CROATICA CHEMICA ACTA CCACAA **75** (2) 357–369 (2002)

ISSN-0011-1643
CCA-2805 *Original Scientific Paper*

Molecular Graphs with Minimal and Maximal Randić Indices*

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Received November 27, 2000; revised February 26, 2001; accepted March 9, 2001

The Randić index χ is the sum of the terms $1/\sqrt{\delta(u)\delta(v)}$ over all pairs of adjacent vertices, where δ stands for the degree of the respective vertex of the respective molecular graph. We determine the (n,m)-molecular graphs (*i.e.*, connected graphs with n vertices, m edges, $n-1 \leq m \leq 2n$, and maximal vertex degree not exceeding 4), having the greatest possible and the smallest possible Randić indices.

Key words: molecular graph, Randić index, topological indices.

INTRODUCTION

In this paper we characterize molecular graphs having maximal and minimal values of the Randić connectivity index. Let G be a graph and let $\delta(v)$ be the degree (= number of first neighbors) of the vertex v of G. Then the Randić index[1] $\chi = \chi(\mathrm{G})$ is the sum of the terms $1/\sqrt{\delta(u)\delta(v)}$ over all pairs of adjacent vertices of G. Note that although the investigation of the Randić index is usually restricted to molecular graphs, it is well defined for all graphs.

Graphs representing the carbon-atom skeleton of organic molecules must, for obvious chemical reasons, possess the following properties: they must be connected and none of their vertices must have degree greater than four. Such graphs are referred to as molecular graphs.[2,3]

The graph invariant χ was put forward by Randić a quarter of century ago.[1] Eventually it became one of the most popular topological indices and

* Dedicated to Professor Milan Randić on the occassion of his 70th birthday.

certainly the structure-descriptor that found the greatest number of applications in QSPR and QSAR studies. Details along these lines can be found in the two monographs[4,5] entirely devoted to χ and its various generalizations, as well as in numerous other books[1,6,7] and reviews.[8,9]

Initially the Randić index was studied only by chemists, but recently it attracted the attention also of mathematicians.[10,11] One of the most obvious mathematical questions occurring in connection with χ is which graphs (from a given class) have maximal and minimal χ-values. The solution of such problems turned out to be difficult, and only a few partial results have been achieved so far.

Bollobàs and Erdős[10] obtained the following:

Theorem 1. Among graphs with a fixed number of vertices, and without isolated vertices, the star has minimal Randić index.

Araujo and de la Pena[11] characterized the graphs with maximal χ-values:

Theorem 2. Among graphs with a fixed number of vertices, the graphs in which all components are regular of non-zero degree have maximal (mutually equal) Randić indices.

In the paper[12] the trees with maximal Randić indiced were identified:

Theorem 3. Among trees with a fixed number of vertices, the path has maximal Randić index.

According to Theorem 1 the tree with minimal χ-value is the star.

Trees whose maximal vertex degree does not exceed 4, with minimal, second minimal, third minimal, maximal, second maximal and third maximal Randić indices were also recently characterized.[13,14]

In this paper we offer a general solution of the problem of the characterization of molecular graphs with minimal and maximal Randić indices. By this we extend and sharpen some of our earlier findings.[15]

In order to arrive at our main results (stated below as Theorems 4 and 5) we need some preparations.

TOWARDS THE MAIN RESULTS

In what follows it is assumed that the graph G considered is a molecular graph on n vertices and that $n \geq 5$. Then the number m of edges of G must satisfy $n - 1 \leq m \leq 2n$. If $m = n - 1$ then the respective graph is a tree; if $m = 2n$ then the respective graph is regular of degree 4. From now on, it will be understood that G is an (n,m)-molecular graph and this detail will not be everywhere repeated.

