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# Wiener-Type Topological Indices

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A unified approach to the Wiener topological index and its various recent modifications, is presented. Among these modifications particular attention is paid to the Kirchhoff, Harary, Szeged, Cluj and Schultz indices, as well as their numerous variants and generalizations. Relations between these indices are established and methods for their computation described. Correlation of these topological indices with physico-chemical properties of molecules, as well as their mutual correlation are examined.

## INTRODUCTION

Half a century ago, in 1947, Harold Wiener published a paper[1] entitled *»Structural Determination of Paraffin Boiling Points«*. In this work the quantity $W_e$, eventually named Wiener index or Wiener number was introduced for the first time. (Note that in the great majority of chemical publications dealing with the Wiener number it is denoted by $W$. Nevertheless, in this paper we use the symbol $W_e$ in order to distinguish between the Wiener index and other Wiener-type indices.) Using the language which in theoretical chemistry emerged several decades after Wiener, we may say that $W_e$ was conceived as the sum of distances between all pairs of vertices in the molecular graph of an alkane, with the evident aim to provide a measure of the compactness of the respective hydrocarbon molecule.

In 1947 and 1948, Wiener published a whole series of papers[1–5] showing that there are excellent correlations between $W_e$ and a variety of physico-chemical properties of organic compounds. Nevertheless, progress in this field of research was by no means fast. It took some 15 years until Stiel and

Thodos[6] became the first scientists apart from Wiener to use $W_e$. Only in 1971 Hosoya[7] gave a correct and generally applicable definition of $W_e$. In 1975/76 Rouvaray and Crafford[8,9] re-invented $W_e$, which shows that even at that time the Wiener-number-concept was not widely known among theoretical and mathematical chemists.

Finally, somewhere in the middle of the 1970s, the Wiener index began to rapidly gain popularity, resulting in scores of published papers. In the 1990s, we are witnesses of another phenomenon: a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to $W_e$.

The aim of this article is to provide an introduction to the theory of the Wiener index and a systematic survey of various Wiener-type topological indices and their interrelations.

In order to achieve this goal, we first need to remind the readers of a few elementary facts of the chemical graph theory.

## MOLECULAR GRAPHS

The branch of mathematics that studies graphs is called graph theory.[10] A graph is a mathematical object that consists of two sorts of elements: vertices and edges. Every edge corresponds to a pair of vertices, in which case the respective two vertices are said to be adjacent. Not every pair of vertices need to be adjacent.

It is usual (although not necessary) to represent a graph by means of a diagram. In such a diagram the vertices are drawn either as small cycles or as big dots. The edges are then indicated by means of lines which connect the respective two adjacent vertices.

In Figure 1, three graphs, $G_1$, $G_2$ and $G_3$, are depicted. Graphs $G_1$ and $G_2$ have 12 vertices each whereas $G_3$ has 11 vertices.

Nowadays, graph theory has numerous applications in such diverse fields as electrotechnics, sociology, nuclear physics, computer science, ethnology, engineering, geography, linguistics, biology, transportation, and par-

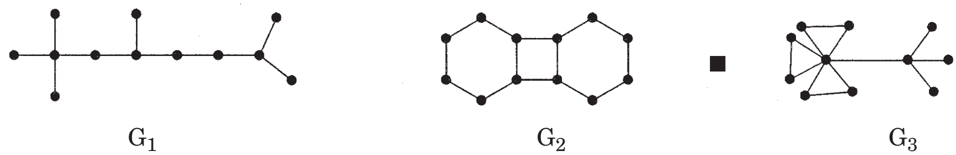
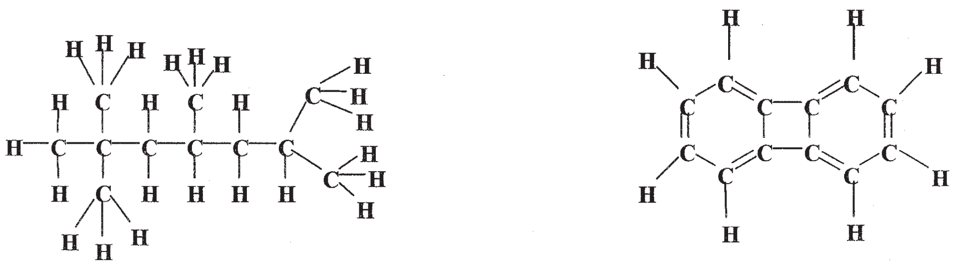



Figure 1. Examples of graphs; note that $G_1$ and $G_2$ are molecular graphs whereas $G_3$ is not.

ticularly in chemistry. Numerous books[11–18] and review articles[19–23] have been written on the applications of graphs in chemistry. The applications are based on the fact that a very close analogy exists between a structural formula and a graph. In Figure 2, the structural formulas of 2,2,4,6-tetramethylheptane (**I**) and diphenylene (**II**) are depicted. These formulas should be compared with graphs $G_1$ and $G_2$. Evidently, $G_1$ and $G_2$ can be understood as the graph representations of the carbon-atom skeletons of 2,2,4,6-tetramethylheptane and biphenylene, respectively. In this respect, we say that $G_1$ is the molecular graph of 2,2,4,6-tetramethylheptane whereas $G_2$ is the molecular graph of biphenylene. (Note that the hydrogen atoms and the double bonds are disregarded in $G_1$ and $G_2$. This is not necessary, but has proved to be very convenient in practice). Recall that a molecular graph is necessarily connected. [14,16]

There are, of course, graphs that are not molecular graphs; an example is $G_3$ in Figure 1.



**I** **II**

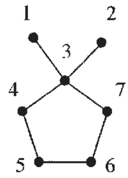
Figure 2. Structural formulas of 2,2,4,6-tetramethylheptane and diphenylene; their molecular graphs are $G_1$ and $G_2$ from Figure 1.

