we have

$$*M_2\,(S(18,5,2)) = \frac{68}{9}\cdot(2+1)!+\frac{1}{18}+\frac{1}{6}\cdot 2=\frac{823}{18}\,;$$

$$*M_2\,(S(12,2,3)) = \frac{68}{9}\cdot(2+1)!+\frac{1}{18}+\frac{1}{6}\cdot 2=\frac{826}{18}$$

so indeed

$$\chi(S(18,5,2)) = \chi(S(12,2,3))$$
$$*M_2(S(18,5,2)) \neq *M_2(S(12,2,3))$$

THEOREM 6. Let m be any natural number. There is a set F' of m benzenoid systems so that for each pair of benzenoid systems S_1, $S_2 \in$ F' we have

$$n(S_1) = n(S_2)$$

$$\left[{}^*M_2(S_1) < {}^*M_2(S_2)\right] \text{ if and only if } \left[\chi(S_1) > \chi(S_2)\right].$$

PROOF. Let us consider the following set of benzenoid systems

$$F' = \left\{ G(m+3,x,6) : x \in \{2,\dots,m+1\} \right\}.$$

For each $x \in \{2,...,m+1\}$ we have

$$n(G(m+3,x,6)) = 36 \cdot (m+3).$$

It is sufficient to prove that for each $x_1, x_2 \in \{2,...,m+1\}$, we have

$$(x_1 < x_2) \Rightarrow (\chi(m+3,x_1,6) < \chi(m+3,x_2,6)) \qquad (4)$$

$$(x_1 < x_2) \Rightarrow ({}^*M_2(m+3,x_1,6) > {}^*M_2(m+3,x_2,6)) \qquad (5)$$

Let us calculate for each $x \in \{2,...,m+1\}$, $r(G(m+3,x,6))$ and $h(G(m+3,x,6))$.

$$h(G(m+3,x,6)) = 6 \cdot (m+3) + 5 \cdot x$$

$$r(G(m+3,x,6)) = 2 \cdot (m+3) \cdot 6 - 2 \cdot x \cdot 5 - 2 \cdot 6 = 12m + 24 - 10x.$$

Let us prove (4). Suppose that $x_1, x_2 \in \{2,...,m+1\}$ and $x_1 < x_2$. We have

$$\chi(G(m+3,x_1,6)) = \frac{n(G(m+3,x_1,6))}{2} - \frac{5-2\sqrt{6}}{6} r(G(m+3,x_1,6)) = \frac{36 \cdot (m+3)}{2} - \frac{5-2\sqrt{6}}{6} \cdot (12m+24-10x_1) = 18 \cdot (m+3) - (5-2\sqrt{6}) \cdot (2m+4) + \frac{5 \cdot (5-2\sqrt{6})}{3} x_1.$$

Completely analogously, we get the following expression:

$$\chi(G(m+3,x_2,6)) = 18 \cdot (m+3) - (5-2\sqrt{6}) \cdot (2m+4) + \frac{5 \cdot (5-2\sqrt{6})}{3} x_2,$$

therefore

$$\chi(G(m+3,x_1,6)) < \chi(G(m+3,x_2,6))$$

which proves (4).

Let us prove (5). Suppose that $x_1, x_2 \in \{2,...m+1\}$ and $x_1 < x_2$. We have

$${}^*M_2(G(m+3,x_1,6)) = \frac{1}{4} n(G(m+3,x_1,6)) - \frac{1}{6} h(G(m+3,x_1,6)) - \frac{1}{36} r(G(m+3,x_1,6)) + \frac{1}{6} = \frac{1}{4} \cdot 36 \cdot (m+3) - \frac{1}{6} \cdot (6 \cdot (m+3) + 5 \cdot x_1) - \frac{1}{36}\left(12m+24-10x_1\right) + \frac{1}{6} = \frac{23}{3} m + \frac{47}{2} - \frac{5}{9} x_1.$$

Completely analogously, we get

$${}^*M_2(G(m+3,x_1,6)) = \frac{23}{3} m + \frac{47}{2} - \frac{5}{9} x_2,$$

and

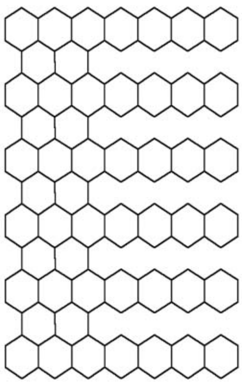
$${}^*M_2(G(m+3,x_1,6)) > {}^*M_2(G(m+3,x_2,6))$$

which proves (5).

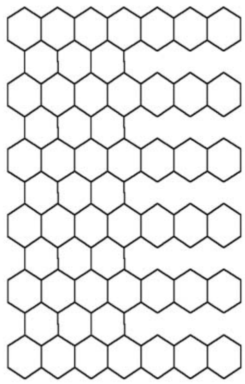
The application of Theorem 6 is demonstrated by the example given below.