Denote by m_{ij} the number of edges of G that connect vertices of degrees i and j. Then

$$\chi(\mathrm{G}) = \sum_{1 \le i \le j \le 4} \frac{m_{ij}}{\sqrt{ij}} \ . \tag{1}$$

Note that $m_{11} = 0$ whenever G is connected and $n \ge 3$. Therefore the case $i = j = 1$ needs not be considered any further. Consequently, the right-hand side of Eq. (1) is a linear function of the nine variables m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34} and m_{44}.

Let n_i be the number of vertices of G having degree i, $i = 1,2,3,4$. Then the following »book-keeping« relations are obeyed:

$$n_1 + n_2 + n_3 + n_4 = n \tag{2}$$

$$m_{12} + m_{13} + m_{14} = n_1 \tag{3}$$

$$m_{12} + 2m_{22} + m_{23} + m_{24} = 2n_2 \tag{4}$$

$$m_{13} + m_{23} + 2m_{33} + m_{34} = 3n_3 \tag{5}$$

$$m_{14} + m_{24} + m_{34} + 2m_{44} = 4n_4 \tag{6}$$

and, in addition to them:

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m. \tag{7}$$

Recall that the left-hand side of Eq. (7) is just the sum of the vertex degrees of G.

Relations (2)–(7) are linearly independent. Their linear independence follows from the fact that the parameter n occurs only in Eq. (2), the parameters m_{22}, m_{33} and m_{44} only in Eqs. (4), (5) and (6), respectively, whereas the parameter m only in Eq. (7). In addition, Eq. (3) contains none of the parameters n, m_{22}, m_{33}, m_{44} and m.

Assuming that the parameters n and m are fixed, Eqs. (2)–(7) may be understood as a system of six linear equations in thirteen unknowns: n_1, n_2, n_3, n_4, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34} and m_{44}.

MOLECULAR GRAPHS WITH MINIMAL RANDIĆ INDICES

By solving the system (2)–(7) in the unknowns n_1, n_2, n_3, n_4, m_{14} and m_{44} we obtain

$$m_{14} = \frac{4n-2m}{3} - \frac{4}{3}m_{12} - \frac{10}{9}m_{13} - \frac{2}{3}m_{22} - \frac{4}{9}m_{23} - \frac{1}{3}m_{24} - \frac{2}{9}m_{33} - \frac{1}{9}m_{34} \tag{8}$$

and

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

which combined with Eq. (1) yields

$$\chi(\mathrm{G}) = \frac{4n+m}{12} + \left(\frac{1}{\sqrt{2}} - \frac{7}{12}\right)m_{12} + \left(\frac{1}{\sqrt{3}} - \frac{19}{36}\right)m_{13} + \frac{1}{12}m_{22} +$$

$$\left(\frac{1}{\sqrt{6}} - \frac{13}{36}\right)m_{23} + \left(\frac{1}{2\sqrt{2}} - \frac{1}{3}\right)m_{24} + \frac{1}{36}m_{33} + \left(\frac{1}{2\sqrt{3}} - \frac{5}{18}\right)m_{34} =$$

$$\frac{4n+m}{12} + 0.1238m_{12} + 0.0496m_{13} + 0.0833m_{22} + 0.0471m_{23} +$$

$$0.0202m_{24} + 0.0278m_{33} + 0.0109m_{34} \quad . \quad (10)$$

Our considerations are based on the fact that all multipliers on the right-hand side of (10) are positive-valued. Define therefore a non-negative auxiliary quantity Δ as:

$$\Delta = \chi(\mathrm{G}) - \frac{4n+m}{12} = 0.1238m_{12} + 0.0496m_{13} + 0.0833m_{22} + 0.0471m_{23} +$$

$$0.0202m_{24} + 0.0278m_{33} + 0.0109m_{34} \quad (11)$$

Now, $\chi(\mathrm{G})$ will attain its smallest values if Δ is equal to zero or if it is as close to zero as possible. This will be achieved if the parameters m_{ij}, occurring on the right-hand side of (11), have non-negative integer values, as close to zero as possible. Furthermore, these parameters must be chosen in a »graphical« manner, namely so that there exist graphs pertaining to them.

