Topological Indices Derived From Parts of a Universal Matrix

Anton Perdih*, Franc Perdih

Department of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, SI-1000 Ljubljana, Slovenia.
E-mail: Anton.Perdih@email.si

Abstract

Using the approach of mutual contribution of vertices to the value of topological indices derived from parts of a universal matrix gave the idea how to develop new topological indices. Some of the newly developed indices are useful indices of Octane Numbers and of Critical Pressure of alkanes of equal carbon number, giving rise to abs(R_{fit}) > 0.99. Using them we estimated the missing data of Octane Numbers of 2,3-dimethyl butane and 2,2,3,3-tetramethyl butane, as well as of nonanes and decanes. The best analogous indices derived from the reverse variants of this universal matrix are in general less useful. Some types of newly developed indices are also useful for structural interpretation of several known indices.

Key words: alkane, index, octane number, structural interpretation, topological matrix

Introduction

In a previous study,[1] several groups of indices were presented, which were derived from a generalized form of the vertex-degree vertex-distance matrix, denoted there as the **G**(a,b,c) matrix. This matrix is a universal matrix since it includes the distance matrix, the adjacency matrix, the reciprocal and several other types of matrices[1-10] and one of the reviewers suggested that it should be better denoted as the **U**(a,b,c) matrix. From this matrix can be derived a number of previously known indices, for example the Wiener index[11], the Randić index[12] as well as those introduced in ref.[13-22] In the same direction, by varying the exponent on the degree of vertices acted subsequently also Milićević and Nikolić,[23] who developed the variable Zagreb indices. Their $^{v}M_1$ resp. $^{v}M_2$ indices are equal to some W(m,n) indices[2] resp. to some Vij(m,n) indices.[8]

However, this universal matrix was introduced first by Ivanciuc[13,24] as the **Dval** matrix and its properties were described as well.[25] Therefore, wherever in present paper is mentioned the universal matrix, it is the **Dval**[13,24] matrix, but the indices derived from it are presented in the I(a,b,c) notation (a ≡ q, b ≡ r, c ≡ p) for easier comparison with the previously[1] tested ones.

In present paper are considered topological indices derived from this matrix by summation of *some* of its non-diagonal elements. Few groups of them, i.e. the VC(a,b,c) and VN_L(a,b,c) indices,[1] as well as the ΔV(a,b,c) indices[1,7] were presented earlier. Here are introduced some additional groups of them.

Data and notations

Physicochemical properties (PP)

The data for the boiling point (BP), density (d), the critical data Tc, Pc, Vc, Zc, αc, and dc, 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[26] or from Lange's Handbook.[27] The data for the liquid molar volume (Vm), the intrinsic molar volume (Vi), the intermolecular volume (V"), the ratios Tc²/Pc and Tc/Pc used instead of the van der Waals parameters a_0 and b_0, the ratio BP/Tc (reduced BP), the molar refraction (MR), cohesive energy density (CED) and its square root, the solubility parameter (Sol. par.) were calculated from data presented in the handbooks. The data for Octane Numbers (BON, MON, RON) were taken from: Balaban and Motoc,[28] Gutman et al.,[22] and Morley;[29] those for vapour pressure (logVP) from Goll and Jurs,[30] and those for the entropy (S) and quadratic mean radius (R^2) from Ren.[31] Surface tension (ST) data were taken from Li.[32]

Quality of results

The quality of linear relationships is expressed by fitted statistical parameters: number of data in the set, N, the correlation coefficient, R_{fit}, the standard error of estimate, S_{fit}, and Fisher's ratio, F. The results are also cross(internally)-validated by a leave-out-one, root mean square procedure, which is reflected in the sign of the cross-validated statistical parameters. Statistical

parameters for the cross-validated linear relationships are denoted R_{cv} and S_{cv}, where the subscript cv denotes cross-validation.

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.

Derivation of additional groups of indices from parts of a universal matrix

Lučić et al.[33] demonstrated the usefulness of structural interpretation[34-36] of topological indices for the development of new and better indices. However, structural interpretation introduced by Randić et al.[34-36] should be performed with caution, since it may happen that incomparable results are compared.[37] For the indices derived from *some* of the non-diagonal elements of the universal matrix, for example the VC(a,b,c), VN_L(a,b,c), and ΔV(a,b,c) indices,[1] the principle of the mutual contribution of graph vertices to the value of index[37] has been found appropriate to interpret these indices. Among these indices, the approach using the mutual contribution of graph vertices to the value of index gives rise to some symmetry related patterns in their structures, which are demonstrated in Figure 1 for pentanes. This type of symmetry relations is well expressed also among the structures of higher alkanes.

The symmetric pattern observed in Figure 1 at 2M4 is observed generally at 2-methyl alkanes, 3-ethyl alkanes, etc. Another interesting case is 3-ethyl-2-methyl pentane, which gives the pattern of what would be 3-*iso*propyl pentane. Furthermore, vertices of degree one contribute mutually only to the VC(a,b,c) indices, together with several other cases of mutual contribution of vertices of equal degree. Some exclusive mutual contributions of vertex pairs of different degree to the VN_L(a,b,c) and ΔV(a,b,c) indices have been observed as well.

Another reviewer raised the question, in which relation are mentioned indices to the symmetric and anti-symmetric part of the universal matrix. The answer is that the V(a,b,c) indices[1,8] can be derived from the symmetric part of the universal matrix but they contain all the information present in the universal matrix. The ΔV(a,b,c) indices,[1,7] on the other hand, can be derived from the anti-symmetric part of the universal matrix and they *do* contain the information of the anti-symmetric part of it. The VC(a,b,c) or VN_L(a,b,c) indices can not be derived from the symmetric or the anti-symmetric part of the universal matrix. They are defined to be derived from the left half of it.[1]

From the observation of the exclusive mutual contribution of vertex pairs of equal resp. different
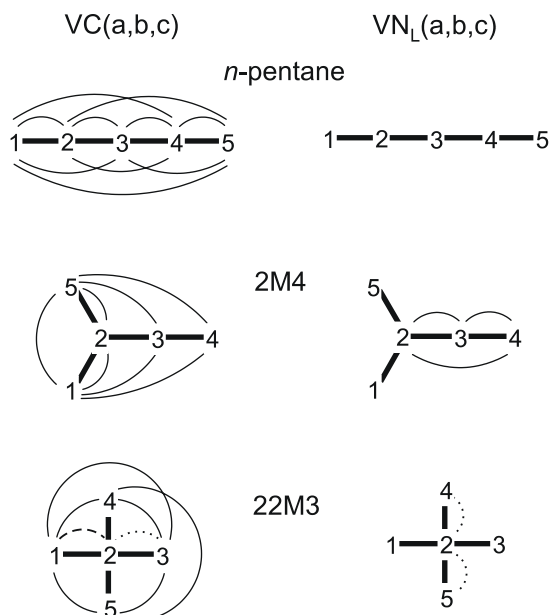
Figure 1. Mutual contribution of pairs of vertices (connected by curved lines) to the VC(a,b,c) resp. VN_L(a,b,c) indices in pentanes.

