SOME TOPOLOGICAL INDICES DERIVED FROM THE $v^m d^n$ MATRIX. PART 9. THE Mj(m,n) AND Mij(m,n) INDICES

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Abstract

The Mj(m,n) and Mij(m,n) indices considered here are derived from the $v^m d^n$ matrix by multiplication of its non-diagonal elements. A general characteristic of the Mj(m,n) and Mij(m,n) indices is the transition domain in the plane of exponents **m** and **n**, which is placed along the diagonal characterized by **m** = -**n**. Above this diagonal transition domain the values of the Mj(m,n) and Mij(m,n) indices of alkanes increase with the size of the molecule and decrease with branching, whereas the reverse is true below the diagonal. Correlation of tested Mj(m,n) and Mij(m,n) indices with the physicochemical properties of alkanes is better than $|r| = 0.9$ in 15 resp. 13 of 23 cases when alkanes from propane to octanes inclusive are considered, as well as in 12 resp. 8 of 24 cases when only octanes are taken into account. There is a number of Mj(m,n) and Mij(m,n) indices that have a regular sequence of isomers due to increasing branching. In the plane of exponents **m** and **n** they are positioned in the regions characterized by **m** ≤ -1, -1 ≤ **n** < 1 and **m** ≥ 1, -1 < **n** ≤ 1 among the Mj(m,n) indices, as well as -6 ≤ **m** ≤ $^1/_3$, -4 ≤ **n** < 1 and **m** ≥ $^1/_3$, -1 < **n** ≤ 2 among the Mij(m,n) indices.

Introduction

In our recent papers we studied several groups of topological indices derived from the $v^m d^n$ matrix, which is a generalized vertex-degree, vertex distance matrix. The indices were derived from it either by summation of its elements[1-5] or they were the largest eigenvalues of said matrix.[6-8] Narumi[9] presented an index, which is the product of vertex degrees. Gutman et al.[10] introduced an index, derived by multiplication of the elements of the matrix and described its characteristics. This prompted us to study also the indices derived from the $v^m d^n$ matrix by multiplication of its elements.

Data and notations

The data for the boiling point (BP), density (d), the critical data Tc, Pc, Vc, Zc, αc, and dc, as well as the standard enthalpy of formation for the ideal gas (ΔHf°g), the enthalpy of vaporisation (ΔHv), the Antoine constants A, B, and C, as well as the Pitzer's acentric factor (ω) and the refractive index (n_D) were taken from the CRC Handbook[11] or

from Lange's Handbook[12]. The data for the liquid molar volume (Vm), the ratios Tc^2/Pc and Tc/Pc used instead of the van der Waals parameters a_0 and b_0, the ratio BP/Tc (reduced BP), and the molar refraction (MR) were calculated from data presented in the handbooks. The data for Motor Octane Numbers (MON) was taken from Pogliani[13] and Gutman et al.,[10] that for vapour pressure (logVP) from Goll and Jurs,[14] and that for the entropy (S) and quadratic mean radius (R^2) from Ren.[15]

The structures of alkanes are presented in shorthand, e.g. Hp is *n*-heptane, Oct is *n*-octane, 223M5 is 2,2,3-trimethylpentane, 3E2M5 is 3-ethyl-2-methylpentane, etc.

Methods

Susceptibility for the increase in carbon number

The susceptibility[16] for the increase in carbon number, $S_{a,a+1} = X_{a+1}/X_a - 1$, where X is an index and subscript *a* refers to the structure of an alkane having a particular carbon number (number of vertices) as well as a number, position and type of branches. Thus, the two alkanes taken into account differ in carbon number by one. For example, in $S_{7,8}$ the digit 8 means any octane having the same number and type of branches as a heptane which is represented by the digit 7. In $S_{Hp,Oct}$ the data of *n*-heptane (Hp) and *n*-octane (Oct) is used. In $S_{2M6,2M7}$ the data of 2-methyl hexane (2M6) and 2-methyl heptane (2M7) is used, etc.

Relative contribution of a structural feature to the value of the index

The relative contribution of a structural feature to the value of the index when the size of the molecule increases, is estimated as follows. The contribution of the number of branches is estimated by $S_{33M5,33M6} - S_{3M7,3M6}$. The contribution of the position of branches is estimated by $^1/_2(S_{33M5,33M6} - S_{22M5,22M6})$. The contribution of the separation between branches is estimated by $S_{24M5,24M6} - S_{23M5,23M6}$. The contribution of the change of the substituent from methyl to ethyl is estimated by $S_{3E5,3E6} - S_{3M6,3M7}$.

The relative contribution of a structural feature to the value of the index when the branching of the molecule increases is estimated with help of the following differences in values of the indices Mj(m,n) or Mij(m,n), as applicable: The contribution of the number of branches is estimated by the difference: $b = M(m,n)_{33M6} - M(m,n)_{3M6}$. The contribution of the position of branches is estimated by $c = M(m,n)_{34M6} - M(m,n)_{23M6}$.

The contribution of the separation between branches is estimated by s = $M(m,n)_{24M6}$ - $M(m,n)_{23M6}$. The contribution of the change of the substituent from methyl to ethyl is estimated by e = $M(m,n)_{3E2M5}$ - $M(m,n)_{23M6}$. The contributions are labelled with letters b, c, s, and e, respectively. The uppercase letter is used to label the structural feature having the highest contribution to the value of index in question. The results of estimations of the relative contribution of structural features are checked by the sequences of isomers obtained by sorting $S_{7,8}$ or the values of indices $Mj(m,n)$ or $Mij(m,n)$ of octanes.

Results and discussion

$Mj(m,n)$ and $Mij(m,n)$ indices and the source matrices

The $Mj(m,n)$ and $Mij(m,n)$ indices are derived by multiplication of all the non-diagonal elements of the matrix having the main diagonal elements $\mathbf{g_{ii}} = 0$. The non-diagonal elements used to derive the $Mj(m,n)$ indices are $\mathbf{g_{ij}}$ $(i{\neq}j) = v_j^{\mathbf{m}}{\times}d_{ij}^{\mathbf{n}}$. Those used to derive the $Mij(m,n)$ indices are $\mathbf{g_{ij}}$ $(i{\neq}j) = v_i^{\mathbf{m}}{\times}v_j^{\mathbf{m}}{\times}d_{ij}^{\mathbf{n}}$, where v_i and v_j is the degree of vertex i and j, respectively, (in alkanes it is the number of C-C bonds the carbon in question is involved in) and d_{ij} is the shortest distance from vertex i to vertex j (in alkanes it is the smallest number of bonds between the carbons in question), cf. ref.[1] They are labelled as $Mj(m,n)$ and $Mij(m,n)$ indices. The π index[10] is identical to $Mj(0,1)^{1/2}$ and $Mij(0,1)^{1/2}$. From the matrices having the non-diagonal elements $\mathbf{g_{ij}}$ $(i{\neq}j) = v_i^{\mathbf{m}}{\times}d_{ij}^{\mathbf{n}}$, there could be derived the $Mi(m,n)$ indices, but $Mi(m,n) = Mj(m,n)$.

The $Mj(m,n)$ as well as the $Mij(m,n)$ indices of methane are equal to zero by definition. The $Mj(m,n)$ as well as the $Mij(m,n)$ indices of ethane are equal to 1. Whenever an exponent, **m** or **n**, or both, is equal to -∞, the values of the $Mj(m,n)$ as well as the $Mij(m,n)$ indices of other alkanes are equal to 0.

The $Mj(m,n)$ and $Mij(m,n)$ indices which are integers

Among the tested $Mj(m,n)$ and $Mij(m,n)$ indices are integers those ones having exponent **m** or **n** or both equal to -∞; for ethane they are equal to 1 and for the other alkanes they are equal to 0. $Mj(0,0)$ and $Mij(0,0)$ is equal to 1 in all cases. Integers seem to be also the $Mj(m,n)$ and $Mij(m,n)$ indices when **m** is equal to 0 or an integer and **n** is equal to 0 or $^1/_2$ or an integer.

The degeneration of Mj(m,n) *and* Mij(m,n) *indices*

How much data of the tested Mj(m,n) and Mij(m,n) indices is degenerated, i.e. equal to at least one more, is presented in Table 1 for all alkanes from propane to octanes inclusive in the plane of exponents **m** and **n**. Totally degenerated are the indices having **m** or **n** equal to -∞, as well as Mj(0,0) and Mij(0,0). Highly degenerated are other Mj(m,0) and Mij(m,0) indices, whereas some degeneration is also observed among some Mj(m,n) or Mij(m,n) indices placed on or near the diagonal, characterized by the relation **m** = -**n**. In the latter group, the identity and the extent of degeneration of Mj(m,n) indices differs from that of Mij(m,n) indices. They are two different groups of indices in this respect.