## THE WIENER INDEX

In order to define the Wiener index, we have to explain the notion of distance in a graph.

Let G be an undirected connected graph and let its vertices be labeled by 1,2, ...,$n$. Let $i_0$, $i_1$, $i_2$, ..., $i_k$ be $k$+1 distinct vertices of graph G, so that for $j$ = 1,2, ...,$k$, $i_{j-1}$ and $i_j$ are adjacent. Then, vertices $i_0$, $i_1$, $i_2$, ..., $i_k$ form a path in graph G, whose length is $k$. The length of the shortest path connecting vertices $x$ and $y$ is called the distance between these vertices and is denoted by $D_{xy}$. In G, the distance is a metric, hence the following relations hold: $D_{xy} = 0$ if and only if $x = y$; $D_{xy} = D_{yx}$ and $D_{xy} + D_{yz} \geq D_{xz}$.

Consider graph $G_4$ depicted in Figure 3 as an example, this is the molecular graph of 1,1-dimethylcyclopentane. The sequence 2,3,7,6,5 is a path in $G_4$ connecting vertices 2 and 5 and having length 4. This, however, is not the shortest path between 2 and 5. There is, namely, another path 2,3,4,5 that has a length of only 3. Because 2,3,4,5 is the shortest path between vertices 2 and 5, we have $D_{25} = 3$.




$G_4$

Figure 3. The molecular graph of 1,1-dimethylcyclopentane.

At this point, the reader may check that for graph $G_4$,

$$\begin{aligned} D_{12} = 2,\ D_{13} = 1,\ D_{14} = 2,\ D_{15} = 3,\ D_{16} = 3,\ D_{17} &= 2 \\ D_{23} = 1,\ D_{24} = 2,\ D_{25} = 3,\ D_{26} = 3,\ D_{27} &= 2 \\ D_{34} = 1,\ D_{35} = 2,\ D_{36} = 2,\ D_{34} &= 1 \\ D_{45} = 1,\ D_{46} = 2,\ D_{47} &= 2 \\ D_{56} = 1,\ D_{57} &= 2 \\ D_{67} &= 1\ . \end{aligned}$$

Numbers $D_{xy}$, $x = 1,2, ..., N$, $y =1,2, ..., N$ define a square symmetric matrix of order $N$, which in this paper will be denoted by $\mathbb{D}_e$.

Now, the Wiener index is equal to the sum of distances between all pairs of vertices of the respective graph:

$$W_e = W_e(G) = \Sigma_{x<y} D_{xy}\ . \tag{1}$$

In view of the above calculated distances in graph $G_4$, we have,

$$\begin{aligned} W_e(G_4) = {} & (2 + 1 + 2 + 3 + 3 + 2) + (1 + 2 + 3 + 3 + 2) + \\ & + (1 + 2 + 2 + 1) + (1 + 2 + 2) + (1 + 2) + (1) = 39. \end{aligned}$$

Such a direct calculation of the Wiener number may look very easy, and it is so only when the number of vertices of the graph considered is small. In the case of larger molecular graphs it would be very hard and impractical to compute the Wiener number from its definition, Eq. (1). Therefore, various methods[24] have been designed, by which $W_e$ can be obtained in a much more efficient way, usually by means of computers. These computational details will not be outlined here.

## CHEMICAL APPLICATIONS OF THE WIENER INDEX

In his first paper[1] Wiener used his index, $W_e$, for the calculation of the boiling points of alkanes. Wiener's formula for the boiling points (bp) reads:

$$\mathrm{bp} = \alpha W_e + \beta P + \gamma \tag{2}$$

where $\alpha$, $\beta$ and $\gamma$ are empirical constants and $P$, the polarity number, is the number of pairs of vertices whose distance is equal to 3. In a subsequent series of papers,[2–5] Wiener pointed out the versatility of his index $W_e$ in structure-property investigations.[3] He used $W_e$ to predict boiling points, molar volumes, refractive indices, heats of isomerization and heats of vaporization of alkanes.

Since 1976, the Wiener number has found a remarkable variety of chemical applications. These, as well as the underlying mathematical theory, are outlined in due detail in several monographs[12,13,15] and numerous review articles.[18,22,24–27] Anyway, the Wiener index happens to be one of the most frequently and most successfully employed structural descriptors that can be deduced from the molecular graph.

It has been recently demonstrated[28] that the Wiener index measures the area of the surface of the respective molecule and thus reflects its compactness. As a consequence, $W_e$ is related to the intermolecular forces,[18,29,30] especially in the case of hydrocarbons where polar groups are absent.

Physical and chemical properties of organic substances, which can be expected to depend on the area of the molecular surface and/or on the branching of the molecular carbon-atom skeleton, are usually well correlated with $W_e$. Among them are the heats of formation, vaporization and atomization, density, boiling point, critical pressure, refractive index, surface tension and viscosity of various, acyclic and cyclic, saturated and unsaturated as well as aromatic hydrocarbon species, velocity of ultra sound in alkanes and alkohols, rate of electroreduction of chlorobenzenes *etc*.[27] Correlations between $W_e$ and melting points were also reported, but here the results were not completely satisfactory. Of particular practical importance is the prediction of the behaviour of organic substances in gas chromatography. For instance, chromatographic retention times (CRT) of monoalkyl- and *o*-dialkylbenzenes can be modeled by $W_e$:[31]

$$\mathrm{CRT} = \alpha {W_e}^{\beta} + \gamma \tag{3}$$

where $\alpha$, $\beta$ and $\gamma$ are empirically determined parameters (different, of course, from those in Eq. (2)). Some other examples can be given.