Dashed line (- - - -): contribution beyond any doubt, but other vertex pairs are to be checked for their inclusion to the VC(a,b,c) or VN_L(a,b,c) indices

Dashed-dotted line (- · - · - ·): contribution of vertex pairs either equivalent to those marked with the dashed line to the VC(a,b,c) indices or those not equivalent to them to VN_L(a,b,c) indices on grounds of structural similarity or dissimilarity

Dotted line (· · · · ·): contribution to the VC(a,b,c) or VN_L(a,b,c) indices based on the distance from the diagonal element 2-2 in the matrix

degree mentioned above, combining it with the idea of structural interpretation using the contribution of interior and terminal vertices[34-36] of the alkane graph, followed the idea:

1. Let us join the mutual contributions of pairs of interior vertices of equal degree,
2. Let us join the mutual contributions of pairs of interior vertices of different degree,
3. Let us join the mutual contributions of all vertices of different degree, which are not considered under point 2,
4. Let us join the mutual contributions of pairs of terminal vertices of degree one.

Doing it, we have four additional groups of indices, for which the mutual contribution of graph vertices to their value is indicated in Figure 2 for the structure of the 2,3-dimethyl pentane:

A(a,b,c): (Sum of matrix elements having $v_i = v_j > 1$)$_{left}$

B(a,b,c): (Sum of matrix elements having $v_i \neq v_j$ where (v_i *and* v_j) > 1)$_{left}$

C(a,b,c): (Sum of matrix elements having $v_i = 1$ and $v_j > 1$, or *vice versa*)$_{\text{left}}$

D(a,b,c): (Sum of matrix elements having $v_i = v_j = 1$)$_{\text{left}}$

These indices can be combined to give additional groups of indices:

$$AB(a,b,c) = A(a,b,c) + B(a,b,c)$$
$$AC(a,b,c) = A(a,b,c) + C(a,b,c)$$
$$AD(a,b,c) = A(a,b,c) + D(a,b,c)$$
$$BC(a,b,c) = B(a,b,c) + C(a,b,c)$$
$$BD(a,b,c) = B(a,b,c) + D(a,b,c)$$
$$CD(a,b,c) = C(a,b,c) + D(a,b,c)$$
$$ABC(a,b,c) = A(a,b,c) + B(a,b,c) + C(a,b,c)$$
$$ABD(a,b,c) = A(a,b,c) + B(a,b,c) + D(a,b,c)$$
$$ACD(a,b,c) = A(a,b,c) + C(a,b,c) + D(a,b,c)$$
$$BCD(a,b,c) = B(a,b,c) + C(a,b,c) + D(a,b,c)$$
$$ABCD(a,b,c) = A(a,b,c) + B(a,b,c) + C(a,b,c) +$$
$$D(a,b,c) \equiv V_L(a,b,c) \ (\text{ref.}[1])$$

VC(a,b,c)   VN$_L$(a,b,c)

A(a,b,c)   B(a,b,c)

C(a,b,c)   D(a,b,c)
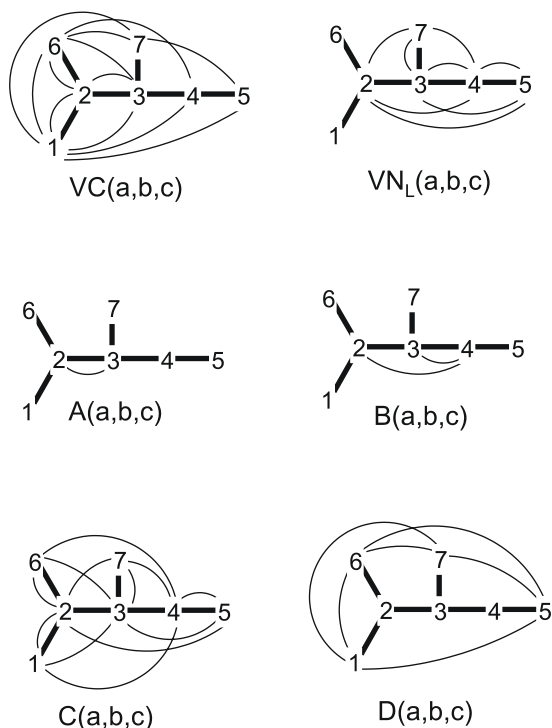
Figure 2. Mutual contribution of pairs of vertices (connected by curved lines) to the indices VC(a,b,c), VN$_L$(a,b,c), A(a,b,c), B(a,b,c), C(a,b,c), and D(a,b,c) in 2,3-dimethyl pentane (23M5).

The A(a,b,c), B(a,b,c), C(a,b,c), and D(a,b,c) indices of *n*-alkanes can be expressed analytically:

$$A(a,b,c)_n = 2^{a+b} \sum_{y=3}^{N-1} (N-y)(y-2)^c$$

$$B(a,b,c)_n = 0$$

$$C(a,b,c)_n = (2^a + 2^b) \sum_{y=2}^{N-1} (N-y)^c$$

$$D(a,b,c)_n = (N\text{-}1)^c$$

$$\begin{vmatrix} 0 \\ 3^a & 0 \\ 3^a\,2^c & \mathbf{3^a3^b} & 0 \\ 2^a\,3^c & \mathbf{2^a3^b\,2^c} & \mathbf{2^a3^b} & 0 \\ 4^c & 3^b\,3^c & 3^b\,2^c & 2^b & 0 \\ 2^c & 3^b & 3^b\,2^c & 2^b\,3^c & 4^c & 0 \\ 3^c & 3^b\,2^c & 3^b & 2^b\,2^c & 3^c & 3^c & 0 \end{vmatrix}$$

Figure 3. Left half of the universal (**Dval**[14,24]) matrix of 2,3-dimethylpentane in the (a,b,c) notation.

<u>**Bold**</u>: Matrix elements contributing to the A(a,b,c) indices
<u>**Bold**</u>: Matrix elements contributing to the B(a,b,c) indices
Italics: Matrix elements contributing to the C(a,b,c) indices
Normal script: Matrix elements contributing to the D(a,b,c) indices

Matrix elements, which at the 2,3-dimethylpentane structure contribute to the VC(a,b,c) resp. VN$_L$(a,b,c) indices were presented previously.[1] Those ones which contribute to the A(a,b,c), B(a,b,c), C(a,b,c), resp. D(a,b,c) indices are presented in Figure 3, from which can be deduced also the combinations that contribute to additional groups of indices defined above. At particular structures, the value of some indices is equal to zero: The indices A(a,b,c) of propane (Pr), 2M3, 2M4, 22M3, 22M4, 223M4, 224M5, 223M5, and 233M5, as well as the indices B(a,b,c) of *n*-alkanes, 2M3, 22M3, 23M4, 234M5, and 2233M4.

An infinite number of reverse analogues of the above-mentioned indices [$^{\text{BR}}$I(a,b,c) and $^{\text{IR}}$I(a,b,c) indices] can be derived from the universal matrix using the Reverse Distance Matrix[38] approach of Balaban et al.[19] where $d = d_{\text{max}} - d_{ij}$, which in our case becomes $^{\text{BR}}d_{ij} = d_{\text{max}} - d_{ij}$, and the Complementary Distance Matrix approach of Ivanciuc et al.[20] where $d = d_{\text{max}} + d_{\text{min}} - d_{ij}$, which in our case becomes $^{\text{IR}}d_{ij} = 1 + d_{\text{max}} - d_{ij}$.

Some of the newly derived indices present a clear structural characteristic:

Indices AB(a,b,c) represent the mutual contributions of all *interior* vertices. Indices C(a,b,c) represent the mutual contributions of vertex pairs composed of an *interior* and a *terminal* vertex. The D(a,b,c) indices represent the mutual contributions of all *terminal* vertices. Thusly, the indices AB(a,b,c), C(a,b,c), and D(a,b,c) can be used for this type of structural interpretation of other indices derived from the left half of the universal matrix. For indices derived from the whole universal matrix by summation of its nondiagonal elements, the indices AB(a,b,c) + AB(b,a,c), C(a,b,c) + C(b,a,c), and 2×D(a,b,c) can be used.

