CROATICA CHEMICA ACTA
CCACAA **77** (3) 501–508 (2004)

ISSN-0011-1643
CCA-2953
Original Scientific Paper

Valence Connectivity *versus* Randić, Zagreb and Modified Zagreb Index: A Linear Algorithm to Check Discriminative Properties of Indices in Acyclic Molecular Graphs

Damir Vukičević[a,*] and Ante Graovac[b,c]

[a]*Department of Mathematics, Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia*

[b]*Department of Chemistry, Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia*

[c]*Ruđer Bošković Institute, P.O. Box 180, HR-10002 Zagreb, Croatia*

RECEIVED JANUARY 23, 2004; REVISED JULY 5, 2004; ACCEPTED JULY 22, 2004

Key words
valence connectivity
acyclic molecular graphs
topological indices

Valence connectivity in molecular graphs is described by 10-tuples μ_{ij} where μ_{ij} denotes the number of edges connecting vertices of valences *i* and *j*. A shorter description is provided by 4-tuples containing the number of vertices and values of Randić, Zagreb and modified Zagreb indices. Surprisingly, these two descriptions are in one-to-one correspondence for all acyclic molecules of practical interest, *i.e.*, for all those having no more than 100 atoms. This result was achieved by developing an efficient algorithm that is linear in the number of 10-tuples.

INTRODUCTION

One of the central notions in chemistry is that of the valence of atoms. Atoms of various valences form chemical bonds. Let n_i denote the number of vertices of degree *i* and let μ_{ij} denote the number of bonds whose terminal atoms are of valences *i* and *j*. The collection of all μ_{ij}s is termed valence connectivity.[1–4]

Molecules are conveniently represented by molecular graphs where hydrogen atoms are usually omitted.[5–6] In most molecules, like those of organic chemistry valences are at most 4, and accordingly the valence connectivities are conveniently represented by 10-tuples of the form $\mu = (\mu_{11}, \mu_{12}, \mu_{13}, \mu_{14}, \mu_{22}, \mu_{23}, \mu_{24}, \mu_{33}, \mu_{34}, \mu_{44})$. Of course, $\mu_{11} \neq 0$ is only rarely encountered, like *e.g.* in a graph depicting ethylene. Graph theoretical terms are parallel to the chemical ones, and instead of molecules, atoms, bonds, valences, *etc*., one speaks respectively of graphs, vertices, edges, vertex degrees, *etc*.

When the topology of bonding in molecules is contracted to a number, one speaks of a molecular descriptor or topological index.[7] Thus far, hundreds of topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.[8–9]

Here, we consider three indices, which are fully defined by knowing only the valence connectivity in a graph G. These are the Randić index, χ:[10]

$$\chi = \chi(\mathrm{G}) = \sum_{1 \le i \le j \le 4} \frac{\mu_{ij}(\mathrm{G})}{\sqrt{i \cdot j}}, \qquad (1)$$

the Zagreb index, M_2:[12]

* Author to whom correspondence should be addressed. (E-mail: vukicevi@pmfst.hr)

$$M_2 = M_2(\mathrm{G}) = \sum_{1 \le i \le j \le 4} i \cdot j \cdot \mu_{ij}(\mathrm{G}) \qquad (2)$$

and the modified Zagreb index $^*M_2$:[12–13]

$$^*M_2 = {}^*M_2(\mathrm{G}) = \sum_{1 \le i \le j \le 4} \frac{\mu_{ij}(\mathrm{G})}{i \cdot j}. \qquad (3)$$

The number of vertices, n, and the number of edges in G, l, are simply related to μ_{ij}s as follows:

$$n = n(\mathrm{G}) = \sum_{1 \le i \ge j \le 4} \left(\frac{1}{i} + \frac{1}{j}\right) \cdot \mu_{ij}(\mathrm{G}) \qquad (4)$$

$$l = l(\mathrm{G}) = \sum_{1 \le i \ge j \le 4} \mu_{ij}(\mathrm{G}) \qquad (5)$$

Besides, 10-tuples of μ_{ij}s, 4-tuples (n, χ, M_2, $^*M_2$) represent another way of describing the topology of molecular graphs. Obviously, the knowledge of 10-tuples uniquely determines 4-tuples, but the opposite does not hold. From here on, we restrict ourselves to acyclic molecules, *i.e.*, to trees, where $l = n - 1$ holds.

The main objective of this paper is to determine when 4-tuples uniquely determine 10-tuples in such graphs. In order to do so, an algorithm is developed here, which for fixed n checks whether there is one-to-one correspondence between 4- and 10- tuples. Trivial checking would require testing of all possible pairs of 10-tuples, *i.e.*, it is quadratic in the number of 10-tuples. The algorithm presented here (after all 10-tuples of m_{ij}s are generated) is linear in that the number and the execution of this algorithm take about three hours on a PC with Celeron 800 processor.

RESULTS

First, we start with a few auxiliary results. Using the theory of the finite extensions of the field of rational numbers or simple, but tedious elementary calculation, it can be shown that:

Lemma 1. – Let $a, b, c, d \in \mathrm{Q}$. If $a + b\sqrt{2} + c\sqrt{3} + d\sqrt{6} = 0$, then $a = b = c = d = 0$, where Q is the set of rational numbers.

