SOME TOPOLOGICAL INDICES DERIVED FROM THE $v^m d^n$ MATRIX. PART 6. SUMMATION-DERIVED DIFFERENCE TYPE INDICES OF BI_A CLASS

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Abstract

The $^{\Delta}W_A(m,n)$ indices derived from the $v^m d^n$ matrix form a different group of topological indices of BI_A class than the $^{S}W_A(m,n)$ indices. Some of the $^{\Delta}W_A(m,n)$ indices correlate with the physicochemical properties ω, Tc^2/Pc, C, BP/Tc, and ΔHv having $|r| > 0.9$.

Introduction

Several hundred topological indices have been developed and tested for their performance as branching indices or indices of substances' properties.[1,2] Some succesful cases are for example the Wiener index,[3] the Randić index,[4] the largest eigenvalue of the adjaceny matrix,[5,6] etc. Important steps towards having better indices are also the VTI indices,[7] several new molecular matrices and other approaches to derive new indices,[8-20] as well as the development of a matrix that enables derivation of an infinite number of indices.[21]

The majority of these indices belongs to the so-called BI_M class indices. The BI_M class indices obey the *Methane based* definition of branching.[22] There has been proposed also the *n-Alkane based* definition of branching, which is a subdefinition of the *Methane based* definition of branching, expected to be more familiar to chemists working in this field. The indices obeying the *n-Alkane based* definition of branching were labelled BI_A class indices.

Two sets of BI_A indices have been tested recently, those derived from a set of most popular topological indices,[23,24] as well as the $^{S}W_A(m,n)$ indices,[25] which are the susceptibilities for branching of the W(m,n) indices.[26] The W(m,n) indices were derived by summation of the elements of the so-called $v^m d^n$ matrix.

In the present paper are evaluated the BI_A indices derived directly from the $v^m d^n$ matrix. This generalized matrix allows the derivation of an infinite number of indices and we present here the properties of 225 indices derived from it.

Data and methods

Notations

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. The other terms are explained on 2,2-, 2,3- and 2,5-dimethyl hexane (22M6, 23M6 and 25M6) as examples. The two branches (i.e. the number of branches, *Nbr* = 2) in 22M6 are positioned on a quaternary carbon (i.e. the number of branches on quaternary carbons, *Nq* = 2) placed on the periphery (*per*) of the molecule. The two branches in 23M6 and 25 M6 are positioned on tertiary carbons (i.e. the number of branches on tertiary carbons, *Nt* = 2). In 23M6 the branches are adjacent (*adj*) and those in in 25M6 are distant (*dist*). The branches on carbons No. 2 and 5 are placed on the periphery of the molecule, and the one on carbon No. 3 is placed near the centre (*ctr*) of the molecule.

The alkanes

Data for alkanes from propane through octanes were tested. Presented are the results obtained with octanes.

The physicochemical properties

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 refractivity index (n_D) were taken from the CRC Handbook[27] or from Lange's Handbook.[28] 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 (i.e. reduced BP), and the molar refraction (MR) were calculated from data presented in the handbooks.

The $^{\Delta}W_A(m,n)$ *indices*

The $^{\Delta}W_A(m,n)$ indices are topological indices derived from the so-called $v^m d^n$ matrix[26] by summing its elements separately on the right side of the main diagonal and separately on the left side of it, Eq. 1 and 2:

$$w_R = \sum(v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}})_{right} \quad (1)$$

$$w_L = \sum(v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}})_{left} \quad (2)$$

where v_j is the degree of vertex *j* (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). The difference of the calculated sums of matrix elements is then defined as the ${}^{\Delta}W_A(m,n)$ index, Eq. 3:

$${}^{\Delta}W_A(m,n) = w_L - w_R \quad (3)$$

Results

In a previous paper[26] we studied the W(m,n) indices, which were derived from the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix by summation of its elements. They are the BI_M class of indices, i.e. they obey the *Methane based* definition of branching. To derive the BI_A class of W(m,n) indices, i.e. the indices obeying the *n-Alkane based* definition of branching and labelled here as $W_A(m,n)$ indices, we have several possibilities. One of them is to use the susceptibility for branching[29] of the W(m,n) indices[26] as a group of $W_A(m,n)$ indices, the ${}^{S}W_A(m,n)$ indices.[25]