EXAMPLE. Take $m = 4$. Then F' consists of the following four graphs:

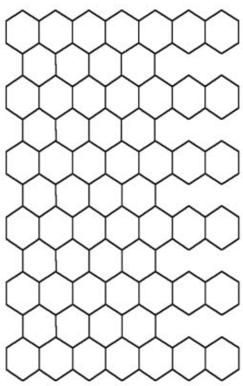
S(7,2,6)



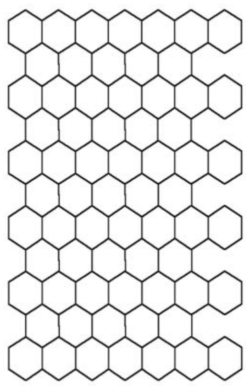
S(7,3,6)



S(7,4,6)



S(7,5,6)



We have (after a straightforward calculation) inequalities:

$$\chi(S(7,2,6)) < \chi(S(7,3,6)) < \chi(S(7,4,6)) < \chi(S(7,5,6))$$

$$*M_2(S(7,2,6)) > *M_2(S(7,3,6)) > *M_2(S(7,4,6)) > *M_2(S(7,5,6))$$

as predicted by Theorem 6.

CONCLUSIONS

The modified Zagreb M_2 index was explicitly derived for benzenoid systems in terms of the number of vertices, the number of hexagons and the number of inlets, following the work by Rada *et al.*[14] who derived an explicit formula for the Randić connectivity index for benzenoids. The two main results that show that the modified Zagreb M_2 index differs, to a great extent, from the Randić connectivity index can be summarized as: (i) for any arbitrary large m there is a number n and a set of m benzenoid systems with n vertices such that every one of them posseses the same Randić connectivity index, but no two graphs exist with the same modified Zagreb M_2 index, and (ii) for any arbitrary large m there is a number n and a set of m benzenoid systems with n vertices so that (a) every pair of graphs possesses a different Randić connectivity index, (b) every pair of graphs has a different modified Zagreb M_2 index, and (c) Randić connectivity indices order these graphs reversely with respect to modified Zagreb M_2 indices.

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REFERENCES

1. N. Trinajstić, *On Modified Zagreb* M_2 *Index*, reported at the *MATH/CHEM/COMP 2002*, Dubrovnik, June 24–29, 2002.
2. I. Gutman and N. Trinajstić, *Chem. Phys. Lett*. **17** (1973) 535–545.
3. I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, Jr., *J. Chem. Phys*. **62** (1975) 3399–3405.
4. E. Estrada, L. Rodriguez, and A. Gutierrez, *MATCH – Comm. Math. Comput. Chem.* **35** (1997) 145–156.
5. E. Estrada, *Chem. Phys. Lett*. **336** (2001) 248–252.
6. A. T. Balaban (Ed.), *From Chemical Topology to Three-Dimensional Geometry*, Plenum Press, New York, 1997.
7. J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.
8. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley – VCH, Weinheim, 2000.
9. S. C. Basak, D. K. Harriss, and V. R. Magnuson, POLLY 2.3, copyright of the University of Minnesota, 1988.
10. R.Todeschini, V. Consonni, and M. Pavan, DRAGON 2.1, 2002. http://www.disat.unimib.it/chm/Dragon.htm
11. M. Vedrina, S. Marković, M. Medić-Šarić, and N. Trinajstić, *Comput. Chem*. **21** (1997) 355–361.
12. M. Randić, *J. Am. Chem. Soc*. **97** (1975) 6609–6615.
13. I. Gutman and S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, Berlin, 1989.
14. J. Rada, O. Araujo, and I. Gutman, *Croat. Chem. Acta* **74** (2001) 225–235.

SAŽETAK

Modificirani zagrebački M_2 indeks – usporedba s Randićevim indeksom povezanosti za benzenoidne sustave

Damir Vukičević i Nenad Trinajstić

Izvedena su dva teorema za benzenoidne sustave iz kojih slijedi (i) za bilo koji proizvoljno veliki broj m (npr. m = 1000000) postoji broj n i skup s m benzenoidnih sustava i n čvorova tako da svaki par posjeduje identični Randićev indeks povezanosti, ali ne postoje dva benzenoidna sustava s jednakim modificiranim zagrebačkim M_2 indeksom i (ii) za bilo koji proizvoljno veliki m (npr. m = 10000000) postoji broj n i skup s m benzenoidnih sustava i n čvorova tako da (a) svaki par grafova posjeduje različiti Randićev indeks povezanosti, (b) svaki par grafova posjeduje različiti modificirani zagrebački M_2 indeks i (c) Randićevi indeksi povezanosti poredaju te grafove u suprotnom redu nego to čine modificirani zagrebački M_2 indeksi. S ta dva teorema pokazano je da se modificirani zagrebački M_2 indeks fundamentalno razlikuje od Randićevoga indeksa povezanosti premda su njihovi algebarski izrazi slični.