Since the pharmacological activity of a substance is related to some of its physico-chemical properties, it is not surprising that attempts have been made to use $W_e$ in designing new drugs.[32–34] Lukovits established correlations between $W_e$ and cytostatic and antihistaminic activities of certain pharmacologically interesting compounds, as well as between $W_e$ and their estron-binding affinities.[33] Recently he employed $W_e$ in the study of the $n$-octanol/water partition coefficient (indicator of transport characteristics and interaction between receptor and bioactive molecule),[34] a physico-chemical parameter of profound importance for the forecasting of pharmacological activity of many compounds.

For work on the Wiener index of benzenoid hydrocarbons see the recent review.[35]

## WIENER MATRIX, HYPER-WIENER INDEX AND RELATED QUANTITIES

For acyclic structures, the Wiener index[1] $W_e$ and its extension, the hyper-Wiener index[36], $W_p$, can be defined as

$$W_e = W_e(\mathrm{G}) = \Sigma_e\, N_{i,e}\, N_{j,e} \tag{4}$$

$$W_p = W_p(\mathrm{G}) = \Sigma_p\, N_{i,p}\, N_{j,p} \tag{5}$$

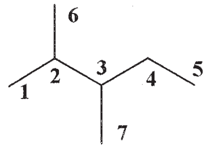
where $N_i$ and $N_j$ denote the number of vertices lying on two sides of the edge **e** or path **p,** respectively; here and later **e** and **p** denote an edge and a path, respectively, having endpoints **i** and **j**. Eq. (4) follows the method of calculation given by Wiener himself[1]: »Multiply the number of carbon atoms on one side of any bond by those on the other side; $W_e$ is the sum of those values for all bonds«.

Edge and path contributions, $N_{i,e}\, N_{j,e}$ and $N_{i,p}\, N_{j,p}$ are just entries in the Wiener matrices,[37,38] $\mathbb{W}_\mathrm{e}$ and $\mathbb{W}_\mathrm{p}$, (see Figure 4) from which $W_e$ and $W_p$, can be calculated by:

$$W_e = (1/2)\ \Sigma_i\, \Sigma_j\, [\mathbb{W}_\mathrm{e}]_{ij} \quad \text{and} \quad W_p = (1/2)\ \Sigma_i\, \Sigma_j\, [\mathbb{W}_\mathrm{p}]_{ij}\,. \tag{6}$$

Recall that by definition $[\mathbb{W}_\mathrm{e}]_{ii} = [\mathbb{W}_\mathrm{p}]_{ii} = 0$ for all **i**. Also, if **i** and **j** are not adjacent vertices, then the ($ij$)-entry of matrix $\mathbb{W}_\mathrm{e}$ is zero. Note that $\mathbb{W}_\mathrm{e}$ is the Hadamard product[39] (see symbol •) between $\mathbb{W}_\mathrm{p}$ and the adjacency matrix: $\mathbb{W}_\mathrm{e} = \mathbb{W}_\mathrm{p} \bullet \mathbb{A}$. Recall that the ($ij$)-entry of the Hadamard product of matrices $\mathbb{X}$ and $\mathbb{Y}$ is equal to the product of the ($ij$)-entries of $\mathbb{X}$ and of $\mathbb{Y}$.

Note that, in the above formulas, numbers (*i.e.,* topological indices) are denoted by boldface italic symbols derived from the name of matrices, whereas matrices (and their entries) by special capital letters. The reason




$G_5$

$\mathbb{D}_e$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 2 | 3 | 4 | 2 | 3 | 15 |
| 2 | 1 | 0 | 1 | 2 | 3 | 1 | 2 | 10 |
| 3 | 2 | 1 | 0 | 1 | 2 | 2 | 1 | 9 |
| 4 | 3 | 2 | 1 | 0 | 1 | 3 | 2 | 12 |
| 5 | 4 | 3 | 2 | 1 | 0 | 4 | 3 | 17 |
| 6 | 2 | 1 | 2 | 3 | 4 | 0 | 3 | 15 |
| 7 | 3 | 2 | 1 | 2 | 3 | 3 | 0 | 14 |

$W_e = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_e]_{ij} = 46$

$\mathbb{W}_e$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 6 |
| 2 | 6 | 0 | 12 | 0 | 0 | 6 | 0 | 24 |
| 3 | 0 | 12 | 0 | 10 | 0 | 0 | 6 | 28 |
| 4 | 0 | 0 | 10 | 0 | 6 | 0 | 0 | 16 |
| 5 | 0 | 0 | 0 | 6 | 0 | 0 | 0 | 6 |
| 6 | 0 | 6 | 0 | 0 | 0 | 0 | 0 | 6 |
| 7 | 0 | 0 | 6 | 0 | 0 | 0 | 0 | 6 |

$W_e = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{W}_e]_{ij} = 46$

$\mathbb{D}_p$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 3 | 6 | 10 | 3 | 6 | 29 |
| 2 | 1 | 0 | 1 | 3 | 6 | 1 | 3 | 15 |
| 3 | 3 | 1 | 0 | 1 | 3 | 3 | 1 | 12 |
| 4 | 6 | 3 | 1 | 0 | 1 | 6 | 3 | 20 |
| 5 | 10 | 6 | 3 | 1 | 0 | 10 | 6 | 36 |
| 6 | 3 | 1 | 3 | 6 | 10 | 0 | 6 | 29 |
| 7 | 6 | 3 | 1 | 3 | 6 | 6 | 0 | 25 |