Another possibility is to derive the BI_A class indices directly from the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix by summing the matrix elements separately on the right side of the main diagonal and separately on the left side of it, Eq. 1 and 2. Their difference is then defined as a new BI_A class index, the ${}^{\Delta}W_A(m,n)$ index, Eq. 3. The choice of difference in Eq. 3 is arbitrary. There could also be $w_R - w_L$. In any case are some indices negative. Later in the paper we shall show that the absolute value of the difference should be defined as the ${}^{\Delta}W_A(m,n)$ index, Eq. 4:

$${}^{\Delta}W_A(m,n) = abs(\sum(v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}})_{left} - \sum(v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}})_{right}) \quad (4)$$

Characteristics of ${}^{\Delta}W_A(m,n)$ *indices*

The ${}^{\Delta}W_A(m,n)$ indices of *n*-alkanes are equal to zero since the matrices presenting their structure are symmetric. The ${}^{\Delta}W_A(m,n)$ indices of other alkanes are equal to zero when **m** = 0 for the same reason. The ${}^{\Delta}W_A(m,n)$ indices are integers only when **n** = -∞

or 0 or an integer and **m** = -∞ or an integer. As a consequence of their definition, the sign of the ${}^{\Delta}W_A(m,n)$ indices is the same as the sign of the exponent **m**. Other properties of the ${}^{\Delta}W_A(m,n)$ indices are presented below taking octanes as examples.

Degenerated ${}^{\Delta}W_A(m,n)$ *indices*

All ${}^{\Delta}W_A(0,n)$ indices are degenerated for reasons presented above. Highly degenerated are the ${}^{\Delta}W_A(-\infty,n)$ and the ${}^{\Delta}W_A(m,-\infty)$ indices. Few ${}^{\Delta}W_A(m,n)$ indices are degenerated when **m** = 2 or 3 and **n** = -2 or -1 or 1 or 2.

How the values of ${}^{\Delta}W_A(m,n)$ *indices depend on exponents* **m** *and* **n**

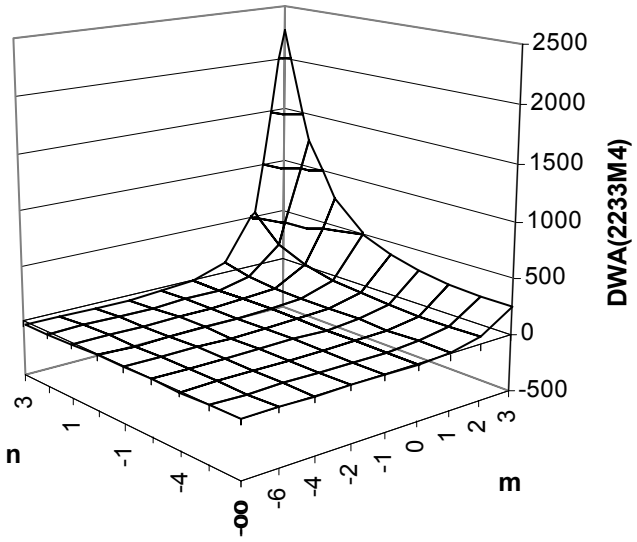

Fig. 1. The values of ${}^{\Delta}W_A(m,n)$ indices of 2,2,3,3-tetramethyl butane in the plain of exponents **m** and **n**. DWA ≡ ${}^{\Delta}W_A(m,n)$.

Fig. 1 serves as an illustration that the dependence of values of the ${}^{\Delta}W_A(m,n)$ indices on exponents **m** and **n** is train-like, whereas that of the ${}^{S}W_A(m,n)$ indices[25] has been shown to be saddle-like. The values of ${}^{\Delta}W_A(m,n)$ indices are high at high **m** and high **n** where they are for several orders of magnitude higher than the values of the ${}^{S}W_A(m,n)$ indices. The comparison of values of the ${}^{\Delta}W_A(m,n)$ indices of some octanes, e.g. 2M7 > 234M5 > 223M4 > 4M7 > etc., suggests that some structural features greatly influence the values of these indices. For example, when **m** ≤ 1 and **n** = 3, the most

different from the value of *n*-octane is the abs($^{\Delta}W_A(m,n)$) of 2-methyl heptane. When **m** = -6 and **n** = 2 this is true for 2,5-dimethyl hexane, when **m** ≥ 2 and **n** = 3 as well as when **m** ≥ -6 and **n** = 1 or 2 this is true for 2,2-dimethyl hexane, when **m** ≤ 4 and 0 < **n** <1 this is true for 2,2,4-trimethyl pentane, when -∞ < **m** ≤ -4 and **n** ~ 0 this is true for 2,3,4-trimethyl pentane, when -2 ≤ **m** ≤ 1 and 0 < **n** < 1 this is true for 2,2,3-trimethyl pentane, when **m** ≤ -2 and -1 < **n** < 0 this is true for 2,3,3-trimethyl pentane, and in other cases this is true for 2,2,3,3-tetramethyl butane.