On the other hand, the AD(a,b,c) indices can be used to assess some symmetric aspects of other indices derived from the left half of the universal matrix, whereas the BC(a,b,c) indices can be used to assess some asymmetric aspects of other indices derived from the left half of the universal matrix. The $\Delta V(a,b,c)$ indices[1,7] (for whole-matrix indices like $V(a,b,c)$;[1] whereas $\frac{1}{2}\Delta V(a,b,c)$ for half-matrix indices like $V_L(a,b,c)$,[1]), can be used to assess the anti-symmetric aspects of other indices derived from the universal matrix, but only when the exponent $\mathbf{a} \neq \mathbf{b}$, which is not the case among many well-known indices, since they are derived from symmetric matrices.

From the universal matrix it is possible to derive also the indices, which represent a special case in structural interpretation, i.e. the concept of mutual contribution of vertices forming the *terminal bonds*.[34,35] These are the $C(a,b,-\infty)$ indices. Structures of all *n*-alkanes give rise to equal values of the terminal bond indices; therefore these indices are useful for the structural interpretation of indices of alkanes of the same size. However, while the $C(a,b,-\infty)$ indices represent the mutual contribution of vertices forming the terminal bonds, the $ABCD(a,b,-\infty)$ $(\equiv V_L(a,b,-\infty)$,[1]) indices represent the mutual contribution of all adjacent vertices, i.e. of all those forming the CC bonds in the alkane in question. Consequently, the difference $ABCD(a,b,c) - ABCD(a,b,-\infty)$ gives the mutual contribution of the non-adjacent vertices, whereas the difference $ABCD(a,b,c) - C(a,b,-\infty)$ gives the mutual contribution of all the vertices which do not form the terminal bonds.

The reverse analogues of terminal bond indices are $^{IR}T(a,b,c) = C(a,b, -\infty)*(d_{max} - 1)^c$, as well as $^{BR}T(a,b,c) = C(a,b, -\infty)*(d_{max} - 2)^c$, where $d_{max} = N - N_p + 1$; N is the carbon number of the alkane in question and N_p is the number of primary carbons in its structure (i.e. the number of vertices of degree one in its graph).

In a similar way as the summation-derived indices considered above, also the multiplication-derived indices can be derived and used. If we define:

$P_{[A]}(a,b,c)$: (Product of elements having $v_i = v_j > 1)_{left}$

$P_{[B]}(a,b,c)$: (Product of elements having $v_i \neq v_j$ where $(v_i$ *and* $v_j) > 1)_{left}$

$P_{[C]}(a,b,c)$: (Product of elements having $v_i = 1$ and $v_j > 1$, or *vice versa*$)_{left}$

$P_{[D]}(a,b,c)$: (Product of elements having $v_i = v_j = 1)_{left}$

Then,

$P_{[AB]}(a,b,c) = P_{[A]}(a,b,c) \times P_{[B]}(a,b,c)$

$P_{[ABCD]}(a,b,c) = P_{[A]}(a,b,c) \times P_{[B]}(a,b,c) \times P_{[C]}(a,b,c) \times P_{[D]}(a,b,c) [\equiv P_L(a,b,c), ref.^1]$

and the fractions of contributions interesting for interpretation are

$P_{[AB]}(a,b,c)/(P_{[ABCD]}(a,b,c))^{1/3}$,
$P_{[C]}(a,b,c)/(P_{[ABCD]}(a,b,c))^{1/3}$, and
$P_{[D]}(a,b,c)/P_{[ABCD]}(a,b,c))^{1/3}$.

Their product is equal to one.

Usefulness of new indices

The usefulness of indices derived from parts of the universal matrix by summation of the corresponding elements, based on data of 29 physicochemical properties of alkanes from propane to octanes inclusive is presented in Table 1 and 2, whereas the usefulness based on 31 physicochemical properties of octanes is presented in Table 3 and 4, where the absolute value of the highest observed correlation coefficient, $abs(R_{fit})_{max}$, of linear relationship of that type of index to the physicochemical property in question is indicated as a guide. The index giving rise to $abs(R_{fit})_{max} > 0.99$ accounts for > 98% of variance in the data set.

Among the physicochemical properties MR, Tc/Pc, and ω, the correlations of best ABC(a,b,c) indices are equal to those of best $V_L(a,b,c)$ indices. In both types of indices they appear at the same values of exponents **a**, **b**, and **c**. From this fact we can conclude that in these cases the mutual contribution of terminal vertices doesn't contribute any important information. Among BP/Tc, BP, ΔHv, ΔHf°g, Tc²/Pc, and logVP, the correlations of the best ABC(a,b,c) indices are better than those of the best $V_L(a,b,c)$ indices. In these cases, the mutual contribution of terminal vertices deteriorates the usefulness of the index. At Vc, the correlation of the best ABC(a,b,c) index is slightly worse than that of the best $V_L(a,b,c)$ index. Interesting is also that an AB(a,b,c) index indexes the best the surface tension of alkanes (ST), but only to $R_{fit} = 0.975$, which is worse than $R_{fit} = -0.986$ of $V^{2/N}(-\infty, 4.8, 3.0)$.[1]

The situation is quite different considering only octanes, Table 3 and 4. Besides some $V_L(a,b,c)$ indices, also some indices of the groups C(a,b,c), AB(a,b,c), BC(a,b,c), CD(a,b,c), ABC(a,b,c), and ABD(a,b,c) give rise to $abs(R_{fit})_{max} > 0.99$. This observation differs from that in the previous paper,[1] where among topological indices derived from the whole universal matrix or from its halves there was as a rule of thumb, $abs(R_{fit})_{max}$ at *n*-alkanes >> all alkanes from propane to octanes inclusive > octanes. Interesting is that most of the best members of these new index groups are the best indices of Octane Numbers (BON, MON, and/or RON), of BP/Tc and Pc, but not of Tc/Pc or Tc²/Pc. The best of them are BC(1.40, -0.50, 2.6) correlating to BON with $R_{fit} = -0.997$, ABC(1.14, 1.15, -3.1) correlating to BP/Tc with $R_{fit} = -0.997$, AB(1.41, 1.14, 0.53) correlating to RON with $R_{fit} = 0.995$, AB(1.50, 0.96, 1.42) correlating to MON with $R_{fit} = 0.994$, and ABD(1.83, 1.84, 1.68) correlating to Pc with $R_{fit} = 0.994$.