Table 1. Degeneration of Mj(m,n) indices (in parentheses degeneration of Mij(m,n) indices) for alkanes from propane to octanes inclusive expressed as the number of data equal to at least one more among the 38 possible ones.

m	-∞	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3	T	(4)		2					24						
2	T	2 (2)	(4)	6 (2)	2				24						
1	T	(2)		(4)	6 (2)	2			24						
$\mathbf{\frac{1}{2}}$	T				(2)	6 (2)	2		24						
$\mathbf{\frac{1}{3}}$	T			(2)	(2)	2	6		24						
$\mathbf{\frac{1}{4}}$	T					(4)		6	24						
0	T								T						
$\mathbf{-\frac{1}{4}}$	T								24	6					
$\mathbf{-\frac{1}{3}}$	T								24		6 (2)				
$\mathbf{-\frac{1}{2}}$	T								24	2	2	6 (2)	(2)		
-1	T								24			2	6 (2)	(4)	2 (2)
-2	T								24				2	6 (2)	2
-4	T								24					2	
-6	T								24						2
-∞	T	T	T	T	T	T	T	T	T	T	T	T	T	T	T

	-∞	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
									n						

T   Totally degenerated. All values are equal

If only octanes are considered (not shown), there are the same indics as above totally degenerated, whereas highly degenerated are the Mj(m,0) and Mij(m,0) indices. Other tested Mj(m,n) and Mij(m,n) indices of octanes are not degenerated. From these observations follows that degeneration observed on or near the above mentioned diagonal is caused exclusively by alkanes of different carbon number.

If we compare Table 1 with tables presenting the degeneration of other indices derived from the $v^m d^n$ matrix,[1-8] we can see an interesting difference. Whereas among the Mj(m,n) and Mij(m,n) indices we observe the degeneration in the row characterized by **m** = -∞, in the columns characterized by **n** = -∞ and **n** = 0, as well as on or near the diagonal, characterized by the relation **m** = -**n**, the summation derived indices and the largest eigenvalues of the same matrices do not give rise to degeneration on or near the diagonal, characterized by the relation **m** = -**n**.

Correlation between Mj(m,n) *and* Mij(m,n) *indices*

Correlation between the Mj(m,n) and Mij(m,n) indices is very high, except when **m** ≈ -**n**, where it is very low. This holds true when the size of the molecules has the main influence as well as when it has no influence. One of the reasons is indicated in Table 1, where a different degree of degeneration along this diagonal is observed.

Correlation of Mj(m,n) *indices with* W(m,n) *and* L(m,n) *indices*

Assuming a linear relationship, the correlation between the Mj(m,n) indices and W(m,n) indices[1] or L(m,n) indices[6] is not good in general. If only octanes are considered, there are nine cases out of 225 tested ones where r > 0.9. These indices are placed around Mj(0,0) near the above mentioned diagonal. The Mj(m,n) indices are thus essentially different from W(m,n) and L(m,n) indices although they are derived from the same matrices.

Correlation of Mij(m,n) *indices with* Vij(m,n) *and* Lij(m,n) *indices*

Assuming a linear relationship, the correlation between the Mij(m,n) indices and Vij(m,n) indices[5] is in general not good, except at (**m,n**) combinations $(^1/_3, -^1/_2)$ and $(^1/_4, -^1/_3)$. If only octanes are considered, a good correlation with Vij(m,n) indices[5] is observed only at Mij$(^1/_4, -^1/_2)$, Mij$(-^1/_4, ^1/_4)$, Mij$(-^1/_4, ^1/_3)$, Mij$(-^1/_4, ^1/_2)$, Mij$(-^1/_3, ^1/_3)$, and Mij$(-^1/_3, ^1/_2)$. There are several **m,n** combinations where the correlation is low. Similar is the situation in correlation between the Mij(m,n) and Lij(m,n) indices[8].

Dependence of values of Mj(m,n) *and* Mij(m,n) *indices of n-alkanes on the increase of size of the molecule*

Table 2 indicates whether the Mj(m,n)$_n$ indices, i.e. the Mj(m,n) indices of *n*-alkanes increase or decrease with the increasing size of molecule. We can see that on

the diagonal in the plane of exponents **m** and **n**, characterized by **m** = -**n**, the values of indices for propane are equal to those of ethane; the values of indices for other *n*-alkanes are decreasing when **n** < 0 and consequently **m** > 0, whereas they are increasing when **n** > 0 and consequently **m** < 0.

Table 2. The changes of values of Mj(m,n) indices of *n*-alkanes on increasing carbon number. Tested were the carbon numbers from C_2 to C_8.

m	$-\infty$	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3	0	-	-	Bu^	+	+	+	+	+	+	+	+	+	+	+
2	0	-	-	=,-	Hp^	+	+	+	+	+	+	+	+	+	+
1	0	-	-	-	=,-	Hp^	+	+	+	+	+	+	+	+	+
$\frac{1}{2}$	0	-	-	-	-	=,-	Bu^	+	+	+	+	+	+	+	+
$\frac{1}{3}$	0	-	-	-	-	-	=,-	Bu^	+	+	+	+	+	+	+
$\frac{1}{4}$	0	-	-	-	-	-	-	=,-	+	+	+	+	+	+	+
0	0	-	-	-	-	-	-	-	1	+	+	+	+	+	+
$-\frac{1}{4}$	0	-	-	-	-	-	-	-	-	=,+	+	+	+	+	+
$-\frac{1}{3}$	0	-	-	-	-	-	-	-	-	Bu˅	=,+	+	+	+	+
$-\frac{1}{2}$	0	-	-	-	-	-	-	-	-	Hp˅	Bu˅	=,+	+	+	+
-1	0	-	-	-	-	-	-	-	-	-	-	Hp˅	=,+	+	+
-2	0	-	-	-	-	-	-	-	-	-	-	-	Hp˅	=,+	+
-4	0	-	-	-	-	-	-	-	-	-	-	-	-	Hp˅	Bu˅
-6	0	-	-	-	-	-	-	-	-	-	-	-	-	-	Hp˅
$-\infty$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

n

+   The value of Mj(m,n) index increases with carbon number
-        The value of Mj(m,n) index decreases with carbon number
=   Mj(m,n)$_{Et}$ = Mj(m,n)$_{Pr}$
Bu^   The highest value of the Mj(m,n) index among *n*-alkanes is observed at *n*-butane
Bu˅   The lowest value of the Mj(m,n) index among *n*-alkanes is observed at *n*-butane

Above that diagonal, the values of Mj(m,n)$_n$ indices increase with carbon number, whereas below the diagonal they decrease. Near that diagonal there is a transition domain where an U-shaped or an inverted U-shaped dependence is observed. This diagonal separation seems to be a general characteristic of the Mj(m,n) indices.

Table 3 indicates whether the Mij(m,n)$_n$ indices, i.e. the Mij(m,n) indices of *n*-alkanes increase or decrease with the increasing size of molecule. We can see that the values of indices increase with carbon number above the diagonal in the plane of exponents **m** and **n**, characterized by **m** = -**n**, whereas below the diagonal they decrease. On the diagonal and near it there is a transition domain where, on the one side, the value

of some Mij(m,n) indices of propane is equal to that of ethane, whereas on the other hand, an U-shaped or an inverted U-shaped dependence is observed. This diagonal separation seems to be a general characteristic of the Mij(m,n) indices, too.