$W_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_p]_{ij} = 83$

$\mathbb{W}_p$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 6 | 4 | 2 | 1 | 1 | 1 | 15 |
| 2 | 6 | 0 | 12 | 6 | 3 | 6 | 3 | 36 |
| 3 | 4 | 12 | 0 | 10 | 5 | 4 | 6 | 41 |
| 4 | 2 | 6 | 10 | 0 | 6 | 2 | 2 | 28 |
| 5 | 1 | 3 | 5 | 6 | 0 | 1 | 1 | 17 |
| 6 | 1 | 6 | 4 | 2 | 1 | 0 | 1 | 15 |
| 7 | 1 | 3 | 6 | 2 | 1 | 1 | 0 | 14 |

$W_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{W}_p]_{ij} = 83$

$\mathbb{SZ}_u$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | 3 | 3 | 1 | 3 | 12 |
| 2 | 6 | 0 | 3 | 3 | 5 | 6 | 3 | 26 |
| 3 | 4 | 4 | 0 | 5 | 5 | 4 | 6 | 28 |
| 4 | 4 | 2 | 2 | 0 | 6 | 4 | 2 | 20 |
| 5 | 2 | 2 | 1 | 1 | 0 | 2 | 2 | 10 |
| 6 | 1 | 1 | 1 | 3 | 3 | 0 | 3 | 12 |
| 7 | 4 | 1 | 1 | 1 | 5 | 4 | 0 | 16 |
| | 21 | 11 | 9 | 16 | 27 | 21 | 19 | |

$SZ_e = \Sigma_e\ [\mathbb{SZ}_u]_{ij}\ [\mathbb{SZ}_u]_{ji} = 46$

$SZ_p = \Sigma_p\ [\mathbb{SZ}_u]_{ij}\ [\mathbb{SZ}_u]_{ji} = 151$

$\mathbb{SZ}_u$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 6 |
| 2 | 6 | 0 | 3 | 3 | 3 | 6 | 3 | 24 |
| 3 | 4 | 4 | 0 | 5 | 5 | 4 | 6 | 28 |
| 4 | 2 | 2 | 2 | 0 | 6 | 2 | 2 | 16 |
| 5 | 1 | 1 | 1 | 1 | 0 | 1 | 1 | 6 |
| 6 | 1 | 1 | 1 | 1 | 1 | 0 | 1 | 6 |
| 7 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 6 |
| | 15 | 10 | 9 | 12 | 17 | 15 | 14 | |

$CJ_e = \Sigma_e\ [\mathbb{CJ}_u]_{ij}\ [\mathbb{CJ}_u]_{ji} = 46$

$CJ_p = \Sigma_p\ [\mathbb{CJ}_u]_{ij}\ [\mathbb{CJ}_u]_{ji} = 83$

Figure 4. Distance-, Wiener-, Szeged- and Cluj-type matrices and derived Wiener-type indices for graph $G_5$.

for such a notation comes from the aim to suggest that different graph-theoretical properties are related to particular matrices.

Indices $W_e$ and $W_p$ count all »external« paths[40] passing through the two endpoints of all edges and paths, respectively, in the graph.

Attempts have been made to extend the »edge contribution« definition (4) to cycle-containing structures,[41–43] such as:

$$W_e = (1/2)\ \Sigma_{i\Sigma j}\ C^e_{ij} \,/\, C_{ij} \tag{7}$$

where $C_{ij}$ is the number of the shortest paths joining vertices **i** and **j**, and $C^e_{ij}$ denotes the number of those shortest paths between **i** and **j** which contain edge **e**. For the $W_p$ contributions, Lukovits and Linert[40] have proposed a definition, which resulted in a variant of the hyper-Wiener index.

Another definition[7,44] of Wiener-type numbers is based on the distance matrix, which, for reasons that will become clear later on, will be denoted by $\mathbb{D}_{\mathrm{e}}$ (see Figure 4). Following the procedure of Klein, Lukovits and Gutman,[40] the path analogue of the distance matrix is defined[44] as

$$[\mathbb{D}_{\mathrm{p}}]_{ij} = \binom{[\mathbb{D}_{\mathrm{e}}]_{ij} + 1}{2}. \tag{8}$$

Then,

$$W_e = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_{\mathrm{e}}]_{ij} \quad \text{and} \quad W_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_{\mathrm{p}}]_{ij}\ . \tag{9}$$

Recall that Wiener himself defined the path number as »the sum of the distances between any two carbon atoms in the molecule, in terms of carbon-carbon bonds.« In other words, $W_e$ is given as a sum of elements above the diagonal of the distance matrix.[7] In opposition to the bond/path contribution definition, (see Eqs. (4) and (5)), relation (9) is valid both for acyclic and cycle-containing structures.

The Wiener index of a path graph, $P_N$, is given by the well known relation:[45]

$$W_e = \binom{N}{2} + \binom{N}{3} = \binom{N+1}{3}. \tag{10}$$

In trees, the branching introduced by vertices $r$, of degree $d_r > 2$, will lower the value of $W_e$, as given by the Doyle-Graver formula:[45–48]

$$W_e = \binom{N}{2} + \binom{N}{3} - \sum_r \sum_{1 \le i < j < k \le d_r} n_i n_j n_k \tag{11}$$

where $n_1, n_2, \ldots, n_{dr}$ are the number of vertices in branches attached to vertex $r$; $n_1+n_2+\ldots+n_{dr}+1=N$, and summation runs as follows: first summation over all branching points in the graph and the second one over all $\binom{d_r}{3}$ triplet products around a branching point. In Eqs. (10), and (11), the first term appears to be the »size« term while the second (and the third) give/s account of the »shape« of a structure.[47]

A relation similar to Eq. (10) can be written for the hyper-Wiener index of the path graph:

$$W_p = \binom{N+1}{3} + \binom{N+1}{4} = \binom{N+2}{4}. \tag{12}$$

Klein, Lukovits and Gutman[40] have decomposed the hyper-Wiener number of trees by a relation which can be written as:

$$W_p = (\mathrm{Tr}(\mathbb{D}_{\mathrm{e}}^2)/2 + W_e)/2 \tag{13}$$

where $(\mathrm{Tr}(\mathbb{D}_{\mathrm{e}}^2)$ is the trace of the squared distance matrix. Relation (13) is nowadays regularly used as the definition for the hyper-Wiener index of cycle-containing graphs.