To the author's best knowledge a precise algebraic characterization of the conditions that the parameters m_{ij} must satisfy in order to be »graphical« is not known. Analogous conditions for n_1, n_2, n_3, n_4 are long known,[16–20] but it is not clear how they could be utilized in the present problem.

From Eq. (11) it is seen that if $n_2 = 2$ and $n_3 = 0$ then Δ is at least $4 \times 0.0202 = 0.0809$. If $n_2 = 1$ and $n_3 = 1$ then Δ is at least $2 \times 0.0202 + 3 \times 0.0109 = 0.0731$. If $n_2 = 0$ and $n_3 = 2$ then Δ is at least $6 \times 0.0109 = 0.0654$. In summary, if $n_2 + n_3 = 2$ then Δ cannot be less than 0.0654. Clearly, Δ will exceed the value 0.0654 also if $n_2 + n_3 > 2$.

We now consider the case when $n_2 + n_3 \leq 1$ and search for graphically feasible combinations of m_{12}, m_{13}, m_{22}, m_{23}, m_{24}, m_{33} and m_{34} for which Δ is less than 0.0654. There are exactly three such combinations:

n_2	n_3	non-zero m_{ij}'s	Δ
0	0		0
0	1	$m_{34} = 3$	0.0327
1	0	$m_{24} = 2$	0.0404

From Eqs. (2) and (7) we obtain

$$2(m + n) = 3n_1 + 4n_2 + 5n_3 + 6n_4 = 3(n_1 + n_2 + 2n_3 + 2n_4) + n_2 - n_3 \ .$$

This implies

$$2(n + m) \equiv n_2 - n_3 \pmod 3$$

and therefore

$$n + m \equiv n_3 - n_2 \pmod 3.$$

Thus, the congruence class modulo 3 to which $n + m$ belongs depends solely on the number of vertices of degree two and three. Consequently, among the combinations for which $\Delta < 0.0654$, there is one with $n + m \equiv 0 \pmod 3$, one with $n + m \equiv 1 \pmod 3$, and one with $n + m \equiv 2 \pmod 3$. This means that these combinations completely determine the (n,m)-molecular graphs with the smallest Randić indices (except for the first few values of n, see below). We thus arrive at:

Theorem 4. If n is sufficiently large (as specified below), then for any value of m, $n - 1 \leq m \leq 2n$, the following is true.

(a) If $n + m \equiv 0 \pmod 3$, then molecular graphs without vertices of degree two and three (that is, the graphs possessing only vertices of degree one and four) have the smallest Randić indices, equal to $(4n + m)/12$.

(b) If $n + m \equiv 1 \pmod 3$, then the molecular graphs without vertices of degree two and with a single vertex of degree three, adjacent to three vertices of degree four, have the smallest Randić indices, equal to $(4n + m)/12 + (3\sqrt{3} - 5)/6$.

(c) If $n + m \equiv 2 \pmod 3$, then the molecular graphs without vertices of degree three and with a single vertex of degree two, adjacent to two vertices of degree four, have the smallest Randić indices, equal to $(4n + m)/12 + (3\sqrt{2} - 4)/6$.

What »sufficiently large n« is depends of the value of m and the congruence class of $n + m$. Below are given the smallest values of n for which Theorem 4 holds in the case of acyclic, unicyclic, bicyclic and tricyclic molecular graphs.