Table 3. The changes of values of Mij(m,n) indices of *n*-alkanes on increasing carbon number. Tested were the carbon numbers from C_2 to C_8.

m	-∞	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3	0	=,-	Bu^	+	+	+	+	+	+	+	+	+	+	+	+
2	0	-	=,-	Hp^	+	+	+	+	+	+	+	+	+	+	+
1	0	-	-	=,-	Hp^	+	+	+	+	+	+	+	+	+	+
$\mathbf{\frac{1}{2}}$	0	-	-	-	=,-	Hp^	+	+	+	+	+	+	+	+	+
$\mathbf{\frac{1}{3}}$	0	-	-	-	-	Bu^	+	+	+	+	+	+	+	+	+
$\mathbf{\frac{1}{4}}$	0	-	-	-	-	=,-	Bu^	+	+	+	+	+	+	+	+
0	0	-	-	-	-	-	-	-	1	+	+	+	+	+	+
$\mathbf{-\frac{1}{4}}$	0	-	-	-	-	-	-	-	-	Hp˅	Bu˅	Pr˅	+	+	+
$\mathbf{-\frac{1}{3}}$	0	-	-	-	-	-	-	-	-	-	Hp˅	Bu˅	+	+	+
$\mathbf{-\frac{1}{2}}$	0	-	-	-	-	-	-	-	-	-	-	Hp˅	=,+	+	+
-1	0	-	-	-	-	-	-	-	-	-	-	-	Hp˅	=,+	+
-2	0	-	-	-	-	-	-	-	-	-	-	-	-	Hp˅	Bu˅
-4	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-6	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-∞	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	-∞	**-6**	**-4**	**-2**	**-1**	$\mathbf{-\frac{1}{2}}$	$\mathbf{-\frac{1}{3}}$	$\mathbf{-\frac{1}{4}}$	**0**	$\mathbf{\frac{1}{4}}$	$\mathbf{\frac{1}{3}}$	$\mathbf{\frac{1}{2}}$	**1**	**2**	**3**

n

+   The value of Mij(m,n) index increases with carbon number
-     The value of Mij(m,n) index decreases with carbon number
= $Mij(m,n)_{Et} = Mij(m,n)_{Pr}$
Bu^   The highest value of the Mij(m,n) index among *n*-alkanes is observed at *n*-butane
Bu˅   The lowest value of the Mij(m,n) index among *n*-alkanes is observed at *n*-butane

The farther from the diagonal the more rapid is the increase or the decrease of the values of the Mj(m,n) and Mij(m,n) indices. On the one hand, the value of the Mj(0,0) and Mij(0,0) index for all *n*-alkanes, except for methane, is equal to 1; the value of any Mj(m,n) and Mij(m,n) index for ethane is equal to 1, too. On the other hand, the value for *n*-octane, for example, of Mj(-6,-6) $\approx$ 9.1E-210 and Mj(3,3) $\approx$ 3.3E+104, whereas the value of Mij(-6,-6) $\approx$ 1.3E-285 and Mij(3,3) $\approx$ 2.8E+142.

Changes of values of Mj(m,n) *and* Mij(m,n) *indices of other alkane isomers due to the increase of the size of molecule*

How the values of Mj(m,n) indices of other alkanes change on increasing the size of the molecule when the main chain of the alkane is elongated preserving the branched structure, is presented in Table 4.

Table 4. The changes of values of Mj(m,n) indices of other alkanes on increasing carbon number.

m															
3	0	-	-	-	+	+	+	+	+	+	+	+	+	+	+
2	0	-	-	-	5-	+	+	+	+	+	+	+	+	+	+
1	0	-	-	-	-	5-	+	+	+	+	+	+	+	+	+
$1/2$	0	-	-	-	-	-	-	5-	+	+	+	+	+	+	+
$1/3$	0	-	-	-	-	-	-	-	+	+	+	+	+	+	+
$1/4$	0	-	-	-	-	-	-	-	+	+	+	+	+	+	+
0	0	-	-	-	-	-	-	-	——	+	+	+	+	+	+
$-1/4$	0	-	-	-	-	-	-	-	-	+	+	+	+	+	+
$-1/3$	0	-	-	-	-	-	-	-	-	+	+	+	+	+	+
$-1/2$	0	-	-	-	-	-	-	-	-	4-	+	+	+	+	+
-1	0	-	-	-	-	-	-	-	-	-	-	4-	+	+	+
-2	0	-	-	-	-	-	-	-	-	-	-	-	4-	+	+
-4	0	-	-	-	-	-	-	-	-	-	-	-	-	4-	+
-6	0	-	-	-	-	-	-	-	-	-	-	-	-	-	4-
-∞	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	-∞	**-6**	**-4**	**-2**	**-1**	**$-1/2$**	**$-1/3$**	**$-1/4$**	**0**	**$1/4$**	**$1/3$**	**$1/2$**	**1**	**2**	**3**
									n						

0	The values of index are equal to zero, except for ethane
——	The values of index do not change with carbon number
+	The value of Mj(m,n) increases with carbon number
-	The value of Mj(m,n) decreases with carbon number
1-	The value of Mj(m,n) of one isomer decreases and that of other isomers increase with carbon number

From Table 4 follows that not only among the *n*-alkanes but among the alkanes in general, the values of indices increase with carbon number above the diagonal in the plane of exponents **m** and **n**, characterized by **m** = -**n**, whereas below the diagonal they decrease. On the diagonal and near it there is a transition domain where the values of Mj(m,n) indices for some isomers increase whereas those of other isomers decrease on increasing the size of the molecule.

Table 5. The changes of values of Mij(m,n) indices of other alkanes on increasing carbon number.

m	$-\infty$	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3	0	-	-	+	+	+	+	+	+	+	+	+	+	+	+
2	0	-	-	5-	+	+	+	+	+	+	+	+	+	+	+
1	0	-	-	-	4-	+	+	+	+	+	+	+	+	+	+
$\mathbf{^1/_2}$	0	-	-	-	-	5-	+	+	+	+	+	+	+	+	+
$\mathbf{^1/_3}$	0	-	-	-	-	-	5-	+	+	+	+	+	+	+	+
$\mathbf{^1/_4}$	0	-	-	-	-	-	-	5-	+	+	+	+	+	+	+
0	0	-	-	-	-	-	-	-	—	+	+	+	+	+	+
$\mathbf{-^1/_4}$	0	-	-	-	-	-	-	-	-	4-	+	+	+	+	+
$\mathbf{-^1/_3}$	0	-	-	-	-	-	-	-	-	-	3-	+	+	+	+
$\mathbf{-^1/_2}$	0	-	-	-	-	-	-	-	-	-	-	4-	+	+	+
-1	0	-	-	-	-	-	-	-	-	-	-	-	4-	+	+
-2	0	-	-	-	-	-	-	-	-	-	-	-	-	4-	+
-4	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-6	0	-	-	-	-	-	-	-	-	-	-	-	-	-	-
$-\infty$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

n

0	The values of index are equal to zero, except for ethane
—	The values of index do not change with carbon number
+	The value of Mij(m,n) increases with carbon number
-	The value of Mij(m,n) decreases with carbon number
1-	The value of Mij(m,n) of one isomer decreases and that of other isomers increase with carbon number

The situation is also similar among the Mij(m,n) indices of other alkanes, Table 5. Above the diagonal in the plane of exponents **m** and **n**, characterized by **m** = -**n**, the values of indices increase with carbon number, whereas below the diagonal they decrease. The transition domain, where the values of Mij(m,n) indices for some isomers increase whereas those of other isomers decrease on increasing the size of the molecule, seems to be exactly on the diagonal in the plane of exponents **m** and **n**, characterized by **m** = -**n**, whereas among the Mj(m,n) indices it is not. This seems to reflect the fact, thatthe matrices from which the Mj(m,n) indices are derived, are in general non-

symmetric, whereas those from which the Mij(m,n) indices are derived, are all symmetric.

The pattern of dependence of values of the multiplication-derived Mj(m,n) and Mij(m,n) indices of alkanes on the size of the molecule is very different from that of the summation-derived W(m,n) and Vij(m,n) indices,[1,5] as well as of the largest eigenvalues of the same matrices,[6,8] the L(m,n), and Lij(m,n) indices. This fact indicates that the multiplication-derived indices are in their essence different from the summation-derived ones as well as from the largest eigenvalues of the same matrices, whereas the latter two groups of indices share many similarities. Some essential differences were indicated already by Gutman et al.[10] for the indices W and π.

Contribution of structural features of alkanes to the values of Mj(m,n) *and* Mij(m,n) *indices on increase of the size of the molecule*

Contribution of structural features to the value of Mj(m,n) and Mij(m,n) indices in the situation when the size of the molecule increases from heptane to octane by elongation of the main chain retaining the branched structure is presented in Table 6-9. A higher value of the structural feature contributes either to a higher increase of the value of the index (no sign before the letter) or to a higher decrease of the value of the index (the - sign before the letter). In all cases, this influence is superimposed to the contribution of the increase of the size of the molecule observed at *n*-alkanes and presented above.