Expansion of the second part of Eq. (9), by taking into account the definition of $\mathbb{D}$ matrix,[44,48] Eq. (8), results in a new decomposition (*i.e.*, a new definition) of the hyper-Wiener index, $W_p$:

$$W_p = \sum_{i<j} [\mathbb{D}_{\mathrm{p}}]_{ij} = \sum_{i<j} \binom{[\mathbb{D}_{\mathrm{e}}]_{ij}+1}{2} = \sum_{i<j} [\mathbb{D}_{\mathrm{e}}]_{ij} + \sum_{i<j} \binom{[\mathbb{D}_{\mathrm{e}}]_{ij}}{2}. \tag{14}$$

The first term is just the Wiener index, $W_e$. The second term is the »non-Wiener« part of the hyper-Wiener index, or the contributions of $[\mathbb{D}_{\mathrm{p}}]_{ij}$ when $|p/>1$. It is denoted by $W_\Delta$($D_\Delta$ in Refs. 44 and 48):

$$W_\Delta = \sum_{i<j} \binom{[\mathbb{D}_{\mathrm{e}}]_{ij}}{2}. \tag{15}$$

Thus, the hyper-Wiener index can be written as:

$$W_p = W_e + W_\Delta\ . \tag{16}$$

$W_\Delta$ index is related to the $(\mathrm{Tr}(\mathbb{D}_{\mathrm{e}}^2)$ by:[18]

$$W_\Delta = (\mathrm{Tr}(\mathbb{D}_{\mathrm{e}}^2) - 2W_e)/4\ . \tag{17}$$

$W_\Delta$ has gained the status of a Wiener-type index both by the matrix definition, (Eq. (15)) and by its participation, along with the Wiener index, in the composition of the hyper-Wiener index (Eq. (16)). It is highly correlated ($r$ = 0. 99975) with $W_p$ in the set of octanes.

Wiener indices express the compactness (or the expansiveness) of a molecular graph (see above). Their values (see Table I) decrease as the branching increases within a set of isomers.

TABLE I

Wiener-type and Harary-type indices in octanes

| Graph | $W_e$ | $W_p$ | $W_{W(A,D,1)}$ | $H_{De}$ | $H_{We}$ | $H_{Dp}$ | $H_{Wp}$ | $H_{W(A,D,1)}$ |
|---|---|---|---|---|---|---|---|---|
| **C8** | 84 | 210 | 256 | 13.7429 | 0.6482 | 10.56429 | 5.8593 | 7.4281 |
| **2MC7** | 79 | 185 | 253 | 14.1000 | 0.7077 | 10.86191 | 7.8938 | 7.4450 |
| **3MC7** | 76 | 170 | *209* | 14.2667 | 0.7244 | 10.98095 | 8.5244 | 7.6542 |
| **4MC7** | 75 | 165 | 208 | 14.3167 | 0.7286 | 11.01429 | 8.6897 | 7.6562 |
| **3EC6** | 72 | 150 | 172 | 14.4833 | 0.7452 | 11.13333 | 9.2952 | 7.8529 |
| **25M2C6** | 74 | 161 | 207 | 14.4667 | 0.7673 | 11.16667 | 10.1784 | 7.5312 |
| **24M2C6** | *71* | 147 | 194 | 14.6500 | *0.7839* | 11.30000 | 10.8923 | 7.6650 |
| **23M2C6** | 70 | 143 | 181 | 14.7333 | 0.7881 | 11.36667 | 11.0992 | 7.8140 |
| **34M2C6** | 68 | 134 | *167* | 14.8667 | 0.8006 | 11.46667 | 11.6339 | 7.9382 |
| **3E2MC5** | *67* | 129 | 161 | 14.9167 | *0.8048* | 11.50001 | 11.7881 | 7.9500 |
| **22M2C6** | *71* | 149 | 208 | 14.7667 | *0.7839* | 11.43333 | 10.9589 | 7.5250 |
| **33M2C6** | *67* | 131 | 179 | 15.0333 | *0.8048* | 11.63333 | 11.8548 | 7.7762 |
| **234M3C5** | 65 | 122 | *167* | 15.1667 | 0.8476 | 11.73333 | 13.7587 | 7.8996 |
| **3E3MC5** | 64 | 118 | 145 | 15.2500 | 0.8214 | 11.79999 | 12.5714 | 8.0202 |
| **224M3C5** | 66 | 127 | *209* | 15.1667 | 0.8435 | 11.76667 | 13.5768 | 7.4805 |
| **223M3C5** | 63 | 115 | 164 | 15.4167 | 0.8601 | 11.96667 | 14.4018 | 7.8850 |
| **233M3C5** | 62 | 111 | 147 | 15.5000 | 0.8643 | 12.03334 | 14.5976 | 7.9971 |
| **2233M4C4** | 58 | 97 | 139 | 16.0000 | 0.9196 | 12.50000 | 17.4196 | 7.9643 |

## QUASI-WIENER AND KIRCHHOFF INDICES

The *Quasi-Wiener* index,[49–52] $W^*$, is defined by means of the Laplace matrix:

$$W^* = N\sum_{i=2}^{N}\frac{1}{\lambda_i} \tag{18}$$

where $\lambda_i$, $i$ = 2,3, . . ., $N$ denote the positive eigenvalues of the Laplace matrix. In acyclic structures, $W^* = W_e$, but in cycle-containing graphs the two quantities are different. In benzenoid molecules, a linear (but not particularly good) correlation between these indices was found.[51]