On the other hand, the value of abs($^{\Delta}W_A(m,n)$) the least different from the value for the structure of *n*-octane has 4-methyl heptane when **m** > 1. The same is true for 3-ethyl-2-methyl pentane when **m** ≤ -2 and **n** ≥ 1, whereas in other cases, when 0 ≠ **m** ≠ 1 as well as when **n** ≠ -∞, this is true for 3-ethyl hexane.

How the structural features influence the $^{\Delta}W_A(m,n)$ *indices*

When we studied the physicochemical properties of alkanes we have shown that they are influenced by several structural features, e.g. by the size of molecule, by the number of branches, by the type of the branched structure, by the position of branches, by the separation between branches, etc.[22] By definition (see Eq. 3 and 4) all $^{\Delta}W_A(m,n)$ indices of *n*-alkanes are equal to zero. Thus the direct influence of the size of molecule is excluded. A qualitative presentation of the influence of particular structural features on the $^{\Delta}W_A(m,n)$ indices, based on sequences of isomers, is presented below.

Number of branches

Due to the definition in Eq. 3, the $^{\Delta}W_A(m,n)$ indices have without exception the same sign as the exponent **m**. If the position of the sum of the right part and of the left part of the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix would be interchanged then also the dependence of the sign of the $^{\Delta}W_A(m,n)$ indices on the sign of the exponent **m** would reverse. The sign observed using Eq. 3 has thus no fundamental importance. So the absolute values of the indices, abs($^{\Delta}W_A(m,n)$), calculated by Eq. 4, can be used as indices. Therefore, from this point on we consider only the absolute values of the $^{\Delta}W_A(m,n)$ indices.

Several octane isomers are presented by the $^{\Delta}W_A(m,n)$ indices as more branched than 2,2,3,3-tetramethyl butane, which is the most branched octane. The extreme situation among the tested indices is at the index $^{\Delta}W_A(-\infty,3)$ where 15 out of 18 octanes are presented as being more branched than 2,2,3,3-tetramethyl butane. This fact cannot be explained by the contribution of the number of branches. It shows, on the other hand, that the $^{\Delta}W_A(m,n)$ indices and the $^{S}W_A(m,n)$ indices[25] are two different groups of the BI_A class indices.

Position of branches

Regarding the influence of the position of branches we observe two cases. In a triangle at $\mathbf{m} < 1$ and $\mathbf{n} < 0$, there the octanes having the branches at or near the centre of molecule are presented by the $^{\Delta}W_A(m,n)$ indices as more branched than those having the branches at the periphery of the molecule, but the difference is small. The reverse is true at higher **m** and **n**, and the difference increases with **m** and especially with **n** being the highest at $^{\Delta}W_A(3,3)$. A transition region seems to exist between these regions. Some $^{\Delta}W_A(m,n)$ indices of octanes do not depend on the position of branches. These are the $^{\Delta}W_A(0,n)$ indices, the $^{\Delta}W_A(m,-\infty)$ indices, and the $^{\Delta}W_A(-\infty,0)$ index.

Separation between branches

Regarding the contribution of the separation between branches is the situation among the $^{\Delta}W_A(m,n)$ indices quite simple. The separation between branches does not influence the values of the $^{\Delta}W_A(m,-\infty)$, $^{\Delta}W_A(-\infty,n)$, and $^{\Delta}W_A(0,n)$ indices. The other $^{\Delta}W_A(m,n)$ indices indicate that an octane having a larger separation between branches is less branched. The highest influence in this direction is observed at high **m** and high **n**.

Type of branches

There are also some differences when the branches are of different type, i.e. whether a branch is methyl or ethyl. The indices $^{\Delta}W_A(m,-\infty)$, $^{\Delta}W_A(0,n)$, as well as the index $^{\Delta}W_A(-\infty,n)$ do not distinguish the influence of methyl from that of ethyl group. In majority of $^{\Delta}W_A(m,n)$ indices is presented the structure containing an ethyl group as less branched than a similar one containing a methyl group. Only at $\mathbf{m} > 1$ and $-\infty < \mathbf{n} < -1$

the contrary is the case. The reason for this is not clear at the moment but the difference in the degree of symmetry in molecules as well as in matrices might be expressed during derivation of ${}^{\Delta}W_A(m,n)$ indices since the symmetric parts of the matrices are eliminated during subtraction.