At **n** = 0, only the number of branches and the type of the branched structure (i.e. whether the branch bearing carbon is tertiary or quaternary; it is not indicated in the tables) influence the value of a Mj(m,n) or Mij(m,n) index. This situation is in principle the same as that observed among the W(m,n) and Vij(m,n) indices,[1,5] as well as among the L(m,n) and Lij(m,n) indices.[6,8] It seems to be a general characteristic of the situation when **n** = 0. At other values of exponent **n**, an essentially different situation is observed among the Mj(m,n) and Mij(m,n) indices, than among the W(m,n) and Vij(m,n) indices,[1,5] as well as of the L(m,n) and Lij(m,n) indices,[6,8] when the pattern of the influence of structural features is compared.

Table 6. Two structural features, which have the highest influence on the values of Mj(m,n) indices when the size of molecules increases from heptane to octane.

m	-∞	-6	-4	-2	-1	-1/2	-1/3	-1/4	0	1/4	1/3	1/2	1	2	3
3				Se	Es	E-b	-Be	-Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
2				Sb	Es	Es	E-b	-Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1				Sb	Bs	Es	Es	Es	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/2				Sb	Bs	Be	Es	Es	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/3				Sb	Bs	Be	Be	Eb	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/4				Sb	Bs	Be	Be	Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
0				Bs	Bs	Bs	Be	Be		-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
-1/4				Bs	Bs	Bs	Be	Be	B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
-1/3				Bs	Bs	Bs	Be	Be	B	-E-b	-B-e	-B-e	-B-e	-B-e	-B-e
-1/2					Bs	Bs	Bs	Be	B	-E-s	-E-b	-B-e	-B-e	-B-e	-B-e
-1					Bs	Bs	Bs	Bs	B	-E-s	-E-s	-E-c	-B-e	-B-e	-B-e
-2					Bs	Bs	Bs	Bs	B	B-s	B-c	-B-s	-E-c	-B-e	-B-e
-4										B-c	B-c	B-c	-C-s	-C-e	-E-b
-6												B-c	-C-e	-C-e	
-∞															
	-∞	-6	-4	-2	-1	-1/2	-1/3	-1/4	0	1/4	1/3	1/2	1	2	3

n

b - the influence of the number of branches
c - the influence of the central position compared to the peripheral position of branches
e - the influence of the ethyl vs. the methyl group
s - the influence of separation between branches
- sign: The increase of that structural feature causes a decrease in the value of the index
The most influential structural feature is presented with the uppercase letter:

B-c:	b>-c>..	Be:	b>e>..	-Be:	-b>e>..	-B-e:	-b>-e>..
Bs:	b>s>..	B-s:	b>-s>..	-B-s:	-b>-s>..		
-C-e:	-c>-e>..	-C-s:	-c>-s>..				
Eb:	e>b>..	E-b:	e>-b>..	-E-b:	-e>-b>..	-E-c:	-e>-c>..
Es:	e>s>..	-E-s:	-e>-s>..				
Sb:	s>b>..	Se:	s>e>..				

The situation when the size of the molecule increases from heptane to octane by elongation of the main chain retaining the branched structure, is presented in Table 6 for the Mj(m,n) indices, and in Table 8 for the Mij(m,n) indices. There can be seen that the highest contribution has in most cases the number of branches (indicated by letter B), followed by the type of branches (indicated by letter E).

Table 7. Two structural features, which have the lowest influence on the values of Mj(m,n) indices when the size of molecules increases. Labels are analogous to those in Table 6.

m \ n	$-\infty$	-6	-4	-2	-1	$-\tfrac{1}{2}$	$-\tfrac{1}{3}$	$-\tfrac{1}{4}$	0	$\tfrac{1}{4}$	$\tfrac{1}{3}$	$\tfrac{1}{2}$	1	2	3
3					bc	cb	sc	sc	sc	-s-c	-s-c	-s-c	-s-c	-c-s	-c-s
2					ec	bc	-bc	sc	sc	-s-c	-s-c	-s-c	-s-c	-c-s	-c-s
1					ec	ec	bc	cb	c-b	-s-c	-s-c	-s-c	-s-c	-c-s	-c-s
$\tfrac{1}{2}$					ce	ec	sc	sc	bc	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
$\tfrac{1}{3}$					ce	ec	sc	sc	sc	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
$\tfrac{1}{4}$					ce	ec	sc	sc	sc	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
0				ce	ec	ec	sc	sc	NB	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
$-\tfrac{1}{4}$					ce	ec	ec	sc	sc	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
$-\tfrac{1}{3}$					ce	ec	ec	sc	sc	-s-c	-s-c	-s-c	-c-s	-c-s	-c-s
$-\tfrac{1}{2}$						ce	ec	ec	sc	-c-b	-s-c	-s-c	-c-s	-c-s	-c-s
-1						ce	ce	ec	ec	-cb	-c-b	-s-b	-c-s	-c-s	-c-s
-2						ce	ce	ce	ce	-e-c	-e-s	-sb	-b-s	-c-s	-c-s
-4										-s-e	-s-e	-s-e	-e-b	-b-s	-c-s
-6												-s-e	-s-b	-b-s	
$-\infty$															

bc:	..>b>c	-bc:	..>-b>c	-b-s:	..>-b>-s		
cb:	..>c>b	c-b:	..>c>-b	-cb:	..>-c>b	-c-b:	..>-c>-b
ce:	..>c>e	-c-s:	..>-c>-s				
-e-b:	..>-e>-b	ec:	..>e>c	-e-c:	..>-e>-c	-e-s:	..>-e>-s
-sb:	..>-s>b	-s-b:	..>-s>-b	sc:	..>s>c	-s-c:	..>-s>-c
-s-e:	..>-s>-e						

In majority of cases, the separation between branches (indicated by letter S), and the position of branches (indicated by letter C) have a lower contribution. This differs from the situation among the W(m,n), Vij(m,n), L(m,n), and Lij(m,n) indices,[1,5,6,8] where the separation between branches has the highest contribution in most cases. The situation is surprising, since adjacent vertices of degree one do not contribute to the value of the Mj(m,n) and Mij(m,n) index, whereas in W(m,n), Vij(m,n), L(m,n), and Lij(m,n) indices[1,5,6,8] they contribute the essential information about the importance of the number of branches. The letters E and C, indicating the prevalent influence of the type of branches and of the position of branches, respectively, appear on or near the diagonal mentioned above. The separation between branches, which has among the W(m,n), Vij(m,n), L(m,n), and Lij(m,n) indices,[1,5,6,8] in severel cases the most important contribution, is mostly lower importance among the Mj(m,n) and Mij(m,n) indices.

Table 8. Two structural features, which have the highest influence on the values of Mij(m,n) indices when the size of molecules increases from heptane to octane. Labels are analogous to those in Table 6.

m \ n	-∞	-6	-4	-2	-1	-1/2	-1/3	-1/4	0	1/4	1/3	1/2	1	2	3
3			Sb	Es	E-b	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
2			Sb	Es	Es	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1				Sb	Es	Es	-Be	-Be	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/2				Ec	Bs	Es	Es	Es	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/3				Sb	Bs	Eb	Es	Es	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
1/4				Sb	Bs	Be	Eb	Es	-B	-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
0				Bs	Bs	Bs	Be	Be		-B-e	-B-e	-B-e	-B-e	-B-e	-B-e
-1/4			Cb	Bs	Bs	Bs	Be		B	-E-s	-E-b	-B-e	-B-e	-B-e	-B-e
-1/3				Bs	Bs	Bs	Bs		B	-E-s	-E-s	-E-b	-B-e	-B-e	-B-e
-1/2				Bs	Bs	Bs	Bs		B	-E-s	-E-s	-E-c	-B-e	-B-e	-B-e
-1				Bs	Bs	Bs	Bs		B	-B-s	-B-s	-C-e	-E-c	-B-e	-B-e
-2									B	-B-s	-B-s	-B-s	-S-b	-C-e	-E-b
-4														-C-s	-C-e
-6															
-∞															

Table 9. Two structural features, which have the lowest influence on the values of Mij(m,n) indices when the size of molecules increases. Labels are analogous to those in Table 7.