		$n + m \equiv 0$	$n + m \equiv 1$	$n + m \equiv 2$
acyclic	$m = n - 1$	5	13	9
unicyclic	$m = n$	9	11	7
bicyclic	$m = n + 1$	10	9	8
tricyclic	$m = n + 2$	8	7	9

Anyway, Theorem 4 does not cover the first few values of n, because graphs with the required properties do not exist if n is not large enough. The finding of these »exceptional« graphs (with n-values smaller than what in Theorem 4 is specified as »sufficiently large«) is an easy task for computer-aided search.[12] A complete list of minimal-χ trees and unicyclic molecular graphs has been reported elsewhere.[13,14]

MOLECULAR GRAPHS WITH MAXIMAL RANDIĆ INDICES

In order to find the molecular graphs with maximal χ-values we cannot use a procedure analogous to what was described in the previous section. Namely, such a procedure would lead to graphs composed of several components, each of which being regular of degree 2 and/or 3 and/or 4 (*cf.* Theorem 2). In order to prevent this, a pertinent modification of the method must be designed.

However, due to Theorems 2 and 3 we already know some (n,m)-molecular graphs with maximal χ.

Proposition 1. If $m = n - 1$ and $n \geq 3$, then the molecular graph with maximal Randić index has $n_1 = 2$, $n_2 = n - 3$, $n_3 = n_4 = 0$, $m_{12} = 2$, $m_{22} = n - 3$, *i.e.*, it is the path.

Proposition 2. If $m = n$ and $n \geq 3$, then the molecular graph with maximal Randić index has $n_2 = n$, $n_1 = n_3 = n_4 = 0$, $m_{22} = n$, *i.e.*, it is the cycle.

Proposition 3. If n is even, $n \geq 4$ and $m = 3n/2$ then the molecular graphs with maximal Randić indices are the regular graphs of degree 3 (for which $n_3 = n$, $n_1 = n_2 = n_4 = 0$, $m_{33} = 3n/2$).

Proposition 4. If $m = 2n$ and $n \geq 5$, then the molecular graphs with maximal Randić indices are the regular graphs of degree 4 (for which $n_4 = n$, $n_1 = n_2 = n_3 = 0$, $m_4 = 2n$).

Proposition 5. If $m = 2\,n - 1$ and $n \geq 5$, then the molecular graphs with maximal Randić indices are the graphs obtained by deleting an edge from a regular graphs of degree 4. For such graphs $n_3 = 2$, $n_4 = n - 2$, $n_1 = n_2 = 0$, $m_{34} = 6$, $m_{44} = 2n - 7$.

Some further results of this kind are:

Proposition 6. If $m = n + 1$ and $n \geq 5$, then the molecular graphs with maximal Randić indices are the graphs obtained by adding an edge to the cycle in such a manner that a triangle is formed. For such graphs $n_3 = 2$, $n_2 = n - 2$, $n_1 = n_4 = 0$, $m_{23} = 4$, $m_{33} = 1$ and $m_{22} = n - 5$.

Proposition 7. If n is even, $n \geq 6$ and $m = 3n/2 + 1$, then the molecular graphs with maximal Randić indices are the graphs obtained by adding an edge to a regular graph of degree 3. For such graphs $n_4 = 2$, $n_3 = n - 2$, $n_1 = n_2 = 0$, $m_{34} = 6$, $m_{44} = 1$, $m_{33} = 3n/2 - 6$.

Proposition 8. If n is even, $n \geq 6$ and $m = 3n/2 + 2$, then the molecular graphs with maximal Randić indices are the graphs obtained by adding two edges to a regular graph of degree 3 in such a manner that the subgraph induced by the four vertices of degree 4 is isomorphic to K_4. For such graphs $n_4 = 4$, $n_3 = n - 4$, $n_1 = n_2 = 0$, $m_{34} = 4$, $m_{44} = 6$, $m_{33} = 3n/2 - 8$).

Proposition 9. If n is odd, $n \geq 5$ and $m = \lfloor 3n/2 \rfloor + 1$, then the molecular graphs with maximal Randić indices are the graphs consisting of one vertex of degree four and $n - 1$ vertices of degree 3. For such graphs $m_{34} = 6$, $m_{33} = \lfloor 3n/2 \rfloor - 5$.