For each molecular graph, denote:

$a(\mathrm{G}) = \mu_{11}(\mathrm{G}) + 6\mu_{14}(\mathrm{G}) + 6\mu_{22}(\mathrm{G}) + 4\mu_{33}(\mathrm{G}) + 3\mu_{44}(\mathrm{G})$

$b(\mathrm{G}) = 2\mu_{12}(\mathrm{G}) + \mu_{24}(\mathrm{G})$

$c(\mathrm{G}) = \mu_{13}(\mathrm{G}) + \mu_{34}(\mathrm{G})$

$d(\mathrm{G}) = \mu_{23}(\mathrm{G})$.

From the last Lemma, it directly follows that:

Lemma 2. – Let G be any molecular graph. Then the numbers a(G), b(G), c(G) and d(G) are uniquely determined by χ(G).

Let us prove:

Lemma 3. – Let G_1 and G_2 be two molecular graphs such that:

$$\begin{pmatrix} (\chi(\mathrm{G}_1) = \chi(\mathrm{G}_2)) \text{ and } (M_2(\mathrm{G}_1) = M_2(\mathrm{G}_2)) \text{and} \\ ({}^*M_2(\mathrm{G}_1) = {}^*M_2(\mathrm{G}_2)) \text{ and } (n_2(\mathrm{G}_1) = n_2(\mathrm{G}_2)) \end{pmatrix} \Rightarrow$$

$$(\mu(\mathrm{G}_1) = \mu(\mathrm{G}_2)), \qquad (6)$$

then

1) $\mu_{11}(\mathrm{G}_1) = 0$ and $\mu_{11}(\mathrm{G}_2) = 0$

2) $n_2(\mathrm{G}_1) \neq 0$ and $n_2(\mathrm{G}_2) \neq 0$

3) $n_3(\mathrm{G}_1) \neq 0$ and $n_3(\mathrm{G}_2) \neq 0$.

Proof. – Note that for each molecular graph G with at least three vertices, we have $\mu_{11}(\mathrm{G}) = 0$ and that single graph with 2 vertices is a path of length one, and hence indeed 1) holds.

Now, let us prove 2). Suppose, in contrast, that there are graphs G_1 and G_2 that satisfy (6), but do not satisfy relation 2). Denote $a = a(\mathrm{G}_1) = a(\mathrm{G}_2)$, $b = b(\mathrm{G}_1) = b(\mathrm{G}_2)$ and analogously for c, d, M_2, $^*M_2$ and n. Without loss of generality, we may assume that $n_2(\mathrm{G}_1) = 0$. It follows that $\mu_{12}(\mathrm{G}_1) = \mu_{22}(\mathrm{G}_1) = \mu_{23}(\mathrm{G}_1) = \mu_{24}(\mathrm{G}_1)$, hence $b = d = 0$, and therefore $\mu_{12}(\mathrm{G}_2) = \mu_{24}(\mathrm{G}_2) = \mu_{23}(\mathrm{G}_2) = 0$. Note that for each $i \in \{1, 2\}$, we have:

$6\mu_{14}(\mathrm{G}_i) + 6\mu_{22}(\mathrm{G}_i) + 4\mu_{33}(\mathrm{G}_i) + 3\mu_{44}(\mathrm{G}_i) = a$

$2\mu_{13}(\mathrm{G}_i) + \mu_{34}(\mathrm{G}_i) = c$

$$\begin{pmatrix} \mu_{13}(\mathrm{G}_i) + \mu_{14}(\mathrm{G}_i) + 2\mu_{22}(\mathrm{G}_i)/2 + \\ (\mu_{13}(\mathrm{G}_i) + 2\mu_{33}(\mathrm{G}_i) + \mu_{34}(\mathrm{G}_i))/3 + \\ (\mu_{14}(\mathrm{G}_i) + \mu_{34}(\mathrm{G}_i) + 2\mu_{44}(\mathrm{G}_i))/4 \end{pmatrix} = n$$

$$\mu_{13}(\mathrm{G}_i) + \mu_{14}(\mathrm{G}_i) + \mu_{22}(\mathrm{G}_i) + \mu_{33}(\mathrm{G}_i) + \mu_{34}(\mathrm{G}_i) + \mu_{44}(\mathrm{G}_i) = n - 1$$

$$3\mu_{13}(G_i)+4\mu_{14}(G_i)+4\mu_{22}(G_i)+9\mu_{33}(G_i)+12\mu_{34}(G_i)+16\mu_{44}(G_i)=M_2$$

$$\frac{1}{3}\mu_{13}(G_i)+\frac{1}{4}\mu_{14}(G_i)+\frac{1}{4}\mu_{22}(G_i)+\frac{1}{9}\mu_{33}(G_i)+\frac{1}{12}\mu_{34}(G_i)+\frac{1}{16}\mu_{44}(G_i)={}^*M_2$$

i.e., a system of 6 equations in 6 unknowns μ_{13} (G_i), μ_{14} (G_i), μ_{22} (G_i), μ_{33} (G_i), μ_{34} (G_i) and μ_{44} (G_i). Note that the matrix of the system has a rank equal to 6; hence, there is a unique solution to these equations, and this is in contradiction with $\mu(G_1) \neq \mu(G_2)$.