m \ n	-∞	-6	-4	-2	-1	-1/2	-1/3	-1/4	0	1/4	1/3	1/2	1	2	3
3			bc	cb	sc	sc	sc	sc		-s-c	-s-c	-s-c	-s-c	-s-c	-c-s
2			ec	bc	-bc	sc	sc	sc		-s-c	-s-c	-s-c	-s-c	-s-c	-c-s
1				ec	bc	-bc	sc	sc		-s-c	-s-c	-s-c	-s-c	-c-s	-c-s
1/2				sb	ec	bc	cb	c-b		-sc	-sc	-sc	-sc	-c-s	-c-s
1/3				ec	ec	sc	bc	cb		-sc	-sc	-sc	-sc	-c-s	-c-s
1/4				ce	ec	sc	sc	bc		-sc	-sc	-sc	-sc	-c-s	-c-s
0				ce	ec	ec	sc	sc	NB	-sc	-sc	-sc	-c-s	-c-s	-c-s
-1/4			s	ce	ec	ec	sc			-c-b	-s-c	-sc	-c-s	-c-s	-c-s
-1/3				ce	ec	ec	ec			-c-b	-c-b	-s-c	-c-s	-c-s	-c-s
-1/2				ce	ce	ec	ec			-c-b	-c-b	-s-b	-c-s	-c-s	-c-s
-1				ce	ce	ce	ce			-s-e	-e-s	-sb	-b-s	-c-s	-c-s
-2										-s-e	-s-e	-s-e	-eb	-b-s	-c-s
-4														b-e	-sb
-6															
-∞															

In Table 6-9 is noticed the peculiarity of the combinations of exponents **m** and **n**, which position the respective Mj(m,n) or Mij(m,n) indices on or near the diagonal characterized by relation **m** = -**n**.

The dependence of Mj(m,n) *and* Mij(m,n) *indices on branching*

The increase or decrease with branching

Whether the values of Mj(m,n) and Mij(m,n) indices increase or decrease with branching is presented for octanes in Table 10 and 11. We notice again the intermediate domain around the above-mentioned diagonal, which separates the region above the diagonal, where the values of tested indices decrease with branching, from the region below the diagonal, where the values increase with branching.

Table 10. Schematic presentation of the change of values of Mj(m,n) indices of octanes on increasing branching.

m	-∞	-6	-4	-2	-1	-1/2	-1/3	-1/4	0	1/4	1/3	1/2	1	2	3
3		+	+	4-	-	-	-	-	-	-	-	-	-	-	-
2		+	+	+	12-	-	-	-	-	-	-	-	-	-	-
1		+	+	+	+	12-	-	-	-	-	-	-	-	-	-
1/2		+	+	+	+	+	4-	12-	-	-	-	-	-	-	-
1/3		+	+	+	+	+	+	2-	-	-	-	-	-	-	-
1/4		+	+	+	+	+	+	+	-	-	-	-	-	-	-
0		+	+	+	+	+	+	+	NB	-	-	-	-	-	-
-1/4		+	+	+	+	+	+	+	+	-	-	-	-	-	-
-1/3		+	+	+	+	+	+	+	+	15-	-	-	-	-	-
-1/2		+	+	+	+	+	+	+	+	5-	13-	-	-	-	-
-1		+	+	+	+	+	+	+	+	+	+	5-	-	-	-
-2		+	+	+	+	+	+	+	+	+	+	+	4-	-	-
-4		+	+	+	+	+	+	+	+	+	+	+	+	5-	15-
-6		+	+	+	+	+	+	+	+	+	+	+	+	+	5-
-∞															

n

+ :   The value of all isomers increases on increasing branching

- :   The value of all isomers decreases on increasing branching

4- :   The value of that Mj(m,n) index of four isomers is lower than that of the index of
       n-octane, whereas the value of the index of other isomers is higher

NB: Does not index branching

On or near this diagonal in the plane of exponents **m** and **n**, the values of Mj(m,n) and/or Mij(m,n) indices of some isomers are lower than that of *n*-octane and those of the others are higher than that of *n*-octane. Again is the transition domain among the Mij(m,n) indices closer to the diagonal than among the Mj(m,n) indices. Comparing Table 10 and 11 with Table 2-5 it is evident that the values of most tested Mj(m,n) and Mij(m,n) indices, which increase with the size of the molecule, decrease with branching, or vice versa.

The pattern of dependence of values of the multiplication-derived Mj(m,n) and Mij(m,n) indices of alkanes on branching is very different from that of the summation-derived W(m,n) and Vij(m,n) indices,[1,5] as well as of the largest eigenvalues of the same matrices,[6,8] the L(m,n), and Lij(m,n) indices. This fact corroborates that the multiplication-derived indices are in their essence different than the summation-derived ones and the largest eigenvalues of the same matrices.

Table 11. The schematic presentation of the change of values of Mij(m,n) indices of octanes on increasing branching.

m														
3	+	4-	-	-	-	-	-	-	-	-	-	-	-	-
2	+	+	12-	-	-	-	-	-	-	-	-	-	-	-
1	+	+	+	12-	-	-	-	-	-	-	-	-	-	-
$1/2$	+	+	+	+	12-	-	-	-	-	-	-	-	-	-
$1/3$	+	+	+	+	2-	12-	-	-	-	-	-	-	-	-
$1/4$	+	+	+	+	+	4-	12-	-	-	-	-	-	-	-
0	+	+	+	+	+	+	+	NB	-	-	-	-	-	-
$-1/4$	+	+	+	+	+	+	+	+	+	13-	-	-	-	-
$-1/3$	+	+	+	+	+	+	+	+	+	+	15-	-	-	-
$-1/2$	+	+	+	+	+	+	+	+	+	+	5-	-	-	-
-1	+	+	+	+	+	+	+	+	+	+	+	5-	-	-
-2	+	+	+	+	+	+	+	+	+	+	+	+	4-	15-
-4	+	+	+	+	+	+	+	+	+	+	+	+	+	1-
-6	+	+	+	+	+	+	+	+	+	+	+	+	+	+
-∞														
	-∞	-6	-4	-2	-1	$-1/2$	$-1/3$	$-1/4$	0	$1/4$	$1/3$	$1/2$	1	2	3
									n					

+ : The value of all isomers increases on increasing branching
- : The value of all isomers decreases on increasing branching
4- : The value of that Mij(m,n) index of four isomers is lower than that of the index of
    n-octane whereas the value of the index of other isomers is higher
NB: Does not index branching

Influence of structural features

The comparison of values of Mj(m,n) or Mij(m,n) indices when branching increases allows some conclusions about the contribution of particular structural features. In Table 12 can be seen that the highest contribution to the value of Mj(m,n) indices due to branching has in general the number of branches (indicated by letter B). Only on or near the above-mentioned diagonal in the plain of exponents **m** and **n**, characterized by the relation **m** = -**n**, the presence of ethyl groups (indicated by the letter E) or the separation between branches (indicated by letter S) has a higher contribution. At **n** < 1, the contribution of ethyl groups is the second highest if not the highest one. The situation among the Mij(m,n) indices, Table 13, is quite similar, except around the diagonal.

Table 12. Two structural features having the highest contribution to the value of a Mj(m,n) index due to the increase of branching.

m	-∞	-6	-4	-2	-1	$-\tfrac{1}{2}$	$-\tfrac{1}{3}$	$-\tfrac{1}{4}$	0	$\tfrac{1}{4}$	$\tfrac{1}{3}$	$\tfrac{1}{2}$	1	2	3
3		Eb	Eb	Ec	-Be	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
2		Be	Eb	Eb	Ec	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
1		Be	Be	Eb	Eb	Ec	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\mathbf{\tfrac{1}{2}}$		Be	Be	Be	Be	Be	Ec	Ec	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\mathbf{\tfrac{1}{3}}$		Be	Be	Be	Be	Be	Be	Eb	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\mathbf{\tfrac{1}{4}}$		Be	Be	Be	Be	Be	Be	Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
0		Be	Be	Be	Be	Be	Be	Be	1	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\mathbf{-\tfrac{1}{4}}$		Be	Be	Be	Be	Be	Be	Be	B	-B-e	-B-e	-B-e	-B-e	-Bs	-Bs
$\mathbf{-\tfrac{1}{3}}$		Be	Be	Be	Be	Be	Be	Be	B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\mathbf{-\tfrac{1}{2}}$		Be	Be	Be	Be	Be	Be	Be	B	-Es	-E-c	-B-e	-Bs	-Bs	-Bs
-1		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	-E-c	-Bs	-Bs	-Bs
-2		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	S-e	-Bs	-Bs
-4		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	Bs	S-e	Bs
-6		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	Bs	Bs	S-e
-∞															
	-∞	-6	-4	-2	-1	$-\tfrac{1}{2}$	$-\tfrac{1}{3}$	$-\tfrac{1}{4}$	0	$\tfrac{1}{4}$	$\tfrac{1}{3}$	$\tfrac{1}{2}$	1	2	3
									n						

Labels: The label has four elements, e.g. b>c>e>s. In Table 12 are presented the former two in the form, e.g. Bc meaning b>c>.., whereas in Table 14 are presented the latter two, e.g. in the form "es" meaning ..>e>s

B: b (c = e = s = 0)   Be: b>e>..   -Be: -b>e>..   B-e: b>-e>..
-B-e: -b>-e>..   Bs: b>s>..   -Bs: -b>s>..
Eb: e>b>..   Ec: e>c>..   -E-c: -e>-c>..   -Es: -e>s>..
S-e: s>-e>..