Table 1. Best correlations of indices derived from parts of the universal matrix with tested physicochemical properties of alkanes from **propane** to **octanes** inclusive.

abs(R_{fit})$_{max}$	0.90 → 0.95	0.95 → 0.99	> 0.99
Index			
$V_L(a,b,c)$,[1] ≡ ABCD(a,b,c)	n$_D$, **ST, d, RON**	**αc , C, B, Tc, Vm**	**logVP, Vc, ω, BP/Tc, ΔHf°g, BP, ΔHv, Tc²/Pc, Tc/Pc, MR**
VC(a,b,c)	MON, n$_D$, Pc, BON, αc, C, d, RON, ω, BP/Tc, Vm, B, Tc	BP, ΔHv, ΔHf°g, logVP, MR, Vc, Tc/Pc, Tc²/Pc	
A(a,b,c)	**BON, RON, MON**		
C(a,b,c)	MON, αc, RON, BON, Pc, B, C	**Tc**, BP/Tc, BP, ΔHv, logVP, Vc, Vm, ΔHf°g, Tc/Pc, Tc²/Pc, ω, MR	
D(a,b,c)	**ω, BP/Tc, Vm, ΔHf°g, MR, Tc²/Pc, Vc, Tc/Pc**		
AB(a,b,c)	αc, **ΔHf°g**, C, Vm, BP/Tc, **n$_D$, d**	Vc, **Tc, BP, MON, logVP, Tc/Pc**, ω, MR, **B, BON, ΔHv, RON**, Tc²/Pc, **ST**	
AC(a,b,c)	**ST**, BON, **n$_D$**, d, Pc, αc, C	**BP/Tc, Vm, B, ω, Tc**, logVP, Vc, **BP, ΔHv**, Tc/Pc, MR	**Tc²/Pc**
AD(a,b,c)	**ΔHv, BP, ω, logVP, Vm, BP/Tc, ΔHf°g, Tc/Pc, Vc, Tc²/Pc, MR**		
BC(a,b,c)	BON, C, Vm, Vc, BP/Tc, **B**, Tc/Pc	Tc, MR, ΔHv, ΔHf°g, logVP, BP, ω, Tc²/Pc	
BD(a,b,c)	**BP/Tc, ω, Vm, MR, ΔHf°g, Tc²/Pc, Vc, Tc/Pc**		
CD(a,b,c)	Pc, **d, αc**, C	BP/Tc, ω, **B**, Tc, Vm, **logVP, BP**, ΔHv, ΔHf°g, **Vc**, Tc/Pc, **MR, Tc²/Pc**	
ABC(a,b,c)	**V''**, BON, **ST**, n$_D$, **d, αc**	**C, B, Pc, Vm, Tc**	**logVP, Vc, ω, BP/Tc, BP, ΔHv, ΔHf°g, Tc²/Pc, MR, Tc/Pc**
ABD(a,b,c)	**MON, Pc**, Vm, **n$_D$, RON, αc, d**	C, ΔHf°g, **BP/Tc, BON**, Tc, Vc, **BP**, MR, B, ω, logVP, Tc/Pc, **ST, ΔHv**, Tc²/Pc	
ACD(a,b,c)	n$_D$, Pc, d, αc, C, BP/Tc, ω	Vm, B, Tc, BP, ΔHv, logVP, ΔHf°g, Vc, Tc/Pc, MR, Tc²/Pc	
BCD(a,b,c)	Pc, **d, αc**, C	**BP/Tc, B, ω**, Vm, Tc, ΔHv, **BP, logVP**, ΔHf°g, Vc, Tc/Pc, MR, Tc²/Pc	

B(a,b,c): No abs(R_{fit}) **>** 0.90 has been observed.
AB(a,b,c): The index does not exist at Pr, 2M3, and 22M3. Therefore, its value at these alkanes was set to be equal to zero.
Bold: Better than the best respective indices derived from the reverse types of universal matrix.

Table 2. Best correlations of indices considered here with tested physicochemical properties of alkanes from **propane** to **octanes** inclusive having abs(R_{fit})$_{max}$ > 0.99; ($V_L(a,b,c) ≡$ ABCD(a,b,c)).

PP	I(a,b,c)	N	R_{fit}	R_{cv}	S_{fit}	S_{cv}	F	
Tc/Pc	ABC(0.86, -0.40, -∞)	38	0.9991	0.9990	1.48	1.61	21038	=
	V_L (0.86, -0.40, -∞)	38	0.9991	0.9990	1.48	1.61	21038	
MR	ABC(1.06, -0.093, -∞)	38	0.9988	0.9983	0.304	0.356	15089	=
	V_L (1.06, -0.093, -∞)	38	0.9988	0.9983	0.304	0.356	15089	
Tc²/Pc	ABC(0.182, -0.170, -∞)	38	0.9981	0.9975	1583	1799	9537	>
	V_L (-0.0109, -0.46, -3.4)	38	0.9981	0.9976	1601	1801	9351	
ΔHf°g	ABC(1.61, -0.33, -4.3)	38	0.9974	0.9970	0.525	0.555	6825	>
	V_L (-0.28, 0.136, -∞)	38	0.9934	0.9925	0.830	0.879	2710	
ΔHv	ABC(-0.49, -0.48, -∞)	38	0.9969	0.9961	0.074	0.079	5743	>
	V_L (-0.50, -0.59, -5.09)	38	0.9966	0.9961	0.077	0.082	5330	
BP	ABC(-0.50, -0.37, -6.2)	38	0.9950	0.9940	4.19	4.53	3574	>
	V_L (-0.61, -0.54, -4.7)	38	0.9950	0.9894	4.19	4.56	3559	
BP/Tc	ABC(0.62, -0.92, -∞)	38	0.9945	0.9907	0.0018	0.0020	3254	=
	V_L (0.62, -0.92, -∞)	38	0.9945	0.9907	0.0018	0.0020	3254	
ω	ABC(0.32, -1.12, -∞)	38	0.9936	0.9931	0.0066	0.0068	2789	=
	V_L (0.32, -1.12, -∞)	38	0.9936	0.9931	0.0066	0.0068	2789	
Vc	ABC(1.00, -0.34, -∞)	38	0.9924	0.9917	0.0090	0.0093	2339	<
	V_L (0.98, -0.38, -5.1)	38	0.9924	0.9917	0.0090	0.0093	2346	
logVP	ABC(-0.52, -0.44, -∞)	37	-0.9905	0.9891	0.0941	0.0993	1819	>
	V_L (-0.55, -0.50, -6.1)	37	-0.9905	0.9892	0.0944	0.0996	1811	

=, >, and <, meaning *equal to*, *better than* resp. *worse than*, refer to the absolute values of non-rounded data relative to the half-matrix index $V_L(a,b,c)$ presented in this Table.

Table 3. Best correlations of indices derived from parts of the universal matrix with tested physicochemical properties of **octanes**.