Let us prove 3). Suppose, in contrast, that there are graphs G_1 and G_2 that satisfy (6), but do not satisfy relation 3). Denote $a,b,c,d,M_2,{}^*M_2$ and n as above. Without loss of generality, we may assume that $n_3(G_1) = 0$. It follows that $\mu_{13}(G_1) = \mu_{23}(G_1) = \mu_{33}(G_1) = \mu_{34}(G_1)$; hence $c = d = 0$, and therefore $\mu_{13}(G_2) = \mu_{23}(G_2) = \mu_{34}(G_2) = 0$. Note that for each $i \in \{1, 2\}$, we have:

$$6\mu_{14}(G_i) + 6\mu_{22}(G_i) + 4\mu_{33}(G_i) + 3\mu_{44}(G_i) = a$$

$$2\mu_{12}(G_i) + \mu_{24}(G_i) = b$$

$$\left(\begin{array}{l}\mu_{12}(G_i)+\mu_{14}(G_i)+\\(\mu_{12}(G_i)+2\mu_{22}(G_i)+\mu_{24}(G_i))/2+\\2\mu_{33}(G_i)/3+(\mu_{14}(G_i)+\mu_{24}(G_i)+2\mu_{44}(G_i))/4\end{array}\right)=n$$

$$\mu_{12}(G_i)+\mu_{14}(G_i)+\mu_{22}(G_i)+\mu_{24}(G_i)+\mu_{33}(G_i)+\mu_{44}(G_i)=n-1$$

$$2\mu_{12}(G_i)+4\mu_{14}(G_i)+4\mu_{22}(G_i)+8\mu_{24}(G_i)+9\mu_{33}(G_i)+16\mu_{44}(G_i)=M_2$$

$$\frac{1}{2}\mu_{12}(G_i)+\frac{1}{4}\mu_{14}(G_i)+\frac{1}{4}\mu_{22}(G_i)+\frac{1}{8}\mu_{24}(G_i)+\frac{1}{9}\mu_{33}(G_i)+\frac{1}{16}\mu_{44}(G_i)={}^*M_2$$

i.e., the system of 6 equations in 6 unknowns: μ_{12} (G_i), μ_{14} (G_i), μ_{22} (G_i), μ_{24} (G_i), μ_{33} (G_i) and μ_{34} (G_i). Note that the matrix of the system has a rank equal to 6; hence, there is a unique solution to this equations, and this is in contradiction with $\mu(G_1) \neq \mu(G_2)$.

In our paper,[2] it is shown that:

Theorem 4. – Let $m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44},) \in \mathcal{N}_0^{10}$ where $\mathcal{N}_0^{10}$ is the set of 10-tuples of nonnegative integers. Then, there is an acyclic molecular graph G with at least two vertices such that μ (G) = m if and only if one of the following statements holds:

1) $m = (1,0,0,0,0,0,0,0,0,0)$
2) $m = (0,2,0,0,m_{22},0,0,0,0)$
3) ($m_{11} = 0$) and ($n_2,n_3,n_4 \in \mathcal{N}_0$) and ($q \geq 0$) and ($m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1$) and [($m_{12} + m_{23} + m_{24} \neq 0$) or ($m_{22} = 0$)] and one of the following holds:

3.1) ($m_{44} \leq n_4 - 1$) and ($m_{33} \leq n_3 - 1$) and ($q + m_{33} - m_{24} \leq n_3 - 1$) and ($q + m_{44} - m_{23} \leq n_4 - 1$)

3.2) $n_3 = 0$

3.3) $n_4 = 0$

where

$n_2 = (m_{12} + 2m_{22} + m_{23} + m_{24})/2$
$n_3 = (m_{13} + m_{23} + 2m_{33} + m_{34})/3$
$n_4 = (m_{14} + m_{24} + m_{34} + 2m_{44})/4$
$q = (m_{23} + m_{24} - m_{12})/2$

Now, it readily follows that:

Lemma 5. – Let $m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44},) \in \mathcal{N}_0^{10}$. There are acyclic molecular graphs G_1 and G_2, such that $\mu(G_1) = m$, $\nu(G_1) = \nu(G_2)$, $M_2(G_1) = M_2(G_2)$, ${}^*M_2(G_1) = {}^*M_2(G_2)$, $\chi(G_1) = \chi(G_2)$ and $\mu(G_1) \neq \mu(G_2)$ only if ($m_{11} = 0$) and ($n_2,n_3 \in \mathcal{N}$) and ($n_4 \in \mathcal{N}_0$) and ($q \geq 0$) and ($m_{33} + m_{34} + m_{44} + q = n_3 + n_4 - 1$) and ($m_{12} + m_{23} + m_{24} > 0$) and ($m_{33} \leq n_3 - 1$) and ($q + m_{33} - m_{24} \leq n_3 - 1$) and one of the following holds:

1) ($m_{44} \leq n_4 - 1$) and ($q + m_{44} - m_{23} \leq n_4 - 1$)
2) $n_4 = 0$

where

$n_2 = (m_{12} + 2m_{22} + m_{23} + m_{24})/2$
$n_3 = (m_{13} + m_{23} + 2m_{33} + m_{34})/3$
$n_4 = (m_{14} + m_{24} + m_{34} + 2m_{44})/4$
$q = (m_{23} + m_{24} - m_{12})/2$

Theorem 6. – Let $A, B, C, D, n, M_2, {}^*M_2 \in \mathcal{N}_0$. There are acyclic molecular graphs G_1 and G_2, such that:

$a(G_1) = a(G_2) = A$; $b(G_1) = b(G_2) = B$;
$c(G_1) = c(G_2) = C$; $d(G_1) = d(G_2) = D$;
$\nu(G_1) = \nu(G_2) = n$; $M_2(G_1) = M_2(G_2) = M_2$;
${}^*M_2(G_1) = {}^*M_2(G_2) = {}^*M_2$; $\mu(G_1) \neq \mu(G_2)$

if and only if

$$
\mathrm{card}\left\{ x\in\mathbb{Z}:\max\left\{\begin{matrix}
5/13+6B/13+5C/39-16D/39+\\ 9e/13-4M_2/13-9n/13+7Q/156,\\
-5/3-23B/12-2C-3D/2-2e-\\ 5M_2/3-4n/3-5Q/6,\\
11/7+12B/7+9C/7+4D/21+\\ 15e/7+3M_2/7-3n/7+131Q/252,\\
-1/2-5B/12-2C/3-5D/6-\\ e/3-5M_2/6-5n/6-7Q/24,\\
-5/3-17B/9-2C-14D/9-2e-\\ 5M_2/3-4n/3-Q/3,\\
-3/2-2B-2C-5D/3-2e-\\ 5M_2/3-4n/3-5Q/6
\end{matrix}\right\} \le x \le
\min\left\{\begin{matrix}
-5/3-11B/6-2C-3D/2-2e-5M_2/3-\\ 4n/3-5Q/6,\\
3/13+5B/26-3C/26-7D/13+5e/13-\\ 6M_2/13-9n/13-3Q/52,\\
55/28+9B/4+25C/14+3D/7+\\ 39e/14+3M_2/4-9n/28+41Q/56,\\
5/13+6B/13+11C/78-16D/39+\\ 9e/13-4M_2/13-9n/13+7Q/156,\\
37/34+21B/17+29C/34-D34+\\ 27e/17+5M_2/34-9n/17+127Q/136,\\
27/40+31B/40+17C/40-11D/40+\\ 21e/20-M_2/8-13n/20+143Q/160,\\
1/5+11B/35-17D/35+18e/35-\\ 2M_2/5-24n/35-Q/5,\\
-23/53-23B/53-36C/53-44D/53-\\ 18e/53-44M_2/53-48n/53-13Q/53
\end{matrix}\right\}\right\}
$$

$$
+\alpha\left(\begin{matrix}
\max\left\{\begin{matrix}
5/13+6B/13+5C/39-16D/39+\\ 9e/13-4M_2/13-9n/13+7Q/156,\\
-5/3-23B/12-2C-3D/2-2e-\\ 5M_2/3-4n/3-5Q/6,\\
11/7+12B/7+9C/7+4D/21+\\ 15e/7+3M_2/7-3n/7+131Q/252,\\
-1/2-5B/12-2C/3-5D/6-\\ e/3-5M_2/6-5n/6-7Q/24,\\
-5/3-17B/9-2C-14D/9-2e-\\ 5M_2/3-4n/3-Q/3,\\
-3/2-2B-2C-5D/3-2e-\\ 5M_2/3-4n/3-5Q/6
\end{matrix}\right\}\le\\
\le(20+21B+16C+3D+26e+6M_2-4n)/11\le\\
\le\min\left\{\begin{matrix}
-5/3-11B/6-2C-3D/2-2e-5M_2/3-\\ 4n/3-5Q/6,\\
3/13+5B/26-3C/26-7D/13+5e/13-\\ 6M_2/13-9n/13-3Q/52,\\
55/28+9B/4+25C/14+3D/7+\\ 39e/14+3M_2/4-9n/28+41Q/56,\\
5/13+6B/13+11C/78-16D/39+\\ 9e/13-4M2/13-9n/13+7Q/156,\\
37/34+21B/17+29C/34-D/34+\\ 27e/17+5M_2/34-9n/17+127Q/136,\\
27/40+31B/40+17C/40-11D/40+\\ 21e/20-M_2/8-13n/20+143Q/160
\end{matrix}\right\}
\end{matrix}\right)\ge 2 \qquad (7)
$$

and

$$e \in \mathbb{Z},$$

where

$$Q = 144\cdot {}^{*}M_2$$

$$e=\frac{A-(6+6B+6C+6M_2+6n+Q)}{12}$$

and $\alpha(R)$ is 1 if relation R holds and 0 otherwise. *card* denotes the cardinality of the set and $\mathbb{Z}$ stands for the set of integers.