${}^{\Delta}W_A(m,n)$ *indices having special characteristics*

The values of indices ${}^{\Delta}W_A(0,n)$ are equal to zero. The index ${}^{\Delta}W_A(-\infty,-\infty)$ contains only the information about the number of branches. The indices ${}^{\Delta}W_A(m,-\infty)$, when $\mathbf{m} \neq -\infty$ or $\mathbf{m} \neq 0$, present the information that a structure containing a vertex of degree four is more branched than a structure containing two vertices of degree three (when $-\infty < \mathbf{m} < 1$), or equally branched as a structure containing three vertices of degree three (when $\mathbf{m} = 1$) or even more branched than a structure containing three vertices of degree three (when $\mathbf{m} > 1$). The indices ${}^{\Delta}W_A(-\infty,n)$, when $\mathbf{n} > -\infty$, contain the information about the number of branches, the position of branches as well as the type of branches.

Which ${}^{S}W_A(m,n)$ *indices could be good branching indices?*

There do not exist agreed criteria what characteristics should have a good branching index. Consequently, there exist several definitions of branching. One of the definitions is, for example, based on the Wiener[3] number,[30] some other ones are based on the leading eigenvalue of adjacency matrix,[5,6] or on the leading eigenvalue of path matrix.[11] We presented the *Methane based* definition of branching as well as the *n-Alkane based* one[22] and concluded that branching should not be defined by topological indices but by structural features of molecules as well as that a good branching index should have a regular, possibly an "ideal" sequence of all isomers.[25] In a regular sequence of isomers the influence of the number of branches should be higher than that of the position of branches, followed by the separation between branches and the type of the branched structure. An “ideal” sequence of octanes of increasing branching would be, e.g.,

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

which indicates that a centrally substituted alkane is more branched than a peripherally substituted one, or,

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

which indicates that a peripherally substituted alkane is more branched than a centrally substituted one. The sign can be either < as above, or >.

Among the ${}^{\Delta}W_A(m,n)$ indices, only few ones have a potentially regular sequence of isomers, i.e. those having $-4 < \mathbf{m} < {}^1/_3$ and $\mathbf{n} < -2$. Their sequences are:

n = -6, **m** = -2, -1; **n** = -4, **m** = -1:
Oct < 3E6 < 2M7 < 3M7 < 4M7 < 25M6 < 3E2M5 < 24M6 < 23M6 < 34M6 < 22M6 < 33M6 < 3E3M5 < 234M5 < 224M5 < 223M5 < 233M5 < 2233M4
n = -6, **m** = $-{}^1/_2$, $-{}^1/_3$, $-{}^1/_4$, $+{}^1/_4$; **n** = -4, **m** = $-{}^1/_2$, $-{}^1/_3$, $-{}^1/_4$:
Oct < 3E6 < 2M7 < 3M7 < 4M7 < 25M6 < 24M6 < 3E2M5 < 23M6 < 34M6 < 22M6 < 33M6 < 3E3M5 < 234M5 < 224M5 < 223M5 < 233M5 < 2233M4
n = -4, **m** = -2:
Oct < 3E6 < 2M7 < 3M7 < 4M7 < 25M6 < 3E2M5 < 24M6 < 23M6 < 34M6 < 22M6 < 3E3M5 < 33M6 < 234M5 < 224M5 < 223M5 < 233M5 < 2233M4

The ${}^{\Delta}W_A(m,n)$ indices have thus a lower potential to be good branching indices than the ${}^{S}W_A(m,n)$ indices[25] do.

Correlation between the ${}^{\Delta}W_A(m,n)$ *indices and physicochemical properties*

The intention of this paper is to indicate, which combinations of exponents' **m** and **n** values indicate the region of best correlation between the index values and the values of a number of physicochemical properties of octanes assuming a linear relationship. Fine-tuning of exponents to find the very best case is beyond the scope of present work, therefore only one indicator, the correlation coefficient is used to indicate the region of best exponents' combinations. Only five of 20 tested physicochemical properties correlate with $|r| > 0.9$ with tested ${}^{\Delta}W_A(m,n)$ indices of octanes, Table 1. All of them except ΔHv belong to those physicochemical properties considered as the best available primary references for branching.[29] In all cases in Table 1 the exponent **n** is negative, whereas the exponent **m** may be either positive or negative, depending on the physicochemical property in question. If we compare in this respect the ${}^{S}W_A(m,n)$ indices[25] and the ${}^{\Delta}W_A(m,n)$ indices, then we can see that in most cases the ${}^{S}W_A(m,n)$ indices correlate with tested physicochemical properties at least slightly better than the

$^{\Delta}W_A$(m,n) indices. The exceptions are the physicochemical properties A (r = 0.80), B (r = -0.74), and Tc (r = -0.72).