abs(R_{fit})$_{max}$	0.90 → 0.95	0.95 → 0.99	> 0.99
Index			
V_L(a,b,c),[1] ≡ ABCD(a,b,c)	**BP, ST, ΔHf°g, V", Vm**	ΔHv, **R²**, d, n$_D$, S, Pc, C, Tc²/Pc, BON	**MON, RON, BP/Tc, ω, Tc/Pc**
VC(a,b,c)	BP/Tc, Vm, V", Pc, C, ω, Tc²/Pc, d, S	RON, BON, Tc/Pc, n$_D$, MON	
VN$_L$(a,b,c)	ΔHf°g, BP, BP/Tc, S, ΔHv, R²	MON, ω, Tc²/Pc, BON, C, RON	
A(a,b,c)	**Vm, V", RON, R², BON, MON, d**	**n$_D$**	
C(a,b,c)	**ST, BP, Pc**	**ΔHf°g, ΔHv, R²**, S, **C, BP/Tc, ω, Tc²/Pc**	**RON, Tc/Pc, MON, BON**
D(a,b,c)	**R², BP/Tc, S, C, Pc, ω, BON, Tc²/Pc, RON**	**Tc/Pc, MON**	
AB(a,b,c)	**BP, ΔHf°g, ΔHv, ST, C, S, V", Vm**	**d, R², n$_D$, ω, BP/Tc, Tc/Pc, Tc²/Pc, Pc, MON**	**BON, RON**
AC(a,b,c)	**αc, ST, V", Vm, BP, ΔHf°g, d, ΔHv, Pc**	**S, C, R², n$_D$, ω, BP/Tc, Tc²/Pc, Tc/Pc, BON, RON, MON**	
AD(a,b,c)	**R², BP/Tc, V", Vm, S, C, Pc, d, ω, BON, Tc²/Pc, RON**	**Tc/Pc, MON, n$_D$**	
BC(a,b,c)	**ST, Pc, BP, ΔHf°g, ΔHv**	S, **BP/Tc, R², Tc/Pc**, C, ω, **Tc²/Pc, RON**	**MON, BON**
BD(a,b,c)	**R², BP/Tc, ΔHv, Pc, MON, S**	**C, Tc/Pc, BON, ω, Tc²/Pc, RON**	
CD(a,b,c)	**ST, BP**	**R², ΔHf°g, ΔHv, Pc**, S, **C, BP/Tc, Tc²/Pc, BON**	**MON, Tc/Pc, ω, RON**
ABC(a,b,c)	**BP, ST, ΔHf°g, V", Vm**	**ΔHv, d, R²**, S, **n$_D$**, Pc, C, **Tc²/Pc**	**BON, MON, RON, ω, Tc/Pc, BP/Tc**
ABD(a,b,c)	**BP, ΔHf°g, ΔHv, ST, S, C**	**V", Vm, R², d, n$_D$, ω, BP/Tc, Tc/Pc, Tc²/Pc**	**BON, MON, Pc, RON**
ACD(a,b,c)	**ST, V", Vm, BP, ΔHf°g, d, Pc, ΔHv, R²**, BP/Tc	S, **n$_D$**, C, **Tc/Pc, Tc²/Pc, ω, BON, MON**	**RON**
BCD(a,b,c)	**ST, BP, ΔHf°g, Pc**	**ΔHv, R²**, S, C, **BP/Tc, ω, Tc/Pc, Tc²/Pc, MON, BON**	**RON**

B(a,b,c): No abs(R_{fit}) **>** 0.90 has been observed.
Bold: Better than the best respective indices derived from the reverse types of universal matrix.

Table 4. Best correlations of indices considered here with tested physicochemical properties of **octanes** having abs(R_{fit})$_{max}$ > 0.99.

PP	I(a,b,c)	N	R_{fit}	R_{cv}	S_{fit}	S_{cv}	F	
BON	BC(1.40, -0.50, 2.6)	17	-0.9973	0.9971	2.52	2.60	2790	>
	C(1.07, -0.060, 2.3)	17	0.9956	0.9943	3.23	3.68	1687	>
	ABC(0.77, 0.35, 1.45)	17	-0.9944	0.9926	3.64	4.18	1326	>
	AB(1.30, 1.13, 0.74)	17	0.9924	0.9901	4.24	4.84	974	>
	ABD(1.30, 1.24, 0.42)	17	0.9902	0.9874	4.81	5.41	754	>
	V$_L$(0.69, 0.150, 1.03)	17	-0.9884	0.9852	5.24	5.86	633	
MON	C(1.61, 0.36, 3.0)	17	0.9943	0.9927	3.60	4.11	1307	>
	ABC(1.43, 0.61, 2.1)	17	-0.9941	0.9925	3.65	4.17	1268	>
	AB(1.50, 0.96, 1.42)	17	0.9940	0.9922	3.68	4.25	1248	>
	ABD(1.17, 0.94, 0.92)	17	0.9934	0.9915	3.86	4.42	1133	>
	BC(1.83, -0.37, 3.2)	17	-0.9933	0.9921	3.89	4.24	1115	>
	V$_L$(1.12, 0.109, 2.1)	17	-0.9928	0.9906	4.06	4.65	1025	
	CD(1.58, -0.64, 3.2)	17	-0.9903	0.9875	4.70	5.37	761	<

Table 4. Continued

	I(a,b,c)							
RON	[IR]CD(0.32, -1.44, 0.160)	17	0.9951	0.9939	3.63	4.05	1530	>
	AB(1.41, 1.14, 0.53)	17	0.9950	0.9934	3.69	4.25	1475	>
	CD(-3.2, -1.12, -3.2)	17	0.9941	0.9929	3.99	4.36	1260	>
	V_L(-2.4, -0.67, -3.8)	17	0.9940	0.9926	4.04	4.44	1229	
	ABD(1.40, 1.28, 0.31)	17	0.9938	0.9920	4.08	4.68	1206	<
	ABC(1.03, 0.45, 1.09)	17	-0.9934	0.9918	4.22	4.71	1125	<
	[BR]CD(1.99, 0.71, 0.040)	17	0.9929	0.9909	4.39	4.96	1042	<
	C(1.37, 0.71, -0.42)	17	0.9923	0.9898	4.57	5.28	958	<
BP/Tc	ABC(1.14, 1.15, -3.1)	18	-0.9965	0.9956	0.00073	0.00082	2290	>
	V_L(1.15, 1.10, -2.8)	18	-0.9964	0.9955	0.00074	0.00083	2233	
Tc/Pc	V_L(1.10, 1.02, 1.05)	18	-0.9984	0.9979	0.47	0.54	4951	
	ABC(1.39, 1.35, -0.82)	18	-0.9978	0.9972	0.55	0.62	3614	<
	ABC(1.45, 1.47, 0.40)	18	-0.9976	0.9971	0.57	0.63	3329	<
	C(1.33, 1.15, 1.98)	18	0.9922	0.9900	1.03	1.15	1020	<
	CD(0.52, 0.00, 2.1)	18	0.9907	0.9879	1.13	1.27	847	<
ω	V_L(-0.108, -0.22, -1.20)	18	-0.9973	0.9966	0.0028	0.0031	2914	
	ABC(0.46, 0.76, 3.8)	18	-0.9960	0.9951	0.0034	0.0037	1969	<
	ABC(0.42, 0.52, -4.8)	18	-0.9959	0.9950	0.0034	0.0038	1942	<
Pc	ABD(1.83, 1.84, 1.68)	18	0.9937	0.9919	0.14	0.16	1259	>
	V_L(1.32, 0.67, -1.63)	18	0.9733	0.9641	0.29	0.32	288	

> resp. <, meaning *better than* resp. *worse than*, refer to the absolute values of non-rounded data relative to the half-matrix index V_L(a,b,c) presented in this Table.

Considering only octanes, there perform the best those indices, which present a clear structural characteristic. Among them, the best ones of the indices AB(a,b,c) (presenting only mutual contributions of all *interior* vertices) and the best ones of the indices C(a,b,c) (presenting contributions of vertex pairs composed of an *interior* and a *terminal* vertex) perform better than the best ones of the indices D(a,b,c), which present only the mutual contributions of *terminal* vertices.

Cross-validation supports the validity of results presented in Table 2 and 4. Some members of groups of these indices are thus promising indices of some physicochemical properties of alkanes. Considering the Octane Numbers, Table 5, they give rise to better results than the three-parameter correlations of Hosoya.[39]

Table 5. Best correlations of indices considered here with Octane Numbers of heptanes (C_7) and octanes (C_8).