Proof. From the previous results, it follows that graphs G_1 and G_2 with the required properties exist if and only if there are:

$m_i = (m_{11,i}, m_{12,i}, m_{13,i}, m_{14,i}, m_{22,i}, m_{23,i}, m_{24,i}, m_{33,i}, m_{34,i}, m_{44,i}) \in \mathbb{N}_0^{10}$, $i = 1, 2$

such that:

i,1) $m_{uv,i} \in \mathbb{Z}$, for each $1 \le u \le v \le 4$

i,2) $m_{uv,i} \ge 0$ for each $1 \le u \le v \le 4$, $m_{11,i} = 0$

i,3) $n_{2,i} \in \mathbb{Z}$

i,4) $n_{3,i} \in \mathbb{Z}$

i,5) $n_{4,i} \in \mathbb{Z}$

i,6) $q_i \in \mathbb{Z}$

i,7) $q_i \ge 0$

i,8) $A = 6m_{14,i} + 6m_{22,i} + 4m_{33,i} + 3m_{44,i}$

i,9) $B = 2m_{12,i} + m_{14,i}$

i,10) $C = 2m_{13,i} + m_{34,i}$

i,11) $D = m_{23,i}$

i,12) $m_{33,i} + m_{34,i} + q = n_{3,i} + n_{4,i} - 1$

i,13) $n_{1,i} + n_{2,i} + n_{3,i} + n_{4,i} = n$

i,14) $2m_{12,i} + 3m_{13,i} + 4m_{14,i} + 4m_{22,i} + 6m_{23,i} + 8m_{24,i} + 9m_{33,i} + 12m_{34,i} + 16m_{44,i} = M_2$

i,15) $\frac{1}{2}m_{12,i} + \frac{1}{3}m_{13,i} + \frac{1}{4}m_{14,i} + \frac{1}{4}m_{22,i} + \frac{1}{6}m_{23,i} + \frac{1}{8}m_{24,i} + \frac{1}{9}m_{33,i} + \frac{1}{12}m_{34,i} + \frac{1}{16}m_{44,i} = {}^{*}M_2$

i,16) $m_{12,i} + m_{23,i} + m_{24,i} > 0$

i,17) $m_{33,i} \le n_{3,i} - 1$

i,18) $q_i + m_{33,i} - m_{24,i} \le n_{3,i} - 1$

i,19) $n_{4,i} = 0$ or ($m_{44,i} \le n_{4,i} - 1$ and $q + m_{44,i} - m_{23,i} \le n_{4,i} - 1$)

20) $m_1 \ne m_2$

where

$n_{1,i} = m_{12,i} + m_{13,i} + m_{14,i}$
$n_{2,i} = (m_{12,i} + 2m_{22,i} + m_{23,i} + m_{24,i}) / 2$
$n_{3,i} = (m_{13,i} + m_{23,i} + 2m_{33,i} + m_{34,i}) / 3$
$n_{4,i} = (m_{14,i} + m_{24,i} + m_{34,i} + 2m_{44,i}) / 4$
$q_1 = (m_{23,i} + m_{24,i} - m_{12,i}) / 2$.

Note that relations i,3) and i,8) – i,15) are equivalent to:

i,1*) $m_{11,i} = 0$

i,2*) $m_{12,i} = (-24 - 10A - 42B - 36C - 48D + 24n + Q) / 12 - m_{44,i} / 4$

i,3*) $m_{13,i} = (-348 - 80A - 342B - 264C - 396D - 12M_2 + 348n + 5Q) / 24 + 13m_{44,i} / 8$

i,4*) $m_{14,i} = (348 + 56A + 234B + 180C + 276D + 12M_2 - 204n - 5Q) / 36 - 13m_{44,i} / 12$

i,5*) $m_{22,i} = (456 + 131A + 558B + 450C + 636D + 12M_2 - 528n - 8Q) / 18 - 7m_{44,i} / 6$

i,6*) $m_{23,i} = D$

i,7*) $m_{24,i} = (24 + 10A + 48B + 36C + 48D - 24n - Q) / 6 + m_{44,i} / 2$

i,8*) $m_{33,i} = (-420 - 104A - 450B - 360C - 516D - 12M_2 + 420n + 7Q) / 8 + 21m_{44,i} / 8$

i,9*) $m_{34,i} = (348 + 80A + 342B + 276C + 396D + 12M_2 - 348n - 5Q) - 13m_{44,i} / 4$

Note that $m_{13,i} \in \mathbb{N}$, hence:

$$-348 - 80A - 342B - 264C - 396D - 12M_2 + 348n + 5Q \equiv 0 \pmod 3$$

or equivalently,

$$A \equiv Q \pmod 3 .$$

Note also that $33n_3 + 87n_4 \in \mathbb{Z}$, hence:

$$-270 - 137A - 582B - 474C - 672D + 6M_2 + 618n + 5Q \equiv 0 \pmod 4$$

or equivalently:

$$A \equiv 2 + 2B + 2C + 2M_2 + 2n + Q \pmod 4 .$$

We can rewrite (8)–(9) as:

$$4A \equiv 4Q \pmod{12}$$

$$3A \equiv 6 + 6B + 6C + 6M_2 + 6n + 3Q \pmod{12}$$

It follows that:

$$A \equiv 6 + 6B + 6C + 6M_2 + 6n + Q \pmod{12}$$

therefore $e \in \mathbb{Z}$. Substituting this in relations i,1*) – i,8*), we get:

$$n_{3,i} = \frac{1}{24}(1740 + 1906B + 1744C + 908D + 2216e + 1124M_2 + 380n + 173Q - 25m_{44,i}) .$$