Proposition 10. If n is odd, $n \geq 5$ and $m = \lfloor 3n/2 \rfloor + 2$, then the molecular graphs with maximal Randić indices are obtained by adding an edge to a graph specified in Proposition 9, in such a manner that the subgraph induced by the three vertices of degree 4 is isomorphic to K_3. For such graphs $n_4 = 3$, $n_3 = n - 3$, $n_1 = n_2 = 0$, $m_{34} = 6$, $m_{44} = 3$, $m_{33} = \lfloor 3n/2 \rfloor - 7$.

Proposition 11. If $m = 2n - 2$ and $n \geq 5$, then the molecular graphs with maximal Randić indices are the graphs obtained by deleting two edges from a regular graph of degree 4 in such a manner that the subgraph induced by the four vertices of degree 3 is isomorphic to C_4. For such graphs $n_3 = 4$, $n_4 = n - 4$, $n_1 = n_2 = 0$, $m_{34} = 4$, $m_{33} = 4$, $m_{44} = 2n - 8$.

Propositions 1–11 cover the »exceptional« choices of the parameters n and m, namely choices for which graphs mentioned in Theorems 5a and 5b do not exist. By direct construction we easily verify the following:

Proposition 12. A molecular graph with $n_1 = n_4 = 0$ and $m_{23} = 2$ exist for all values of n and m, such that $n \geq 5$ and $n + 2 \leq m \leq \lceil (3n - 1)/2 \rceil$, and only for these values.

Proposition 13. A molecular graphs with $n_1 = n_2 = 0$ and $m_{34} = 2$ exist for all values of n and m, such that $n \geq 9$ and $\lceil (3n + 5)/2 \rceil \leq m \leq 2n - 2$, and only for these values.

We are now prepared to seek for molecular graphs with maximal Randić index. The following two cases need to be considered separately: (A) $n + 2 \leq m \leq [(3n - 1)/2]$ and (B) $\lceil (3n + 5)/2 \rceil \leq m \leq 2n - 2$. Other choices of m are covered by Propositions 1–11.

Case A: $n + 2 \leq m \leq \lceil (3n - 1)/2 \rceil$

In order to avoid graphs in which one component is a regular graph of degree 2, we require that

$$\begin{aligned} m_{22} &< n_2 \qquad \text{if} \quad n_2 > 1 \\ m_{22} &= 0 \qquad \text{if} \quad n_2 = 0. \end{aligned}$$

Subcase A1: $n_2 > 0$

If $n_2 > 0$, then we introduce an auxiliary non-negative variable ξ, satisfying

$$m_{22} + \xi = n_2 - 1. \tag{12}$$

Consider now the system of equations (2)–(7) and (12) and solve it in n_1, n_2, n_3, n_4, m_{22}, m_{23} and m_{33}. This gives

$$n_1 = m_{12} + m_{13} + m_{14}$$

$$n_2 = 3n - 2m - 2m_{12} - 2m_{13} - \frac{7}{4}m_{14} + \frac{1}{4}m_{24} + \frac{1}{4}m_{34} + \frac{1}{2}m_{44}$$

$$n_3 = 2m - 2n + m_{12} + m_{13} + \frac{1}{2}m_{14} - \frac{1}{2}m_{24} - \frac{1}{2}m_{34} - m_{44}$$

$$n_4 = \frac{1}{4}m_{14} + \frac{1}{4}m_{24} + \frac{1}{4}m_{34} + \frac{1}{2}m_{44}$$

$$m_{22} = 3n - 2m - 1 - 2m_{12} - 2m_{13} - \frac{7}{4}m_{14} + \frac{1}{4}m_{24} + \frac{1}{4}m_{34} + \frac{1}{2}m_{44} - \xi$$

$$m_{23} = 2 - m_{12} - m_{24} + 2\xi$$

$$m_{33} = 3m - 3n - 1 + 2m_{12} + m_{13} + \frac{3}{4}m_{14} - \frac{1}{4}m_{24} - \frac{5}{4}m_{34} - \frac{3}{2}m_{44} - \xi$$