Table 1. Combinations of tested exponents in the $^{\Delta}W_A$(m,n) indices that give rise to the best correlations with values of selected physicochemical properties.

	m,n	r	**m,n**	r	**m,n**	r	**m,n**	r	**m,n**	r
ω	$^1/_2$,-4	-0.975	$^1/_3$,-4	-0.975	1,-4	-0.974	$^1/_4$,-4	-0.974	$^1/_2$,-6	-0.973
BP/Tc	1,-2	-0.930	$^1/_2$,-4	-0.928	$^1/_3$,-4	-0.928	$^1/_4$,-4	-0.928	$^1/_2$,-2	-0.928
Tc^2/Pc	-1,-4	0.969	-1,-6	0.969	-2,-4	0.969	-1,-∞	0.969	-2,-6	0.968
C	1,-∞	0.965	1,-6	0.965	1,-4	0.964	$^1/_2$,-∞	0.963	$^1/_2$,-6	0.962
ΔHv	$^1/_4$,-∞	-0.915	$^1/_3$,-∞	-0.915	$^1/_2$,-∞	-0.914	-$^1/_4$,-∞	0.914	-$^1/_3$,-∞	0.913

The information presented by the $^{\Delta}W_A$(m,n) *indices*

If we consider the information presented by the $^{\Delta}W_A$(m,n) indices we should start with the indices having the most reduced information content, the $^{\Delta}W_A$(0,n) indices. These indices present no information since $^{\Delta}W_A$(0,n) = 0 for all alkanes taken into consideration. Next to them is to be considered the index $^{\Delta}W_A$(-∞,-∞). It bears the information about the number of branches, *Nbr*, in the structure of the alkane, which is the most fundamental information regarding branching. This index can be considered as the most simple or primitive or degenerated, but a true branching index presenting only the most important contribution to branching of alkanes, cf. also ref.[26]

The simplest branching index, $^{\Delta}W_A$(-∞,-∞), is a member of two groups of indices, $^{\Delta}W_A$(m,-∞) and $^{\Delta}W_A$(-∞,n). For the indices of the group $^{\Delta}W_A$(m,-∞) it is easy to show that they are, Eq. 5,

$$^{\Delta}W_A(m,-\infty) = Nq\times(4^{\mathbf{m}}-1) + Nt\times(3^{\mathbf{m}}-1) \qquad 5$$

showing clearly that one branch on a quaternary carbon contributes more than one branch on a tertiary carbon. Thus, the indices $^{\Delta}W_A$(m,-∞) bear the information of the number of branches (*Nbr* = *Nq* + *Nt*) as well as of the type of the branched structure, i.e. whether the branch bearing carbons are tertiary (*t*) or quaternary (*q*), but nothing else.

The information contained in indices $^{\Delta}W_A$(-∞,n) is not as straightforward. For 3-ethyl-3-methyl pentane and 2,2,3,3-tetramethyl butane it can be shown that $^{\Delta}W_A(-\infty,n) = -(Nbr + 2^{n+2})$. For the other isomers only some qualitative conclusions can

be drawn at the moment. The type of the branched structure, i.e. whether the branch bearing carbons are tertiary or quaternary, as well as the separation between branches do not influence the ${}^{\Delta}W_A(-\infty,n)$ indices. On the other hand, isomers having equal number of branches as well as some similarities in the position of branches (equal distances of branches from the centre of the main chain regardless the side they are placed) have equal ${}^{\Delta}W_A(-\infty,n)$: 22M6 and 25M6, 23M6 and 24M6, 33M6 and 34M6, 223M5 and 234M5. At the same number of branches, when $\mathbf{n} > 0$, peripherally placed branches give rise to higher values of ${}^{\Delta}W_A(-\infty,n)$ than the centrally placed ones, etc. The reverse is true when $\mathbf{n} < 0$. Ethyl substituted isomers have in any case lower ${}^{\Delta}W_A(-\infty,n)$ values than methyl substituted ones. This is most easily seen at the ${}^{\Delta}W_A(-\infty,0)$ index, where it is also evident that an ethyl group placed on a tertiary carbon has a different contribution than on a quaternary carbon.