A higher value of the structural feature contributes either to a higher increase of the value of the index (no sign before the letter) or to a higher decrease of the value of the index (the - sign before the letter). At **n** = 0, only the number of branches and the type of the branched structure (i.e. whether the branch bearing carbon is tertiary or quaternary) influence the value of index.

The structural features that have a lower contribution than those presented in Table 12 and 13 are presented in Table 14 and 15 for comparison. The indices Mj(m,-∞), Mj(-∞,n) and Mj(0,0), as well as Mij(m,-∞), Mij(-∞,n) and Mij(0,0) do not index any contribution of structural features.

Table 13. Two structural features having the highest contribution to the value of a Mij(m,n) index due to the increase of branching. Labels are analogous to those in Table 12.

m	-∞	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3		Ec	Ec	-Be	-Be	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
2		Eb	Ec	Ec	-Be	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
1		Be	Eb	Eb	Ec	-Be	-Be	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\frac{1}{2}$		Be	Be	Eb	Eb	Ec	Ec	Ec	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\frac{1}{3}$		Be	Be	Be	Be	Eb	Ec	-Be	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$\frac{1}{4}$		Be	Be	Be	Be	Be	Ec	Ec	-B	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
0		Be	Be	Be	Be	Be	Be	Be	1	-B-e	-B-e	-B-e	-Bs	-Bs	-Bs
$-\frac{1}{4}$		Be	Be	Be	Be	Be	Be	Be	B	-E-c	-E-c	-B-e	-Bs	-Bs	-Bs
$-\frac{1}{3}$		Be	Be	Be	Be	Be	Be	Be	B	B-e	-E-c	-B-e	-Bs	-Bs	-Bs
$-\frac{1}{2}$		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	-E-c	-B-e	-Bs	-Bs
-1		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	S-e	-Bs	-Bs
-2		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	Bs	S-e	-Bs
-4		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	Bs	Bs	Bs
-6		Be	Be	Be	Be	Be	Be	Be	B	B-e	B-e	B-e	B-e	B-e	B-e
-∞															
	-∞	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
									n						

Size of the molecule

Among the tested indices, there is observed neither a Mj(m,n) nor a Mij(m,n) index that would index only the size of the molecule. Indexing the size of the molecule as the sole structural feature seems to be a characteristic of a few of the summation-derived indices and of the largest eigenvalues of matrices used here, but not of the multiplication derived indices.

Number of branches

Among the tested indices, there is observed neither a Mj(m,n) nor a Mij(m,n) index that would index only the number of branches or the size of the molecule and the number of branches. Gutman et al.[10] noticed that vertex pairs at distance 1, i.e. adjacent vertices, do not contribute at all to their π index, which completely disregards the short range interactions. That was a special situation since they used the matrix where **m** = 0 and **n** = 1. In general, the degree of vertices of degree one does not contribute to the value of a Mj(m,n) or Mij(m,n) index, contrary to the situation observed among the summation derived[1-5] indices and the largest eigenvalues,[6-8] where the degree of vertices of degree one contributes essentially to the information about the number of branches. This fact can be interpreted also in the way that the outer-most vertices do not contribute directly to the value of a Mj(m,n) or Mij(m,n) index; they do so only indirectly through mutual contributions with the inner ones.

Table 14. Two structural features having the lowest contribution to the value of a Mj(m,n) index due to the increase of branching. Labels are analogous to those in Table 12.

m														
3	c-s	c-s	b-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
2	c-s	c-s	c-s	-b-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
1	c-s	c-s	c-s	c-s	-b-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
$^1/_2$	c-s	c-s	c-s	c-s	c-s	b-s	-b-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
$^1/_3$	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
$^1/_4$	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
0	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
$-^1/_4$	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	s-c	-e-c	-e-c
$-^1/_3$	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-cs	-cs	-e-c	-e-c	-e-c
$-^1/_2$	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cb	-bs	-cs	-e-c	-e-c	-e-c
-1	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-c-s	sb	s-c	-e-c	-e-c
-2	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-c-s	-c-s	-cb	-e-c	-e-c
-4	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-c-s	-c-s	-e-c	-cb	-e-c
-6	c-s	c-s	c-s	c-s	c-s	c-s	c-s		-cs	-c-s	-c-s	-e-c	-e-c	-cb
-∞														
	-∞	**-6**	**-4**	**-2**	**-1**	**$-^1/_2$**	**$-^1/_3$**	**$-^1/_4$**	**0**	**$^1/_4$**	**$^1/_3$**	**$^1/_2$**	**1**	**2**	**3**
									n						

b-s: ..>b>-s   -bs: ..>-b>s   -b-s: ..>-b>-s

-cb: ..>-c>b   c-s: ..>c>-s   -cs: ..>-c>s   -c-s: ..>-c>-s

-e-c: ..>-e>-c

sb: ..>s>b   s-c: ..>s>-c

The contribution of the number of branches to the value of a Mj(m,n) or Mij(m,n) index is indirect but very important as illustrated in Tables 12 and 13 where in most cases the number of branches contributes to the value of a Mj(m,n) or Mij(m,n) index more than other structural features which are contributing to branching.

Indexing the number of branches as the sole structural feature seems to be a characteristic of a few of the summation-derived indices and of the largest eigenvalues of matrices used here, but not of the multiplication derived indices.

Table 15. Two structural features having the lowest contribution to the value of a Mij(m,n) index due to the increase of branching. Label are analogous to those in Table 12.

m	$-\infty$	-6	-4	-2	-1	$-\tfrac{1}{2}$	$-\tfrac{1}{3}$	$-\tfrac{1}{4}$	0	$\tfrac{1}{4}$	$\tfrac{1}{3}$	$\tfrac{1}{2}$	1	2	3
3	b-s	b-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
2	c-s	b-s	-b-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
1	c-s	c-s	c-s	-b-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
$\tfrac{1}{2}$	c-s	c-s	c-s	c-s	-b-s	-b-s	-b-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
$\tfrac{1}{3}$	c-s	c-s	c-s	c-s	c-s	-b-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
$\tfrac{1}{4}$	c-s	c-s	c-s	c-s	c-s	b-s	-b-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
0	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
$-\tfrac{1}{4}$	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-bs	-cs	-e-c	-e-c	-e-c
$-\tfrac{1}{3}$	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	sb	-cs	-e-c	-e-c	-e-c
$-\tfrac{1}{2}$	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	sb	s-c	-e-c	-e-c
-1	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-cb	-e-c	-e-c
-2	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-cb	-e-c
-4	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-e-c	-e-c	-e-c
-6	c-s	c-s	c-s	c-s	c-s	c-s	c-s			-cs	-cs	-cs	-cs	-cs	-cs
$-\infty$															

n

b-s: ..>b>-s   -bs: ..>-b>s   -b-s: ..>-b>-s
-cb: ..>-c>b   -cs: ..>-c>s   c-s: ..>c>-s
-e-c: ..>-e>-c
sb: ..>s>b   s-c: ..>s>-c

Type of the branched structure

The size of molecule, the number of branches as well as the type of the branched structure, i.e. whether the branch bearing carbon is tertiary or quaternary index the Mj(m,0) and Mij(m,0) indices, which are not mentioned above. They indicate that the structure having a quaternary carbon is more branched than that having two tertiary

carbons. Thus, the general characteristics of the indices, derived from the $v^m d^0$ matrix are quite similar regardless the way they are derived.

Type of branches

The label E in Table 12 or 13 indicates that at some combinations of exponents **m** and **n** in the Mj(m,n) or Mij(m,n) indices the exchange of a methyl group for an ethyl group in the structure of an octane contributes to the value of index more than any other structural feature, whereas in several cases (label e) it is the second greatest contribution.

Position of branches

Position of branches contributes to the value of a Mj(m,n) or Mij(m,n) index in most cases less than the number of branches and the type of branches.