which substituted back into Eq. (1) results in:

$$\chi(\mathrm{G}) = \frac{n}{2} + \frac{2}{\sqrt{6}} - \frac{5}{6} + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} - \frac{1}{3}\right) m_{12} + \left(\frac{1}{\sqrt{3}} - \frac{2}{3}\right) m_{13} - \frac{1}{8} m_{14} +$$

$$\left(\frac{1}{\sqrt{8}} - \frac{1}{\sqrt{6}} + \frac{1}{24}\right) m_{24} + \left(\frac{1}{\sqrt{12}} - \frac{7}{24}\right) m_{34} + \left(\frac{2}{\sqrt{6}} - \frac{5}{6}\right) \xi =$$

$$\frac{n}{2} + \frac{2}{\sqrt{6}} - \frac{5}{6} - 0.0345 m_{13} - 0.0853 m_{13} - 0.1250 m_{14} -$$

$$0.0130 m_{24} - 0.0026 m_{34} - 0.0168 \xi$$

Note that the parameters m and m_{44} do not occur on the right-hand side of the latter expression.

Now, in order that $\chi(\mathrm{G})$ be maximal, we have to set

$$m_{12} = m_{13} = m_{14} = m_{24} = m_{34} = \xi = 0 \tag{13}$$

provided this choice is graphically feasible. Also m_{44} must be set equal to zero, because otherwise all vertices of degree 4 would be mutually connected and not connected to other vertices of G, *i.e.*, the graph would possess a component which is regular of degree 4.

From conditions (13) and $m_{44} = 0$ follows $n_1 = n_4 = 0$, $n_2 = 3n - 2m$, $n_3 = 2m - 2n$, $m_{22} = 3n - 2m - 1$, $m_{23} = 2$, $m_{33} = 3m - 3n - 1$. From Proposition 12 we see that graph with such parameters exist for all the required values of m. The Randić indices of these graphs are equal to

$$\chi^{(1)} = \frac{n}{2} + \frac{2}{\sqrt{6}} - \frac{5}{6} \tag{14}$$

which, remarkably, is independent of m.

Subcase A2: $n_2 = 0$

If $n_2 = 0$, then $m_{12} = m_{22} = m_{23} = m_{24} = 0$. The system (2)–(7) has now to be solved in the variables n_1, n_3, n_4, m_{13} and m_{33}. The resulting expression of χ reads:

$$\chi(\mathrm{G}) = \frac{3n}{2}\left(\frac{1}{\sqrt{3}} - \frac{1}{3}\right) + m\left(\frac{2}{3} - \frac{1}{\sqrt{3}}\right) + \left(\frac{11}{24} - \frac{7}{8\sqrt{3}}\right) m_{14} +$$

$$\left(\frac{1}{8\sqrt{3}} + \frac{1}{\sqrt{12}} - \frac{3}{8}\right) m_{34} + \left(\frac{1}{4\sqrt{3}} - \frac{1}{6}\right) m_{44} =$$

$$\frac{3n}{2}\left(\frac{1}{\sqrt{3}}-\frac{1}{3}\right)+m\left(\frac{2}{3}-\frac{1}{\sqrt{3}}\right)-0.0468m_{14}-0.0142m_{34}-0.0223m_{44}.$$

In order that $\chi(G)$ be as large as possible it must be $m_{14} = m_{34} = m_{44} = 0$, in which case the maximal value of χ is:

$$\chi^{(2)}=\frac{3n}{2}\left(\frac{1}{\sqrt{3}}-\frac{1}{3}\right)+m\left(\frac{2}{3}-\frac{1}{\sqrt{3}}\right) . \tag{15}$$

Combining Eqs. (14) and (15) we get

$$\chi^{(1)}-\chi^{(2)}=\frac{1}{6}\left[(3n-2m)(\sqrt{2}-3)+2\sqrt{6}-5\right] .$$