This implies that:

$$m_{44,i} \equiv 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q \pmod{24} .$$

Hence, there are numbers such that:

$$m_{44,i} \equiv 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q + 24x_i .$$

It readily follows that relations i,1*) – i,8*) can be replaced by:

i,1#) $m_{11,i} = 0$

i,2#) $m_{12,i} = -10 - 11B - 12C - 9D - 12e - 10M_2 - 8n - 2Q - 6x_i$

i,3#) $m_{13,i} = -15 - 18B - 5C + 16D - 27e + 12M_2 + 27n + 5Q + 39x_i$

i,4#) $m_{14,i} = 5B - 3C - 2(-3 + 7D - 5e + 6M_2 + 9n + 2Q + 13x_i)$

i,5#) $m_{22,i} = 55 + 63B + 50C + 12D + 78e + 21M_2 - 9n + Q - 28x_i$

i,6#) $m_{23,i} = D$

i,7#) $m_{24,i} = 23B + 2(10 + 12C + 9D + 12e + 10M_2 + 8n + 2Q + 6x_i)$

i,8#) $m_{33,i} = -99 - 108B - 81C - 12D - 135e - 27M_2 + 27n + Q + 63x_i$

i,9#) $m_{34,i} = 36B + 11C - 2(-15 + 16D - 27e + 12M_2 + 27n + 5Q + 39x_i)$

i,10#) $m_{44,i} = 12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q + 24x_i$

i,11#) $x_i \in \mathbb{Z}$

where

$$x_i = \frac{1}{24}(m_{44,i} - (12 + 10B + 16C + 20D + 8e + 20M_2 + 20n + 5Q)) .$$

It is obvious that relation i,1) is satisfied and since the following holds:

$$n_{2,i} = 60 + 69B + 56C + 17D + 84e + 26M_2 - 5n + 2Q - 25x_i$$

$$n_{3,i} = -61 - 66B - 52C - 13D - 81e - 22M_2 + 9n - Q + 29x_i$$

$$n_{4,i} = 20 + 21B + 16C + 3D + 26e + 6M_2 - 4n - 11x_i$$

$$q_i = 30 + 34B + 36C + 28D + 36e + 30M_2 + 24n + 6Q + 18x_i$$

relations i,3) – i,6) are satisfied, too. Relations i,2), i,7) and i,16) – i,18) are equivalent to i,12[#]):

$$\max\left\{\begin{array}{l} 5/13+6B/13+5C/39-16D/39+9e/13- \\ 4M_2/13-9n/13+7Q/156, \\ -5/3-23B/12-2C-3D/2-2e- \\ 5M_2/3-4n/3-5Q/6, \\ 11/7+12B/7+9C/7+4D/21+15e/7+ \\ 3M_2/7-3n/7+131Q/252, \\ -1/2-5B/12-2C/3-5D/6-e/3- \\ 5M_2/6-5n/6-7Q/24, \\ -5/3-17B/9-2C-14D/9-2e-5 \\ M_2/3-4n/3-Q/3, \\ -3/2-2B-2C-5D/3-2e-5M_2/3- \\ 4n/3-5Q/6 \end{array}\right\} \le x_i$$

$$\le \min\left\{\begin{array}{l} -5/3-11B/6-2C-3D/2-2e-5M_2/3- \\ 4n/3-5Q/6, \\ 3/13+5B/26-3C/26-7D/13+5e/13- \\ 6M_2/13-9n/13-3Q/52, \\ 55/28+9B/4+25C/14+3D/7+39e/14+ \\ 3M_2/4-9n/28+41Q/56, \\ 5/13+6B/13+11C/78-16D/39+9e/13- \\ 4M_2/13-9n/13+7Q/156, \\ 37/34+21B/17+29C/34-D/34+ \\ 27e/17+5M_2/34-9n/17+127Q/136, \\ 27/40+31B/40+17C/40-11D/40+ \\ 21e/20-M_2/8-13n/20+143Q/160 \end{array}\right\}$$

Note that statements (connected by *or*) in i,19) are mutually exclusive, *i.e.*, i,19) is equivalent to:

i,13[#]) exactly one of the following statements is true:

i,13[#]a) $x = (20 + 21B + 16C + 3D + 26e + 6M_2 - 4n) / 11$

i,13[#]b) $x \le \min\left\{\begin{array}{l} 1/5+11B/35-17D/35+ \\ 18e/35-2M_2/5-24n/35-Q/5, \\ -23/53-23B/53-36C/53- \\ 44D/53-18e/53-44M_2/53- \\ 48n/53-13Q/53 \end{array}\right\}$