The series of isomers of indices ${}^{\Delta}W_A(-\infty,n>3)$: 0=Oct < 3Et2M5 < 3Et3M5 < 2233M4 < 3Et6 < 233M5 < 4M7 < 33M6 = 34M6 < 223M5 = 234M5 < 224M5 < 3M7 < 23M6 = 24M6 < 22M6 = 25M6 < 2M7 indicates that when $\mathbf{n} > 3$, then the equivalent position of branches relative to the centre of the molecule gives rise to equal values of ${}^{\Delta}W_A(-\infty,n)$.

Discussion

The ${}^{\Delta}W_A(m,n)$ indices considered here were found to be less suitable as branching indices as well as in most cases also less suitable as indices of physicochemical properties than the ${}^{S}W_A(m,n)$ indices,[25] which are the susceptibilities for branching[24,29] of the W(m,n) indices.[26] These groups of indices differ appreciably also in other characteristics. For this reason it can be reasonably expected that the ${}^{\Delta}W_A(m,n)$ indices may be useful in combination with the ${}^{S}W_A(m,n)$ or other indices. There is, on the other hand, also the question, whether the present "one spot" test is representative for all other possible indices of the ${}^{\Delta}W_A(m,n)$ type.

The ${}^{\Delta}W_A(m,n)$ indices considered here were derived from the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrices, which have the main diagonal elements $\mathbf{g}_{ii} = 0$ and the nondiagonal elements $\mathbf{g}_{ij}$ $(i \neq j) = v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}}$. In present case, the $v_j^{\mathbf{m}} \times d_{ij}^{\mathbf{n}}$ elements of the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrices are summed separately on the right side of the main diagonal and separately on the left side of it. The

absolute value of the sums' difference is then defined as a new BI_A class index, the $^{\Delta}W_A(m,n)$ index. This way of index derivation is useful only when the matrices are not symmetric, which is the case with the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix mentioned above. If we consider a more general matrix,[26] having the nondiagonal elements $\mathbf{g}_{ij}$ $(i\neq j) = v_i^{\mathbf{a}}\times v_j^{\mathbf{b}}\times d_{ij}^{\mathbf{c}}$, then in the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix $\mathbf{a} = 0$, $\mathbf{b} = \mathbf{m}$, and $\mathbf{c} = \mathbf{n}$. The matrix having the nondiagonal elements $\mathbf{g}_{ij}$ $(i\neq j) = v_i^{\mathbf{a}}\times v_j^{\mathbf{b}}\times d_{ij}^{\mathbf{c}}$, will be nonsymmetric when $\mathbf{a} \neq \mathbf{b}$, which is the case using the $v^{\mathbf{m}}d^{\mathbf{n}}$ matrix presented above. When $\mathbf{a} \neq \mathbf{b}$, there is in fact given different weight to the contribution of v_i than to v_j. Another way to give different weight to these contributions is to consider the matrices having the nondiagonal elements $\mathbf{g}_{ij}$ $(i\neq j) = (k_i\times v_i)^{\mathbf{a}}\times(k_j\times v_j)^{\mathbf{b}}\times d_{ij}^{\mathbf{c}}$, where k_i and k_j are constants. Whenever $k_i \neq k_j$ and/or $\mathbf{a} \neq \mathbf{b}$, the matrices are not symmetric and they are thus useful to derive the indices of the $^{\Delta}W_A(m,n)$ type. From this consideration follows that it is possible to derive a large number of sets of the $^{\Delta}W_A(m,n)$ indices and prior to concluding that they are all inferior to $^{S}W_A(m,n)$ or other indices, at least some additional sets of them are to be tested. A clue to properly choose the values of constants k_i and k_j, as well as of exponents **a**, **b**, and **c**, may be as follows: **c** should be negative and **a** should not be very different from **b**. By analogy, k_i should not be very different from k_j, but this assumption is still to be tested.

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Povzetek

Indeksi vrste ${}^{\Delta}W_A(m,n)$, izvedeni iz matrik $v^{\mathbf{m}}d^{\mathbf{n}}$, tvorijo drugačno skupino topoloških indeksov tipa BI_A kot indeksi ${}^{S}W_A(m,n)$. Nekateri od indeksov ${}^{\Delta}W_A(m,n)$ korelirajo s fizikokemijskimi lastnostmi ω, Tc^2/Pc, C, BP/Tc in ΔHv $z|r| > 0.9$.