Separation between branches

The separation between branches contributes more than any other structural feature contributing to branching, to the value of only few Mj(m,n) or Mij(m,n) indices. These indices are placed on the above-mentioned diagonal in the plane of exponents **m** and **n**. It has the second greatest contribution to the values of several indices when **n** $\geq$ 1.

Correlation of physicochemical properties with Mj(m,n) *or* Mij(m,n) *indices*

The values of tested Mj(m,n) and Mij(m,n) indices were correlated, assuming a linear relationship of the form y = ax + b, with values of 23 or 24 physicochemical properties, as applicable. The results are presented here in the text for data of alkanes from propane to octanes inclusive and in Fig. 1 and 2 for data of octanes.

The best correlation coefficients for tested data of alkanes from propane to octanes inclusive are in both cases crowded in the plane of exponents **m** and **n** near the diagonal characterized by **m** = -**n** in vicinity of Mj(0,0) or Mij(0,0) where the increase of the Mj(m,n) and Mij(m,n) indices with the size of the molecule is not too rapid. The best correlation coefficients of tested Mj(m,n) indices and data of physicochemical properties of alkanes from propane to octanes inclusive are given in parentheses:

Mj($^1/_3$,-$^1/_4$): Mw (-0.**9**83), MR (-0.**9**82), Vc (-0.**9**76), **Tc^2/Pc** (-0.**9**75), **Tc/Pc** (-0.**9**74), **ΔHf°g** (-0.**9**71), Vm (-0.**9**64), BP (-0.**9**62), logVP (0.**9**53), ΔHv (-0.**9**50), B (-0.**9**41), **BP/Tc** (-0.**9**10), **C** (0.**9**07), αc (-0.893), d (-0.868), ω (-0.840), n_D (-0.820)

Mj($^1/_4$,-$^1/_4$): Tc (-0.**9**58), Pc (0.**9**50), dc (-0.677)   Mj($^1/_2$,0): MON (-0.665)

Mj($^1/_4$,0): A (0.511)   Mij(-$^1/_2$,$^1/_4$): Zc (0.687)

The best correlation coefficients of tested Mij(m,n) indices and data of physicochemical properties of alkanes from propane to octanes inclusive are:

Mij($^1/_4$,-$^1/_3$): Mw (-0.**9**51), MR (-0.**9**52), **ΔHf°g** (0.**9**50), Vc (-0.**9**43), **Tc^2/Pc** (-0.**9**41),
      Tc/Pc (-0.**9**41), αc (-0.847), n$_D$ (-0.801);
Mij($^1/_3$,-$^1/_2$): BP (-0.**9**37), Pc (0.**9**37), Tc (-0.**9**36), Vm (-0.**9**35), ΔHv (-0.**9**14),
      logVP (0.**9**12), B (-0.**9**09), C (0.883), BP/Tc (-0.880), d (-0.841),
      ω (-0.799), dc (-0.665);
Mij($^1/_4$,0): MON (-0.665);   Mij($^1/_3$,-$^1/_4$): A (0.526);   Mij(-$^1/_4$,$^1/_3$): Zc (0.687);

Figure 1. Positions of 24 physicochemical properties in the plane of exponents **m** and **n**, determined by the highest correlation coefficient (data in parentheses, see below) for data of octanes with Mj(m,n) indices.

m	-∞	-6	-4	-2	-1	-$^1/_2$	-$^1/_3$	-$^1/_4$	0	$^1/_4$	$^1/_3$	$^1/_2$	1	2	3
3															
2															
1						VP									
$^1/_2$					d		B								
$^1/_3$					n$_D$										
$^1/_4$						b	MR	a							
0								1	αc						
-$^1/_4$								c	e						
-$^1/_3$								Zc							
-$^1/_2$								h	Tc						
-1															
-2															
-4															
-6															
-∞															

n

Single standing: VP(logVP, r=-0.694), B (0.591) , n$_D$ (0.**9**73) , MR (-0.881), αc (0.743), Zc (0.699), Tc (-0.748)

a: MON (-0.**9**70), **Tc^2/Pc** (0.**9**61), R^2 (0.**9**05), A (0.806), ΔHv (0.887)

b: Pc (0.**9**75), **BP/Tc** (-0.**9**69), **Tc/Pc** (-0.**9**62), ω (-0.**9**15)

c: **C** (0.**9**29), S (-0.**9**29)

d: d (0.**9**62), Vm (-0.**9**51)

e: Vc (0.850), dc (-0.834)

h: **ΔHf°g** (0.875), BP (-0.826)

In most cases the correlation with Mj(m,n) indices is better than with Mij(m,n) indices. This is probably the consequence of the less rapid increase of the Mj(m,n) indices with the size of the molecule. It can be reasonably expected that on fine-tuning of exponents **m** and **n** better results may be obtained.

The pattern of positions of the best correlation coefficients when only octanes are considered is presented in Fig. 1 and 2. As in the case of all tested alkanes, also in the case of octanes the best correlation coefficients are placed near the above-mentioned diagonal in vicinity of **m** = 0 and **n** = 0. The correlations are not very good but it can be reasonably expected that on fine-tuning the exponents the results would be better.

Figure 2. The positions of 24 physicochemical properties in the plane of exponents **m** and **n**, determined by the highest correlation coefficient (data in parentheses, see below) for data of octanes with Mij(m,n) indices.

m \ **n**	$-\infty$	-6	-4	-2	-1	$-\frac{1}{2}$	$-\frac{1}{3}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1	2	3
3															
2															
1															
$\frac{1}{2}$															
$\frac{1}{3}$								h							
$\frac{1}{4}$				d	f			A							
0								c	1	a					
$-\frac{1}{4}$										b	Tc	e			
$-\frac{1}{3}$										Zc					
$-\frac{1}{2}$															
-1															
-2															VP
-4															
-6															
$-\infty$															

Single standing: A (-0.754), Tc (-0.748), Zc (-0.748), logVP (-0.506),

a: **Tc²/Pc** (0.894), R^2 (0.865), αc (0.743)   *b*: **ΔHf°g** (0.874), BP (-0.826)
c: S (-0.**9**61), **BP/Tc** (-0.**9**24), **C** (0.**9**17), ω (-0.**9**11)
d: n$_D$ (0.**9**70), d (0.**9**62), Vm (-0.**9**51)   *e*: Vc (0.823), dc (-0.804)
f: Pc (-0.**9**37), **Tc/Pc** (-0.870), MR (-0.863), MON (-0.662)
h: ΔHv (0.848), B (0.597)

Mj(m,n) *and* Mij(m,n) *indices that might be good branching indices.*

The question of branching indices has been discussed in depth by Randić.[19] An additional step forward was the illustration of a "regular" sequence of dimethylhexane isomers,[20] as well as the suggestion of "regular" sequences of heptane resp. octane isomers.[1,3] The idea of using "regular" sequences of increasing branching is applied in Fig. 3 and 4, where the Mj(m,n) and Mij(m,n) indices, respectively, that may be sources of good branching indices are presented in the plane of exponents **m** and **n**.

The pattern of Fig. 3 and 4 is different from patterns of other groups of indices derived from the $v^m d^n$ matrix. The Mj(m,n) and especially the Mij(m,n) indices having the same sequence of isomers are placed centrosymmetrically regarding the position of the index Mij(0,0) in the plane of exponents **m** and **n**.