Note that all numbers $m_{11,i},\ldots, m_{44,i}$ are uniquely determined by the value of x_i, and hence relation 20) is equivalent to:

i,14[#]) $x_i \ne x_j$

We can conclude that there are graphs G_1 and G_2 with the required properties if and only if there are integers x_1 and x_2, such that i,12[#])– i,14[#]) hold. The existence of these numbers is equivalent to:

$$\mathrm{card}(S) \ge 2$$

where

$$S = \left\{\begin{array}{l} x\in\mathbb{Z}: \max\left\{\begin{array}{l} 5/13+6B/13+5C/39-16D/39+ \\ 9e/13-4M_2/13-9n/13+7Q/156, \\ -5/3-23B/12-2C-3D/2-2e- \\ 5M_2/3-4n/3-5Q/6, \\ 11/7+12B/7+9C/7+4D/21+ \\ 15e/7+3M_2/7-3n/7+131Q/252, \\ -1/2-5B/12-2C/3-5D/6- \\ e/3-5M_2/6-5n/6-7Q/24, \\ -5/3-17B/9-2C-14D/9-2e- \\ 5M_2/3-4n/3-Q/3, \\ -3/2-2B-2C-5D/3-2e- \\ 5M_2/3-4n/3-5Q/6 \end{array}\right\} \le x \\ \le \min\left\{\begin{array}{l} -5/3-11B/6-2C-3D/2-2e- \\ 5M_2/3-4n/3-5Q/6, \\ 3/13+5B/26-3C/26-7D/13+ \\ 5e/13-6M_2/13-9n/13-3Q/52, \\ 55/28+9B/4+25C/14+3D/7+ \\ 39e/14+3M_2/4-9n/28+41Q/56, \\ 5/13+6B/13+11C/78-16D/39+ \\ 9e/13-4M_2/13-9n/13+7Q/156, \\ 37/34+21B/17+29C/34-D/34+ \\ 27e/17+5M_2/34-9n/17+127Q/136, \\ 27/40+31B/40+17C/40-11D/40+ \\ 21e/20-M_2/8-13n/20+143Q/160 \end{array}\right\} \\ \left[\begin{array}{l} x=\dfrac{1}{11}(20+21B+16C+3D+26e+6M_2-4n) \text{ xor} \\ x\le\min\left\{\begin{array}{l} 1/5+11B/35-17D/35+18e/35- \\ 2M_2/5-24n/35-Q/5, \\ -23/53-23B/53-36C/53-44D/53- \\ 18e/53-44M_2/53-48n/53-13Q/53 \end{array}\right\} \end{array}\right] \end{array}\right\};$$

From here, the theorem readily follows.

ALGORITHM

Now we utilize Theorem 6 to check whether the following holds for acyclic graphs:

$$\left(\left(\begin{array}{l} (\chi(G_1)=\chi(G_2)) \text{ and } (M_2(G_1)=M_2(G_2)) \text{ and} \\ ({}^*M_2(G_1)={}^*M_2(G_2)) \text{ and } (n=n(G_1)=n(G_2)) \end{array}\right)\right)\Rightarrow$$

$$(\mu(G_1)) = \mu(G_2))$$

i.e., for which values of n 4-tuples uniquely determine 10-tuples. An algorithm is given in Ref. 2 that for given n generates the set Γ_n of all 10-tuples $m = (m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44})$, which are 10-tuples (*i.e.*, $\mu(G) = m$) of acyclic graphs with n vertices. We use this algorithm in the first line of the pseudocode of the algorithm developed here.

Let us denote the left hand side of inequality (7) by $T(A, B, C, D, n, M_2, {}^*M_2)$. Now, we demonstrate our algorithm:

1) Input n

2) For each $(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}) \in \Gamma_n$

2.1) $A = m_{11} + 6m_{14} + 6m_{22} + 4m_{33} + 3m_{44}$

2.2) $B = 2m_{12} + m_{24}$

2.3) $C = 2m_{13} + m_{34}$

2.4) $D = m_{23}$

2.5) $M_2 = m_{11} + 2m_{12} + 3m_{13} + 4m_{14} + 4m_{22} + 6m_{23} + 8m_{24} + 9m_{33} + 12m_{34} + 16m_{44}$

2.6) $^*M_2 = m_{11} + \frac{1}{2}m_{12} + \frac{1}{3}m_{13} + \frac{1}{4}m_{14} + \frac{1}{4}m_{22} + \frac{1}{6}m_{23} + \frac{1}{8}m_{24} + \frac{1}{9}m_{33} + \frac{1}{12}m_{34} + \frac{1}{16}m_{44}$

2.7) Calculate $T(A, B, C, D, n, M_2, {}^*M_2)$

2.8) If $T(A, B, C, D, n, M_2, {}^*M_2) < 1$ then Error

2.9) If $T(A, B, C, D, n, M_2, {}^*M_2) \geq 2$

2.9.1) Output: There are graphs G_1 and G_2 with n vertices such that

$$\left(\begin{pmatrix} (\chi(G_1)=\chi(G_2)) \text{ and } (M_2(G_1)=M_2(G_2)) \text{ and} \\ (^*M_2(G_1)={}^*M_2(G_2)) \text{ and } (n=n(G_1)=n(G_2)) \end{pmatrix}\right) \text{and}$$

$$(\mu(G_1)) \neq \mu(G_2))$$

2.9.2) Output A, B, C, D, M_2, $^*M_2$ and exit

3) Output:

$$\left(\begin{pmatrix} (\chi(G_1)=\chi(G_2)) \text{ and } (M_2(G_1)=M_2(G_2)) \text{ and} \\ (^*M_2(G_1)={}^*M_2(G_2)) \text{ and } (n=n(G_1)=n(G_2)) \end{pmatrix}\right) \Rightarrow$$

$$(\mu(G_1)) = \mu(G_2))$$

Note that line 2.8) does not solve the required problem, but it is a useful control, which verifies that the algorithm works correctly.