Klein and Randić[53] have recently considered the so-called resistance distances between the vertices of a graph, by analogy to the resistance between the vertices of an electrical network (superimposable on the considered graph and having unit resistance of each edge). The sum of resistance distances is a topological index which was eventually named the *Kirchhoff index*.[54,55] It satisfies the relation[53,54]

$$Kf = N \,\mathrm{Tr}(\mathbb{L}^{\clubsuit}) \tag{19}$$

where $\mathrm{Tr}(\mathbb{L}^{\clubsuit})$ is the trace of the Moore-Penrose generalized inverse[56,57] of the Laplace matrix. Recently, Gutman and Mohar have demonstrated the identity of the quasi-Wiener and the Kirchhoff numbers for any graph.[54]

## HARARY INDICES

If $\mathbb{M}$ is a matrix, then its reciprocal matrix $\mathbb{RM}$ is defined so that $[\mathbb{RM}]_{ij} = 1/[\mathbb{M}]_{ij}$ if $[\mathbb{M}]_{ij}$ is different from zero, and $[\mathbb{RM}]_{ij} = 0$ if $[\mathbb{M}]_{ij} = 0$. *Harary* indice*s* are constructed on the basis of reciprocal matrices, $\mathbb{RM}$, and are called so in honour of Frank Harary[18,24,58–61] They are defined by

$$H_M = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{RM}]_{ij} \tag{20}$$

subscript $M$ being the identifier of matrix $\mathbb{M}$.

The original Harary index, $H_{De}$, is constructed from the reciprocal distance matrix, $\mathbb{RD}_\mathrm{e}$, introduced in Refs. 58 and 61. The entries in $\mathbb{RD}_\mathrm{e}$ suggest interactions between the atoms of a molecule, which decrease as their mutual distances increase. Table I lists $H_{De}$ values for octanes. One can see that they increase with the branching (in contrast to the Wiener number values) within the set of isomers and no degeneracy appears. This index was tested[18,44,62] on correlations with boiling points and van der Waals areas of octanes.

By analogy to $H_{De}$, Diudea[62] has proposed the $H_{We}$ index, derived from the reciprocal Wiener matrix, $\mathbb{RW}_\mathrm{e}$. This number shows excellent correlation with the octane number, ON, both in linear ($r$ = 0.971) and parabolic (r = 0.991) regression. $H_{We}$ values for octanes are given in Table I. They show the same degenerate pairs (marked by italics) as the Wiener index within this set.

Another Harary-type index is $H_{W(A,D,1)}$. It is calculated from the »restricted random walk« matrix of Randić,[64] which is identical to the $\mathbb{RW}_{(\mathrm{A,D,1})}$ matrix,[63] (matrix $\mathbb{W}_{(\mathrm{A,D,1})}$ will be defined by Eq. (51)). Values of this index, for octanes, are listed in Table I, along with the corresponding $W_{W(A,D,1)}$ values.

$W_{W(A,D,1)}$ index correlates with critical pressures, CP, of octanes ($r$ = 0.919) while for 1/ $W_{W(A,D,1)}$ the correlation is higher ($r$ = 0.962); in triple variable regression ($W_p$, *MTI* and 1/ $W_{W(A,D,1)}$), a coefficient of correlation $r$ = 0.994 is obtained (*MTI* being the molecular topological index, discussed in the section »Schultz-type indices«).

*Hyper-Harary numbers* can be constructed by considering the reciprocal of a property collected in a path-defined square matrix:[62]

$$H_{Dp} = (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{RD}_{\mathrm{p}}]_{ij} \tag{21}$$

$$H_{Wp} = (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{RW}_{\mathrm{p}}]_{ij}\ . \tag{22}$$

All the Harary indices are intercorrelated (over $r$ = 0.98 within the set of octanes). The hyper-Harary index, $H_{Wp}$, shows an excellent correlation with the octane number (*e.g.*, linear ($r$ = 0.9620) and parabolic ($r$ = 0.9922) regression). Van der Waals area of octanes is quite well described by the $H_{De}$ and $H_{Dp}$ indices (in two variable regression, $r$ = 0.9204).[63] A variant of hyper-Harary index is proposed in Ref. 60.

## SZEGED INDICES

A Wiener analogue, referred to as the Szeged index, *SZ*, was recently proposed by Gutman.[65–70] It is defined in analogy to Eq. (4), but the sets $N_i$ and $N_j$ are defined so the equation holds both for acyclic and cycle-containing graphs:

$$N_i = |\{\, v\ |v\in V(\mathrm{G});\ [\mathbb{D}_{\mathrm{e}}]_{iv} < [\mathbb{D}_{\mathrm{e}}]_{jv}\ \}| \tag{23}$$

$$N_j = |\{\, v\ |v\in V(\mathrm{G});\ [\mathbb{D}_{\mathrm{e}}]_{jv} < [\mathbb{D}_{\mathrm{e}}]_{iv}\ \}|\ . \tag{24}$$

Thus, $N_i$ and $N_j$ represent the cardinalities of the sets of vertices closer to **i** and to **j**, respectively; vertices equidistant to **i** and **j** are not counted. Note that in $N_i$ and $N_j$, defined by Eqs. (23) and (24), vertices **i** and **j** need to be adjacent. Note also that $N_i$ depends on both **i** and **j**. The same is hold for $N_j$.