ON	I(a,b,c)	C_7		C_8	
		R_{fit}	S_{fit}	R_{fit}	S_{fit}
BON	BC(2.1, -0.057, 2.8)	-0.998	**2.2**	-0.992	4.2
	BC(1.40, -0.50, 2.6)	-0.996	3.2	**-0.997**	**2.5**
	C(1.61, 0.48, 2.5)	-0.996	**3.1**	-0.992	4.3
	C(1.07, -0.060, 2.3)	-0.994	3.8	**-0.996**	**3.2**
MON	BC (1.92, -0.26, 3.3)	**-0.996**	**3.0**	-0.993	3.9
	BC (1.83, -0.37, 3.3)	-0.996	3.1	**-0.993**	**3.9**
	AB(1.17, 0.65, 1.59)	**-0.992**	**4.3**	-0.991	4.6
	AB(1.50, 0.96, 1.42)	-0.990	4.9	**-0.994**	**3.7**
RON	AB(1.27, 0.79, 0.98)	**-0.990**	**5.0**	-0.991	5.0
	AB(1.44, 1.17, 0.51)	-0.983	6.6	**-0.995**	**3.7**

Using the best indices in Table 5 we estimated the missing data of Octane Numbers in the set in use. RON of 2,3-dimethyl butane (23M4) is estimated to be 92.1. For 2,2,3,3-tetramethyl butane (2233M4), the estimation gives the following values: BON = 117.4 and 122.9; MON = 116.0 and 117.2; RON = 137.5. The most promising index derived from the reverse types of the universal matrix, [IR]CD(0.32, -1.44, 0.160), gives rise to RON = 139. Values estimated by extrapolation using the best observed indices have to be checked by independent approaches. In present case few of them are available. On the one hand, RON values of 2233M4 estimated here are comparable to RON = 135 estimated by Hosoya.[39] On the other hand, experimental[29] BON values of 2233M5 and 2233M6 are similar to BON of 2233M4 estimated here. Thusly, our estimated values seem to be quite close to the real ones.

The pattern of Octane Numbers, where the estimated values for 2,2,3,3-tetramethylbutane are also included, is presented in Figure 4 for heptanes and octanes.

Considering all alkanes from propane to octanes inclusive, the best indices derived from the universal (**Dval**[13,24]) matrix are in general better than the best ones derived from the reverse types of this matrix. The physicochemical property, for which the best indices derived from the universal matrix are evidently better than the best ones derived from the reverse types of the universal matrix, is the surface tension of alkanes.

Considering only octanes, there are the best indices derived from the universal matrix in general better than the best ones derived from the reverse types of the universal matrix, as well. Exceptions are noticed mainly at physicochemical properties C, ω, and S, where 0.95 < abs(R_{fit}) < 0.99 is observed.
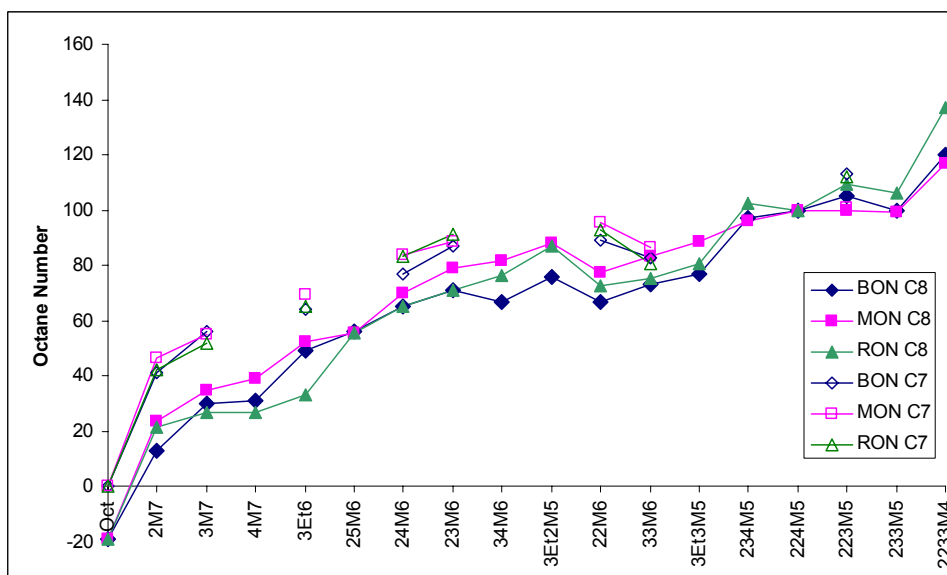
Figure 4. The pattern of Octane Numbers (BON, MON, RON) of heptanes and octanes. For 2233M4 the values estimated by new indices considered here (see text) are taken.

The correlation of the best indices that contain only the information of the mutual contribution of vertices, which are involved in terminal CC bonds, i.e. of the C(a,b,-∞) indices, to the values of physicochemical properties of octanes is remarkable but in all cases abs(R_{fit}) < 0.99. Noticeable is the fact that all of the best indices of this type correlate the best i.a. with measures of the Octane Number.

Estimation of BON of nonanes and decanes

The existence of quite good indices of Octane Numbers of octanes, giving rise to (R_{fit}) = -0.994 to -0.997, S_{fit} = 3.7 to 2.5, Table 5, is encouraging. Namely, since there do exist good indices of Octane Numbers of octanes, then it can be reasonably expected that there exist also good indices of Octane Numbers of nonanes and decanes and that these good indices will be among those ones, which correlate well with available data. However, there are available only few data of Octane Numbers of nonanes and decanes, i.e. six BON data of nonanes[29] as well as of decanes[29] and only three RON data of nonanes.[39] Therefore, the estimation of Octane Numbers of these groups of alkanes is an extremely risky task.

There is also another problem. Besides 2,5,5- and 3,3,5-trimethylheptane, also the values of BON of *n*-nonane and *n*-decane are outliers in the plot of Morley[29] as well as in comparison with other *n*-alkanes.

Nonanes

If, in analogy to *n*-octane, where the change of value proved successful,[39] we estimate the BON value of *n*-nonane to be not -17 as presented by Morley[29] but

possibly around -30, which follows from the regression of Morley's[29] k and BON data, or even -38, which follows from the approx. linear decrease of BON values with the size of *n*-alkane as observed in BON data from *n*-pentane to *n*-octane, then we obtain the best indices for nonanes to be those presented in Table 6.

The pattern of results obtained using these indices is illustrated in Figure 5 based on BON_{Non} = -30. The best C(a,b,c) indices mentioned in Figure 5 seem to

Table 6. The best indices for BON of nonanes.