Figure 3. Mj(m,n) indices that might be a source of good branching indices of the BI$_A$ group. In parentheses: the position of the π index of Gutman et al.[10]

m																
3								*-BI*	*-BI*	*t<q*	-BI	-BI	-BI	-BI		
2									*-BI*	*t<q*	-BI	-BI	-BI			
1										*t<q*	-BI	-BI	-BI			
$^1/_2$										*t>q*						
$^1/_3$										*t>q*						
$^1/_4$										*t>q*						
0														(π)		
$-^1/_4$										*t<q*						
$-^1/_3$										*t<q*						
$-^1/_2$										*t<q*						
-1								BI	BI	*t<q*						
-2							BI	BI	BI	*t<q*	*BI*					
-4						BI	BI	BI	BI	*t<q*	*BI*	*BI*	*BI*			
-6						BI	BI	BI	BI	*t<q*	*BI*	*BI*	*BI*			
-∞																
	-∞	**-6**	**-4**	**-2**	**-1**	**$-^1/_2$**	**$-^1/_3$**	**$-^1/_4$**	**0**	**$^1/_4$**	**$^1/_3$**	**$^1/_2$**	**1**	**2**	**3**
									n						

BI   Oct < 2M7 < 3M7 < 4M7 < 3E6 < 25M6 < 24M6 < 23M6 < 34M6 < 3E2M5 < 22M6 < 33M6 < 3E3M5 < 234M5 < 224M5 < 223M5 < 233M5 < 2233M4

-BI   Oct > 2M7 > 3M7 > 4M7 > 3E6 > 25M6 > 24M6 > 23M6 > 34M6 > 3E2M5 > 22M6 > 33M6 > 3E3M5 > 234M5 > 224M5 > 223M5 > 233M5 > 2233M4

BI   Oct < 3E6 < 4M7 < 3M7 < 2M7 < 3E2M5 < 34M6 < 23M6 < 24M6 < 25M6 <3E3M5 < 33M6 < 22M6 < 234M5 < 233M5 < 223M5 < 224M5 < 2233M4

-BI   Oct > 3E6 > 4M7 > 3M7 > 2M7 > 3E2M5 > 34M6 > 23M6 > 24M6 > 25M6 >3E3M5 > 33M6 > 22M6 > 234M5 > 233M5 > 223M5 > 224M5 > 2233M4

Figure 4. Mij(m,n) indices that might be a source of good branching indices of the BI_A group. In parentheses: the position of the π index of Gutman et al.[10]

m															
3						*-BI*	*-BI*	*-BI*	*t<q*	-BI	-BI	-BI	-BI	-BI	
2						*-BI*	*-BI*	*-BI*	*t<q*	-BI	-BI	-BI	-BI		
1								*-BI*	*t<q*	-BI	-BI	-BI			
$^1/_2$									*t>q*	-BI	-BI				
$^1/_3$									*t>q*	-BI					
$^1/_4$									*t>q*						
0													(π)		
$-^1/_4$									*t<q*						
$-^1/_3$								BI	*t<q*						
$-^1/_2$							BI	BI	*t<q*						
-1						BI	BI	BI	*t<q*	*BI*					
-2					BI	BI	BI	BI	*t<q*	*BI*	*BI*	*BI*			
-4				BI	BI	BI	BI	BI	*t<q*	*BI*	*BI*	*BI*			
-6			BI	BI	BI	BI	BI	BI	*t<q*	*BI*	*BI*	*BI*			
-∞															
	-∞	**-6**	**-4**	**-2**	**-1**	**$-^1/_2$**	**$-^1/_3$**	**$-^1/_4$**	**0**	**$^1/_4$**	**$^1/_3$**	**$^1/_2$**	**1**	**2**	**3**
									n						

BI	Oct < 2M7 < 3M7 < 4M7 < 3E6 < 25M6 < 24M6 < 23M6 < 34M6 < 3E2M5 < 22M6 < 33M6 < 3E3M5 < 234M5 < 224M5 < 223M5 < 233M5 < 2233M4
-BI	Oct > 2M7 > 3M7 > 4M7 > 3E6 > 25M6 > 24M6 > 23M6 > 34M6 > 3E2M5 > 22M6 > 33M6 > 3E3M5 > 234M5 > 224M5 > 223M5 > 233M5 > 2233M4
BI	Oct < 3E6 < 4M7 < 3M7 < 2M7 < 3E2M5 < 34M6 < 23M6 < 24M6 < 25M6 <3E3M5 < 33M6 < 22M6 < 234M5 < 233M5 < 223M5 < 224M5 < 2233M4
-BI	Oct > 3E6 > 4M7 > 3M7 > 2M7 > 3E2M5 > 34M6 > 23M6 > 24M6 > 25M6 >3E3M5 > 33M6 > 22M6 > 234M5 > 233M5 > 223M5 > 224M5 > 2233M4

The indices Mj(m,0) and Mij(m,0), **m** ≠ -∞ and **m** ≠ 0, index the size of the molecule, the number of branches and in addition they indicate that a quaternary structure is more branched than a tertiary one. They are the simplest and degenerated Mj(m,n) and Mij(m,n) indices, which are potential sources of branching indices.

There are also four groups of Mj(m,n) as well as of Mij(m,n) indices having a regular sequence of isomers. Two groups of them (*BI* and *-BI*) indicate that a peripherally substituted alkane is more branched than a centrally substituted one. The other two groups of them (BI and -BI) indicate the reverse.

Conclusions

The Mj(m,n) and Mij(m,n) indices considered here form another group of topological indices to be considered for their usefulness. They are derived from the $v^m d^n$ matrix by multiplication of its non-diagonal elements. One index of this group has been described recently:[10] $\pi \equiv (Mj(0,1))^{1/2} \equiv (Mij(0,1))^{1/2}$. By their characteristics, the Mj(m,n) and Mij(m,n) indices are different from the W(m,n), Vij(m,n), L(m,n) or Lij(m,n) indices derived from the same matrices.

A general characteristic of the Mj(m,n) and Mij(m,n) indices is the transition domain in the plane of exponents **m** and **n** along the diagonal characterized by **m** = -**n**. In this transition domain several peculiarities are observed:

- Maximum or minimum in the dependence of values of indices of *n*-alkanes on the size of the molecule,

- Different signs of dependence of other isomers on the size of the molecule,

- Different signs of dependence of other isomers on branching,

- The highest contribution to the value of an index have other structural features than elsewhere in the plane of exponents **m** and **n**.

Above this diagonal transition domain the values of the Mj(m,n) and Mij(m,n) indices of alkanes increase with the size of the molecule and decrease with branching, whereas the reverse is true below the diagonal.

The Mj(m,n) and Mij(m,n) indices having **m** or **n** equal to -∞, as well as Mj(0,0) and Mij(0,0) do not index anything.

None of the Mj(m,n) or Mij(m,n) indices indexes only the size of the molecule, nor only the number of branches or both.

The size of molecule, the number of branches as well as the type of the branched structure, i.e. whether the branch bearing carbon is tertiary or quaternary, index the Mj(m,0) and Mij(m,0) indices not mentioned above, just like the W(m,0), Vij(m,0), L(m,0), and Lij(m,0) indices studied earlier.

Majority of Mj(m,n) and Mij(m,n) indices contain the information that among the structural features, the contribution of the number of branches to the value of the index is the most important, except in the above mentioned diagonal transition domain, where the contribution of the ethyl groups, or of the position of branches, or of the separation between branches can be higher.

Correlation of tested Mj(m,n) and Mij(m,n) indices with the physicochemical properties of alkanes is not very good due to the too rapid increase or decrease of the index values with the size of molecule and/or branching. But, fine-tuning of exponents **m** and **n** may give better results.

There are several Mj(m,n) and Mij(m,n) indices which are potential sources of branching indices. In the plane of exponents **m** and **n** they are positioned in the regions characterized by:

Mj(m,n): **m** ≤ -1, -1 ≤ **n** < 1 and **m** ≥ 1, -1 < **n** ≤ 1

Mij(m,n): -6 ≤ **m** ≤ 1/3, -4 ≤ **n** < 1 and **m** ≥ 1/3, -1 < **n** ≤ 2.

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Povzetek

Indeksi Mj(m,n) in Mij(m,n) so izvedeni iz matrike v^{m}d^{n} z množenjem njenih nediagonalnih elementov. Zanje je značilno prehodno področje vzdolž diagonale na ravnini eksponentov **m** in **n**, opredeljene z zvezo **m** = -**n**. Nad tem diagonalnim prehodnim področjem vrednosti indeksov Mj(m,n) in Mij(m,n) naraščajo z velikostjo molekule in se manjšajo z naraščajočim razvejanjem. Pod diagonalnim prehodnim območjem je stanje obratno. Korelacije preizkušenih indeksov Mj(m,n) in Mij(m,n) s fizikokemijskimi lastnostmi alkanov presegajo |r| = 0,9 v 15 oz. 13 primerih od 23, ko upoštevamo alkane od propana do vključno oktanov ter v 12 oz. 8 primerih od 24, ko upoštevamo le oktane. Regularno zaporedje izomer pri večanju razvejanosti imajo indeksi Mj(m,n), ko je **m** ≤ -1, -1 ≤ **n** < 1 ter **m** ≥ 1, -1 < **n** ≤ 1 medtem ko je pri indeksih Mij(m,n) to pri -6 ≤ **m** ≤ $^{1}/_{3}$, -4 ≤ **n** < 1 ter **m** ≥ $^{1}/_{3}$, -1 < **n** ≤ 2.