Based on the product $N_iN_j$, two symmetric Szeged matrices, $\mathbb{SZ}_{\mathrm{e}}$ and $\mathbb{SZ}_{\mathrm{p}}$ can be defined. In $\mathbb{SZ}_{\mathrm{e}}$ the ($ij$)-entry is equal to $N_iN_j$ if **i** and **j** are adjacent vertices, and is zero otherwise. In $\mathbb{SZ}_{\mathrm{p}}$ all matrix elements are given by $N_i\ N_j$. Note that $\mathbb{SZ}_{\mathrm{e}}$ is the Hadamard product between $\mathbb{SZ}_{\mathrm{p}}$ and the adjacency matrix, $\mathbb{A}$.

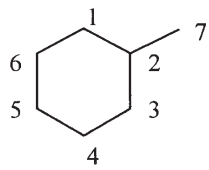
A third, unsymmetric Szeged matrix,[71,72] $\mathbb{SZ}_{\mathrm{u}}$ can be defined (see Figures 4 and 5). The ($ij$)-entry of $\mathbb{SZ}_{\mathrm{u}}$ is equal to $N_i$.

In analogy to the Wiener and hyper-Wiener indices, one defines the Szeged, $SZ_e$ and the hyper-Szeged, $SZ_p$ indices as follows

$$SZ_e = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{SZ}_\mathrm{e}]_{ij} = \Sigma_\mathrm{e}\ [\mathbb{SZ}_\mathrm{u}]_{ij}\ [\mathbb{SZ}_\mathrm{u}]_{ji} \tag{25}$$

$$SZ_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{SZ}_\mathrm{p}]_{ij} = \Sigma_\mathrm{p}\ [\mathbb{SZ}_\mathrm{u}]_{ij}\ [\mathbb{SZ}_\mathrm{u}]_{ji}\ . \tag{26}$$

Numbers $SZ_e$ and $SZ_p$ count the vertices closer to one and the another of the two endpoints of all edges and paths, respectively in a graph.




$G_6$

$\mathbb{D}_\mathrm{e}$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 2 | 3 | 2 | 1 | 2 | 11 |
| 2 | 1 | 0 | 1 | 2 | 3 | 2 | 1 | 10 |
| 3 | 2 | 1 | 0 | 1 | 2 | 3 | 2 | 11 |
| 4 | 3 | 2 | 1 | 0 | 1 | 2 | 3 | 12 |
| 5 | 2 | 3 | 2 | 1 | 0 | 1 | 4 | 13 |
| 6 | 1 | 2 | 3 | 2 | 1 | 0 | 3 | 12 |
| 7 | 2 | 1 | 2 | 3 | 4 | 3 | 0 | 15 |
| | 11 | 10 | 11 | 12 | 13 | 12 | 15 | |

$W_e = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_\mathrm{e}]_{ij} = 42$

$\mathbb{D}_\mathrm{e}$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 3 | 6 | 3 | 1 | 3 | 17 |
| 2 | 1 | 0 | 1 | 3 | 6 | 3 | 1 | 15 |
| 3 | 3 | 1 | 0 | 1 | 3 | 6 | 3 | 17 |
| 4 | 6 | 3 | 1 | 0 | 1 | 3 | 6 | 20 |
| 5 | 3 | 6 | 3 | 1 | 0 | 1 | 10 | 24 |
| 6 | 1 | 3 | 6 | 3 | 1 | 0 | 6 | 20 |
| 7 | 3 | 1 | 3 | 6 | 10 | 6 | 0 | 29 |
| | 17 | 15 | 17 | 20 | 24 | 20 | 29 | |

$W_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_\mathrm{p}]_{ij} = 71$

$\mathbb{SZ}_\mathrm{u}$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 3 | 2 | 4 | 3 | 4 | 3 | 19 |
| 2 | 4 | 0 | 4 | 3 | 4 | 3 | 6 | 24 |
| 3 | 2 | 3 | 0 | 4 | 3 | 4 | 3 | 19 |
| 4 | 3 | 2 | 3 | 0 | 4 | 2 | 4 | 18 |
| 5 | 2 | 3 | 2 | 3 | 0 | 3 | 3 | 16 |
| 6 | 3 | 2 | 3 | 2 | 4 | 0 | 4 | 18 |
| 7 | 1 | 1 | 1 | 3 | 2 | 3 | 0 | 11 |
| | 15 | 14 | 15 | 19 | 20 | 19 | 23 | |

$SZ_e = \Sigma_\mathrm{e}\ [\mathbb{SZ}_\mathrm{u}]_{ij}\ [\mathbb{SZ}_\mathrm{u}]_{ji} = 78$
$SZ_p = \Sigma_\mathrm{p}\ [\mathbb{SZ}_\mathrm{u}]_{ij}\ [\mathbb{SZ}_\mathrm{u}]_{ji} = 182$

$\mathbb{CJ}_\mathrm{u}$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 3 | 2 | 3 | 3 | 4 | 3 | 18 |
| 2 | 4 | 0 | 4 | 3 | 3 | 3 | 6 | 23 |
| 3 | 2 | 3 | 0 | 4 | 3 | 3 | 3 | 18 |
| 4 | 2 | 2 | 3 | 0 | 4 | 2 | 3 | 16 |
| 5 | 2 | 2 | 2 | 3 | 0 | 3 | 2 | 14 |
| 6 | 3 | 2 | 2 | 2 | 4 | 0 | 3 | 16 |
| 7 | 1 | 1 | 1 | 1 | 1 | 1 | 0 | 6 |
| | 14 | 13 | 14 | 16 | 18 | 16 | 20 | |

$CJ_e = \Sigma_\mathrm{e}\ [\mathbb{CJ}_\mathrm{u}]_{ij}\ [\mathbb{CJ}_\mathrm{u}]_{ji} = 78$
$CJ_p = \Sigma_\mathrm{p}\ [\mathbb{CJ}_\mathrm{u}]_{ij}\ [\mathbb{CJ}_\mathrm{u}]_{ji} = 142$

Figure 5. Matrices $\mathbb{D}_\mathrm{e}$, $\mathbb{D}_\mathrm{p}$, $\mathbb{SZ}_\mathrm{u}$ and $\mathbb{CJ}_\mathrm{u}$ and derived indices for graph $G_6$.