BON_{Non}	Index	R_{fit}	S_{fit}
none	ABC(0.96, 2.2, -0.56)	0.999614	0.55
	ABC(0.72, 1.78, -∞)	0.998528	1.07
	V_L(1.07, 2.2, -0.48)	0.999516	0.61
	V_L(-0.51, 1.59, -3.3)	0.998604	1.04
-17[30]	C(1.12, 1.30, -0.160)	0.998385	3.14
	C(0.54, 0.65, -1.13)	0.997915	3.57
	V_L(-1.43, -0.089, -∞)	0.997951	3.53
-30	C(1.08, 1.26, -0.079)	0.998523	3.31
	C(-0.33, 0.113, -∞)	0.997610	4.30
	V_L(-1.52, -0.115, -∞)	0.996665	4.97
	V_L(-∞, -1.29, -3.3)	0.993622	6.87
-38	C(1.02, 1.20, -0.084)	0.998587	3.43
	C(-0.37, 0.088, -∞)	0.997230	4.79
	V_L(-1.57, -0.128, -∞)	0.995749	5.94
	V_L(-∞, -1.20, -3.4)	0.993028	7.60
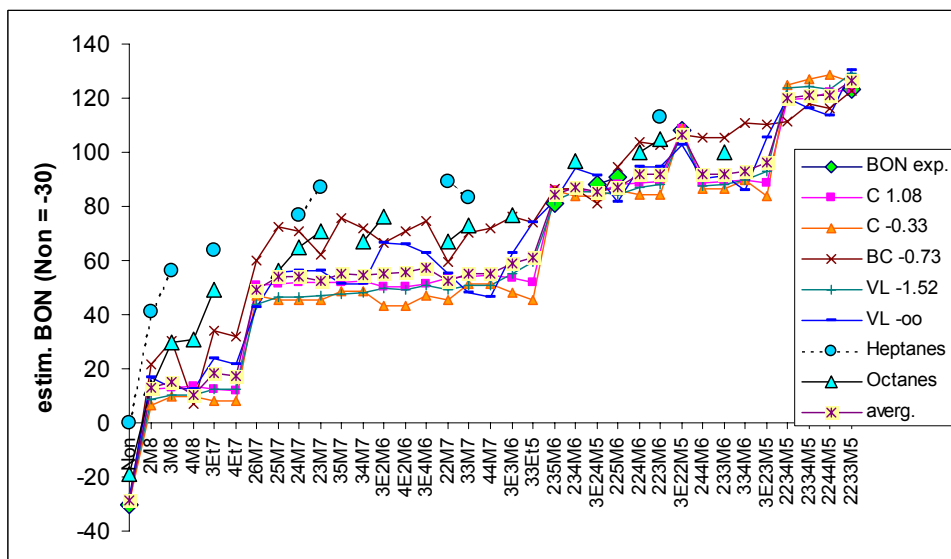
Figure 5. Estimated BON values of nonanes, taking BON_{Non} = -30. Indices: C(1.08, 1.26, -0.079), C(-0.33, 0.113, -∞), BC(-0.73, 0.74, -1.16), V_L(-1.52, -0.115, -∞), V_L(-∞, -1.29, -3.3).

present the *lower limit* of possible BON values. To help judging the upper limit, the BON values of heptanes and octanes having the same type of the branched structure were taken in consideration. Since no octane having the same type of branched structure has a higher BON value than the corresponding heptane, the same rule seems plausible also for nonanes.

Thus, the *upper limit* of plausible BON values of nonanes present the BON values of octanes. To estimate better the Octane Numbers of nonanes, the average of estimated values is taken and it is presented in Table 7.

When no value of *n*-nonane is considered among the input data, only the interpolated results seem promising, whereas those extrapolated towards less branched nonanes are obviously too high, higher than those of octanes since the apparently best indices taken into account do not index all the curvature of the relation of ON vs. structure. As an example: the result for BON_{Non} = 50.

Some other indices, correlating quite well to available BON data of nonanes, proved useless since they give rise to an evidently unacceptable scatter of results. One of them is e.g. V_L(4.6, 1.89, 0.89), correlating to available data of nonanes with R_{fit} = 0.9989, S_{fit}= 3.05, but giving rise to some improbable results such as BON_{2244M5} = 365, BON_{244M6} = 208, BON_{26M7} = 99, BON_{223M6} = -24, BON_{2iPr6} = -48. Among decanes a still worse situation is among V_L(0.35, 0.00, -4.7), correlating to available data of decanes with R_{fit} = -0.9995, S_{fit}= 2.08, but giving rise to BON_{3E22M6} = 1043, $BON_{22344M5}$ = -1417, as well as among V_L(0.79, 0.00, -5.1), correlating to available data of decanes with R_{fit} = -0.9939, S_{fit} = 6.90, but giving rise to BON_{3E22M6} = 674, $BON_{22344M5}$ = -1643.

Table 7. Estimated BON values of nonanes, derived as the average of values calculated from the indices mentioned in text.

BON_{Non}		none	-17	-30	-38
Nonane	BON^{30}				
Non	-17		-16	-29	-36
2M8			18	13	6
3M8			20	15	7
4M8			20	10	7
3Et7			19	18	10
4Et7			18	17	9
26M7			51	49	43
25M7			53	54	47
24M7			53	54	48
23M7			54	53	48
35M7			54	55	48
34M7			55	55	48
3E2M6			54	55	51
4E2M6			53	56	50
3E4M6			55	57	51
22M7			56	53	48
33M7			58	55	48
44M7			59	55	48
3E3M6			59	59	53
33Et5			58	61	56
235M6	81	82	85	84	84
234M6		87	87	87	88
3E24M5	88	87	86	85	87
225M6	91	91	87	87	84
224M6		95	88	92	88
223M6		100	90	92	88
3E22M5	108	108	108	107	107
244M6		92	90	92	88
233M6		98	91	92	88
334M6		99	92	93	89
3E23M5		103	92	96	93
2234M5		109	119	120	123
2334M5		109	121	121	123
2244M5		108	120	121	122
2233M5	123	123	125	126	128

Decanes

If, in analogy to *n*-octane, where the change of value proved successful,[39] we estimate the BON value of *n*-decane to be not -41 as presented by Morley[29] but possibly -30, which follows from the regression of Morley's[29] k and BON data, or -57, which follows from the approx. linear decrease of BON values with the size of *n*-alkane as observed in BON data from *n*-pentane to *n*-octane, we obtain the best indices of BON to be those presented in Table 8.

Table 8. The best indices to indicate BON values of decanes at supposed values of BON_{Dec}.

BON_{Dec}	Index	R_{fit}	S_{fit}
none	C(3.0, -1.59, 2.0)	-0.999739	1.12
	AC(3.0, -∞, 2.1)	-0.999798	0.99
	AC(3.6, -0.71, 1.74)	-0.999385	1.72
	BC(3.0, -4.7, 2.0)	-0.999636	1.32
-31	AC(3.0, -3.2, 2.0)	-0.999092	2.54
-41[30]	C(2.8, -∞, 2.3)	-0.992804	7.53
	AC(3.0, -2.9, 2.1)	-0.998550	3.38
	AC(3.6, -1.14, 2.0)	-0.999395	2.19
	BC(2.6, -∞, 2.1)	-0.992559	7.65
-57	AC(3.2, -1.63, 1.92)	-0.999268	2.62
	AC(3.5, -0.99, 1.85)	-0.999986	0.37

The indices C(2.8, -∞, 2.3) and BC(2.6, -∞, 2.1) seem to give the most plausible results. A similar conclusion holds also in other cases, i.e. when the value of BON_{Dec} is omitted as well as when it is taken to be BON_{Dec} = -31 or -57. The best C(a,b,c) indices seem on the one hand to present the lower limit of possible BON values and on the other hand to indicate on average the most plausible estimated BON values of decanes.

Table 9. Estimated BON values of decanes, means of best results.*

BON_{Dec}**		none	-31	-41	-57
Decane	BON[30]				
Dec	-41	-2	-30	-37	-57
2M9		53	47	37	50
3M9		48	37	30	34
4M9		37	25	20	18
5M9		22	10	5	2
3Et8		52	42	37	39
4Et8		45	36	32	33
4Pr7		42	33	29	32
27M8	20	20	21	14	20
26M8		45	44	38	43
25M8		65	63	58	65
24M8		80	79	72	84
23M8		90	91	83	101
36M8		39	37	33	37
35M8		59	55	52	57
34M8		74	71	66	74
45M8	48	48	44	42	46
5E2M7		45	44	38	51