Because $m \le (3n - 1)/2$ it follows that

$$\chi^{(1)}-\chi^{(2)}\ge\frac{1}{6}(2\sqrt{6}-\sqrt{3}-3)=0.0278>0 .$$

Hence $\chi^{(1)}$ always exceeds $\chi^{(2)}$ and we may assume $n_2 > 0$. Consequently, $\chi^{(1)}$ is the required maximal possible value of the Randić index. Bearing in mind Proposition 12 we can now state:

Theorem 5a. Among the molecular graphs for which $n + 2 \le m \le \lceil(3n - 1)/2\rceil$, maximal Randić index is attained by the graphs with $n_1 = n_4 = 0$, $n_2 = 3n - 2m$, $n_3 = 2m - 2n$, $m_{22} = 3n - 2m - 1$, $m_{23} = 2$ and $m_{33} = 3m - 3n - 1$. This maximal value is equal to $n/2 + 2/\sqrt{6} - 5/6$ (and is, hence, independent of m). Such graphs exist for $n \ge 5$.

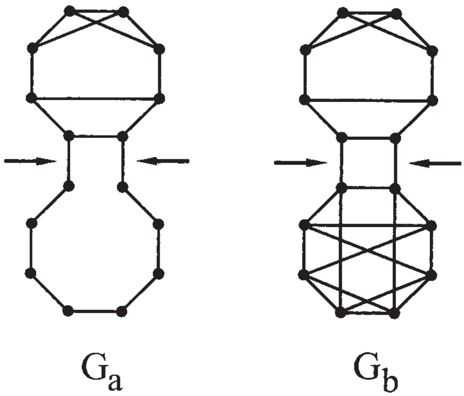

Figure 1. G_a and G_b are examples of graphs with maximal Randić index, specified in Theorems 5a and 5b; these graphs possess exactly two edges (indicated by arrows) connecting vertices of different degrees.

The graph G_a, depicted in Figure 1, illustrates the structure of the graphs described in Theorem 5a.

Case B: $\lceil(3n + 5)/2\rceil \le m \le 2n - 2$

This case is analyzed in a similar manner as the previous one. Instead of condition $m_{22} < n_2$ we now require $m_{44} < 2n_4$. Thus instead of Eq. (12) we introduce a non-negative auxiliary variable ζ, such that

$$m_{44} + \zeta = 2n_4 - 1. \tag{16}$$

The consideration is simplified by the fact that molecular graphs for which $m > 3n/2$ necessarily possess vertices of degree 4. Consequently, the case $n_4 = 0$ needs not be examined at all.

Solving the system (2)–(7) and (16) in n_1, n_2, n_3, n_4, m_{33}, m_{34} and m_{44} results in:

$$n_1 = m_{12} + m_{13} + m_{14}$$

$$n_2 = \frac{1}{2}m_{12} + m_{22} + \frac{1}{2}m_{23} + \frac{1}{2}m_{24}$$

$$n_3 = 4n - 2m - 4m_{12} - 3m_{13} - 3m_{14} - 2m_{22} - m_{23} - m_{24}$$

$$n_4 = 2m - 3n + \frac{5}{2}m_{12} + 2m_{13} + 2m_{14} + m_{22} + \frac{1}{2}m_{23} + \frac{1}{2}m_{24}$$

$$m_{33} = 6n - 3m - 1 - 6m_{12} - 5m_{13} - 4m_{14} - 3m_{22} - 2m_{23} - m_{24} - \zeta$$

$$m_{34} = 2 - m_{14} - m_{24} + 2\zeta$$

$$m_{44} = 4m - 6n - 1 + 5m_{12} + 4m_{13} + 4m_{14} + 2m_{22} + m_{23} + m_{24} - \zeta$$

which substituted back into Eq. (1) yields:

$$\chi(G) = \frac{n}{2} - \frac{7}{12} + \frac{1}{\sqrt{3}} + \left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right)m_{12} + \left(\frac{1}{\sqrt{3}} - \frac{2}{3}\right)m_{13} + \left(\frac{1}{6} - \frac{1}{\sqrt{12}}\right)m_{14} +$$
$$\left(\frac{1}{\sqrt{6}} - \frac{5}{12}\right)m_{23} + \left(\frac{1}{\sqrt{8}} - \frac{1}{\sqrt{12}} - \frac{1}{12}\right)m_{24} + \left(\frac{1}{\sqrt{3}} - \frac{7}{12}\right)\zeta = \tag{17}$$
$$\frac{n}{2} - \frac{7}{12} + \frac{1}{\sqrt{3}} - 0.0429m_{12} - 0.0853m_{13} - 0.1220m_{14} -$$
$$0.0084m_{23} - 0.0185m_{24} - 0.0056\zeta .$$

This time the parameters missing from the right-hand side of Eq. (17) are m and m_{22}.

For getting a maximal value for χ(G), Eq. (17), we have now to set

$$m_{12} = m_{13} = m_{14} = m_{23} = m_{24} = \zeta = 0$$

and, in order to prevent that a regular graph of degree 2 be a component of G, also $m_{22} = 0$. Bearing in mind Proposition 13 we finally arrive at:

Theorem 5b. Among the molecular graphs for which $\lceil (3n - 5)/2 \rceil \le m \le 2n - 2$, maximal Randić index is attained by the graphs with $n_1 = n_2 = 0$, $n_3 = 4n - 2m$, $n_4 = 2m - 3n$, $m_{33} = 6n - 3m - 1$, $m_{34} = 2$ and $m_{44} = 4m - 6n - 1$. This maximal value is equal to $n/2 - 7/12 + 1/\sqrt{3}$ (and is, hence, independent of m). Such graphs exist for $n \ge 9$.

The graph G_b, depicted in Figure 1, illustrates the structure of the graphs described in Theorem 5b.

By Theorems 5a and 5b and by the Propositions 1–11 we characterized the molecular graphs with maximal Randić index for all n, $n \ge 5$, and for all m, $n - 1 \le m \le 2n$.

ON CONSTRUCTION OF GRAPHS WITH MINIMAL AND MAXIMAL RANDIĆ INDICES

Theorems 4 and 5 provide a complete characterization of the molecular graphs with minimal and maximal χ-values. They, however, do not give a recipe how such graphs can actually be constructed. In fact, the construction of representatives of such graphs is quite elementary and should be evident from Figure 1 and well as from the earlier communicated examples.[13,14] The true problem with the (n,m)-molecular graphs having minimal and maximal Randić indices is that these are not unique. Therefore, instead in their construction one should be interested in their enumeration. Of course, the ideal solution of this problem would be a constructive enumeration. This, however, remains a task for the future.

Acknowledgements. – The author thanks the Alexander von Humboldt Foundation for financial help that made him possible to spend the Fall of 2000 in Germany, where this work has been completed. The hospitality of the colleagues at the Institute für Organische Chemie und Biochemie of the Freiburg University, and at the Lehrstuhl II für Mathematik of the Bayreuth University are gratefully acknowledged.

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SAŽETAK

Molekulski grafovi s minimalnim i maksimalnim Randićevim indeksima

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Randićev indeks χ zbroj je članova oblika $1/\sqrt{\delta(u)\,\delta(v)}$ po svim parovima susjednih čvorova, gdje δ označuje stupanj odgovarajućeg čvora u molekulskom grafu. U radu su karakterizirani (n,m)-molekulski grafovi (to jest, povezani grafovi s n čvorova, m grana, $n - 1 \leq m \leq 2n$, takvi da im maksimalni stupanj čvora nije veći od 4), koji imaju najmanje i najveće Randićeve indekse.