APPLICATIONS

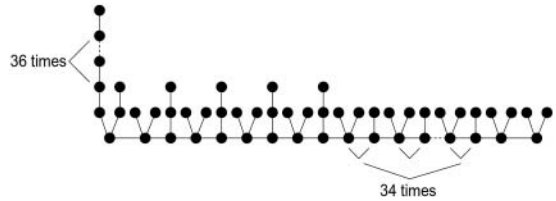
The number of 10-tuples grows rapidly with n. Therefore, we have tested n from 3 up to 100 and have found that for all these values 4-tuples uniquely determine 10-tuples of acyclic graphs. The procedure could be continued for higher values of n, but for some of these values 4-tuples cannot determine uniquely 10-tuples. That it is so shows the following example of two graphs G_1 and G_2 with $n = n(G_1) = n(G_2) = 241$:

$$a(G_1) = a(G_2) = 684;\ b(G_1) = b(G_2) = 12;$$
$$c(G_1) = c(G_2) = 150;\ d(G_1) = d(G_2) = 6;$$

$$^*M_2(G_1) = {}^*M_2(G_2) = 7344/144;$$
$$M_2(G_1) = M_2(G_2) = 1548;$$

$$\mu(G_1) = (0, 6, 36, 78, 36, 6, 0, 0, 78, 0) \neq$$
$$\mu(G_2) = (0, 0, 75, 52, 8, 6, 12, 63, 0, 24).$$

We represent these two graphs by the following figures:



There may be some lower values of n where such a situation is encounteres, but we leave it as an open problem.

CONCLUSIONS

Here, we consider two kinds of objects able to model valence connectivities: 10-tuples and 4-tuples containing the Randić, Zagreb, modified Zagreb indices and the number of vertices. A question is raised here whether there is one-to-one correspondence among 4- and 10-tuples for acyclic molecular graphs with a fixed number of vertices, and an algorithm is developed here which is able to answer this question. The algorithm is linear in the number of 10-tuples. The exhaustive computations have shown that the above one-to-one correspondence holds at least for all acyclic graphs with up to 100 vertices.

REFERENCES

1. I. Gutman, *Croat. Chem. Acta* **75** (2002) 357–369
2. D. Vukičević and A. Graovac, *Croat. Chem. Acta* **77** (2004) 313–319
3. D. Veljan and D. Vukičević, unpublished work.
4. D. Vukičević and N. Trinajstić, unpublished work.
5. A. Graovac, I. Gutman, and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer-Verlag, Berlin, 1977.
6. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1983; 2nd revised edition 1992.
7. H. Hosoya, *Bull. Chem. Soc. Jpn.* **44** (1971), 2332–2339.
8. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
9. M. V. Diudea, I. Gutman, and L. Jantschi, *Molecular Topology*, Nova, Huntington, 2001.
10. M. Randić, *J. Am. Chem. Soc.* **97** (1975), 6609–6615.

11. I. Gutman and N. Trinajstić, *Chem. Phys. Lett.* **17** (1972) 535–538.
12. B. Lučić, A. Miličević, S. Nikolić, and N. Trinajstić, *On Modified Zagreb Indices*, in: A. Graovac, B. Pokrić, and V. Smrečki (Eds.), *MATH/CHEM/COMP 2002 Book of Abstracts*, ISBN 953-6690-22-5, Zagreb, 2002, p. 39.
13. S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, *Croat. Chem. Acta* **76** (2003) 113–124.

Acknowledgement. – Partial support of the Ministry of Science and Technology of the Republic of Croatia (Grant No. 0037117 and Grant No. 0098039) is gratefully acknowledged.

SAŽETAK

Odnos susjednosti valencija i Randićevoga, Zagrebačkoga i modificiranoga Zagrebačkoga indeksa: Linearni algoritam za provjeru diskriminativnih svojstava indeksa u acikličkim grafovima

Damir Vukičević i Ante Graovac

Susjednost valencija u molekularnim grafovima opisana je desetorkama μ_{ij} gdje μ_{ij} označava broj bridova koji povezuju čvorove valencija i i j. Kraći opis susjednosti daju četvorke čiji su elementi broj vrhova u grafu i vrijednosti Randićevoga, Zagrebačkoga i modificiranoga Zagrebačkoga indeksa. Iznenađuje da su ova dva opisa u obostrano jednoznačnoj korespondenciji za sve acikličke molekule od praktičnog interesa, tj. za sve one koje sadrže najviše do 100 atoma. Ovaj rezultat je dobiven primjenom ovdje razvijenoga i opisanoga algoritma koji je linearan u broju desetorki μ_{ij}.