Table 9. Continued

4E2M7	70	69	64	76
5E3M7	47	45	41	50
3E2M7	85	84	78	92
3E4M7	76	73	70	76
4E3M7	70	68	65	72
4iPr7	18	17	18	22
34Et6	71	68	67	73
22M8	94	92	86	95
33M8	76	71	70	68
44M8	45	39	42	32
3E3M7	79	74	74	72
33Et6	80	76	77	76
4E4M7	50	45	49	40
236M7	70	71	68	64
246M7	60	60	58	54
235M7	90	91	88	89
245M7	79	80	78	78
234M7	105	106	103	110
345M7	73	73	72	75
3E25M6	83	83	81	83
4E23M6	84	84	81	92
3E24M6	98	98	96	102
3iPr2M6	44	45	48	50
226M7	74	77	73	84
225M7	94	95	92	100
224M7	109	110	106	114
223M7	119	121	116	127
255M7	31	32	33	38	32
244M7	76	77	79	77
233M7	107	109	106	113
335M7	77	75	75	76	77
334M7	91	90	91	90
344M7	70	69	73	67
4E22M6	82	82	78	92
3E22M6	105	105	102	112
4E33M6	76	75	76	78
4E24M6	63	63	65	67
3E23M6	101	100	100	104
3E34M6	91	91	92	91
33E2M5	90	89	90	95
3iPr24M5	62	62	68	56
2345M6	95	95	95	89
2245M6	98	100	100	104
2235M6	109	111	110	112
2234M6	124	126	124	129
2335M6	97	98	100	94
2344M6	91	93	97	91
2334M6	112	113	114	112
3E224M5	107	108	107	114
3E234M5	103	104	105	104
2255M6	51	52	59	37
2244M6	96	96	100	88
2233M6	126	127	128	128	127
3344M6	77	77	85	70
3E223M5	110	110	111	112
22344M5	102	103	109	98
22334M5	123	124	126	121

* Average values obtained using indices:
**BON_{Dec} = none: C(3.0, -1.59, 2.0), AC(3.0, -∞, 2.1), BC(3.0, -4.7, 2.0)
**BON_{Dec} = -31: AC(3.0, -3.2, 2.0)
**BON_{Dec} = -41: C(2.8, -∞, 2.3), AC(3.0, -2.9, 2.1), BC(2.6, -∞, 2.1)
**BON_{Dec} = -57: AC(3.2, -1.63, 1.92), AC(3.5, -0.99, 1.85)
** Assumed BON_{Dec}

Using these indices, we get the estimation of BON values of decanes, which is presented in Table 9. Having Table 7 and 9, let us wait for additional experimental data to check the validity of derived values. Comparison of known ON data based on structural features of alkanes, however, indicates that several values estimated above are plausible.[40]

Conclusions

Structural interpretation of indices does give better understanding of the background of their characteristics. The new approach to their structural interpretation using the concept of mutual contribution of vertices proved useful for indices derived from parts of halves of a universal (**Dval**[13,24]) matrix. It gave rise to new ideas how to develop new indices from this matrix. Some of these new indices proved useful for structural interpretation of other (e.g. known) indices derived from this matrix, whereas several ones proved to be useful indices of a number of physicochemical properties of alkanes, especially of Octane Numbers.

References

1. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2004**, *51*, 598-609.
2. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2002**, *49*, 67-110.
3. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2002**, *49*, 291-308.
4. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2002**, *49*, 309-330.
5. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2002**, *49*, 467-482.
6. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2002**, *49*, 497-514.
7. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2003**, *50*, 83-94.
8. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2003**, *50*, 95-114.
9. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2003**, *50*, 161–184.
10. A. Perdih, B. Perdih, *Acta Chim. Slov*. **2003**, *50*, 513-538.
11. H. Wiener, *J. Am. Chem. Soc*. **1947**, *69*, 17-20.
12. M. Randić, *J. Am. Chem. Soc*. **1975**, *97*, 6609-6615.
13. O. Ivanciuc, *Rev. Roum. Chim*. **1999**, *44*, 519-528.
14. I. Gutman, N. Trinajstić, *Chem. Phys. Lett*. **1972**, *17*, 535-538.
15. L. Lovasz, J. Pelikan, *Period. Math. Hung*. **1973**, *3*, 175-182.
16. D. M. Cvetković, I. Gutman, *Croat. Chem. Acta* **1977**, *49*, 115-121.
17. O. Ivanciuc, *Rev. Roum. Chim*. **1989**, *34*, 1361-1368.
18. M.V. Diudea, *J. Chem. Inf. Comput. Sci*. **1997**, *37*, 292-299.
19. A. T. Balaban, D. Mills, O. Ivanciuc, S. C. Basak, *Croat. Chem. Acta*. **2000**, *73*, 923-941.
20. O. Ivanciuc, T. Ivanciuc, A.T. Balaban *ACH-Models Chem*. **2000**, *137*, 57-82.
21. O. Ivanciuc, *J. Chem. Inf. Comput. Sci*. **2000**, *40*, 1412-1422.
22. I. Gutman, W. Linert, I. Lukovits, Ž. Tomović, *J. Chem. Inf. Comput. Sci*. **2000**, *40*, 113-116.
23. A. Miličević, S. Nikolić, *Croat. Chem. Acta* **2004**, *77*, 97-101
24. O. Ivanciuc, *Rev. Roum. Chim*. **2000**, *45*, 587-596.
25. O. Ivanciuc, Topological indices. In: *Handbook of Chemoinformatics*, Ed.: J. Gasteiger, Wiley-VCH, 2003, pp. 981-1003.
26. D. R. Lide, *CRC Handbook of Chemistry and Physics*, 76th Ed., CRC Press, Boca Raton 1995-96.
27. J. A. Dean, *Lange's Handbook of Chemistry*, McGraw-Hill, New York 1985.
28. A. T. Balaban, I. Motoc, *MATCH (Commun. Math. Chem.)* **1979**, *5*, 197-218.
29. C. Morley, *Combust. Sci., Technol*. **1987**, *55*, 115-123.
30. E. S. Goll, P.C. Jurs, *J. Chem. Inf. Comput. Sci*. **1999**, *39*, 1081-1089.
31. B. Ren, *J. Chem. Inf. Comput. Sci*. **1999**, *39*, 139-143.
32. X. H. Li, *Chem. Phys. Lett*. **2002**, *365*, 135-139.
33. M. Randić, J. Zupan, *J. Chem. Inf. Comput. Sci*. **2001**, *41*, 550-560.
34. M. Randić, A. T. Balaban, S. C. Basak, *J. Chem. Inf. Comput. Sci*. **2001**, *41*, 593-601.
35. M. Randić, *Indian J. Chem*. **2003**, *42A*, 1207-1218.
36. B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, *Croat. Chem. Acta* **2002**, *75*, 847-868.
37. A. Perdih, B. Perdih, *Indian J. Chem*. **2003**, *42A*, 1219-1226.
38. M. Randić, *New J. Chem*. **1997**, *21*, 945-951.
39. H. Hosoya, *Croat. Chem. Acta*. **2002**, *75*, 433-445.
40. A. Perdih, F. Perdih, *Acta Chim. Slov*. in press.

Povzetek

S pristopom vzajemnega doprinosa parov točk v grafu alkana k vrednosti topoloških indeksov izvedenih iz splošne matrike sva razvila nove topološke indekse iz delov njenih polovic. Nekateri od teh indeksov so videti uporabni indeksi oktanskih števil in kritičnega tlaka alkanov z enakim številom ogljikovih atomov, saj dajejo abs(R_{fit})$_{max}$ > 0.99. Z njihovo pomočjo sva ocenila manjkajoče podatke oktanskih števil za 2,3-dimetil butan, 2,2,3,3-tetrametil butan, nonane in dekane. Indeksi, izvedeni iz obrnjenih oblik splošne matrike so na splošno manj uporabni. Nekateri od novih indeksov so uporabni tudi za razlago znanih indeksov.