In the case of tree graphs, the index defined on edge is identical in Szeged and Wiener matrices (*i.e.* $SZ_e = W_e$) while the index defined on path is different (*i.e.* $SZ_p \surd W_p$). However, in cyclic graphs, the Szeged indices and the Wiener indices are different quantities and it is only accidentally or in special cases[65] (*e.g.* in complete graphs, $SZ_e\,(K_N) = W_e\,(K_N) = N(N–1)/2;\ N>2$) that they show identical values. Values of Szeged indices in octanes and simple cycles are listed in Tables II and III, respectively. Analytical relations for calculating Szeged indices in some classes of graphs can be found in Refs. 63, 65 and 71.

TABLE II

Szeged-type indices in octanes

| Graph | $SZ_e$ | $SZ_p$ | $H_{SZe}$ | $H_{SZp}$ |
|---|---|---|---|---|
| C8 | 84 | 340 | 0.6482 | 2.5024 |
| 2MC7 | 79 | 320 | 0.7077 | 3.5952 |
| 3MC7 | 76 | 307 | 0.7244 | 3.2286 |
| 4MC7 | 75 | 294 | 0.7286 | 3.2286 |
| 3EC6 | 72 | 272 | 0.7452 | 3.3952 |
| 25M2C6 | 74 | 308 | 0.7673 | 4.6464 |
| 24M2C6 | 71 | 288 | 0.7839 | 4.3173 |
| 23M2C6 | 70 | 282 | 0.7881 | 4.2714 |
| 34M2C6 | 68 | 268 | 0.8006 | 4.0298 |
| 2E2MC5 | 67 | 242 | 0.8048 | 4.6381 |
| 22M2C6 | 71 | 280 | 0.7839 | 5.7714 |
| 33M2C6 | 67 | 250 | 0.8048 | 5.1381 |
| 234M3C5 | 65 | 258 | 0.8476 | 5.4032 |
| 3E3MC5 | 64 | 220 | 0.8214 | 5.0714 |
| 224M3C5 | 66 | 254 | 0.8435 | 6.8976 |
| 223M3C5 | 63 | 242 | 0.8601 | 6.5744 |
| 233M3C5 | 62 | 234 | 0.8643 | 6.2476 |
| 2233M4C4 | 58 | 232 | 0.9196 | 8.9821 |

The hyper-Szeged index was tested,[70] with good results, for discriminating ability (*i.e.* separating nonisomorphic isomers) on catafusenes and other cyclic structures. Enthalpies of the formation of (unsubstituted) cycloalkanes are well described by Szeged indices, in single ($SZ_e$, $r = 0.9813$; $SZ_p$, $r = 0.9623$) and two variable ($SZ_e$ & $W_e$, $r = 0.9912$; $SZ_p$ & $W_e$, $r = 0.9910$) correlations.

Reciprocal Szeged matrices,[72] $\mathbb{RSZ}_\mathrm{e}$, $\mathbb{RSZ}_\mathrm{p}$ and $\mathbb{RSZ}_\mathrm{u}$, allow calculation of Harary-type indices, $H_{SZe}$ and $H_{SZp}$

$$H_{SZe} = (1/2)\ \Sigma_i\ _{\Sigma j}\ [\mathbb{RSZ}_\mathrm{e}]_{ij} = \Sigma_\mathrm{e}\,[\mathbb{RSZ}_\mathrm{u}]_{ij}\,[\mathbb{RSZ}_\mathrm{u}]_{ji} \tag{27}$$

$$H_{SZp} = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{RSZ}_p]_{ij} = \Sigma_p\ [\mathbb{RSZ}_u]_{ij}\ [\mathbb{RSZ}_u]_{ji}\ . \tag{28}$$

In trees, $H_{SZe} = H_{We}$ but $H_{SZp} \surd H_{Wp}$. However, in cycle-containing structures, $H_{SZe}$ and $H_{We}$ as well as $H_{SZp}$ and $H_{Wp}$ are distinct quantities. Values of these indices in octanes and simple cycles are listed in Tables II and IV, respectively.

Like other Harary-type numbers, $H_{SZe}$ and $H_{SZp}$ indices correlate quite well ($r$ about 0.88) with the van der Waals areas of octanes. The $H_{SZp}$ index contributes, along with $SW_3$ and $SW_4$ indices,[73] to a correlation of $r = 0.986$; $s = 1.15$ with the boiling points of octanes, in a multilinear regression.

## CLUJ INDICES

Before we proceed with the definition of Cluj indices and Cluj matrices, we remind the reader that the Wiener index $W_e$ and the hyper-Wiener index $W_p$ are constructed by means of numbers $N_{i,e}$ and $N_{i,p}$, see Eqs. (4) and (5). These equations strictly hold for acyclic systems. Generalization of numbers $N_{i,e}$ to cycle-containing graphs leads to numbers $N_i$, Eq. (23), which ultimately resulted in introduction of Szeged indices and Szeged matrices. We now give an analogous generalization of the numbers $N_{i,p}$ which is used in defining the Cluj matrix, $\mathbb{CJ}_u$,[48,74–76]

$$[\mathbb{CJ}_u]_{ij} = N_{i,\,p_k(i,j)} = \max |V_{i,\,p_k(i,j)}| \tag{29}$$

where $|V_{i,\,p_k(i,j)}|$ is the number of elements of the set $V_{i,\,p_k(i,j)}$, where the maximum is taken over all paths $p_k(i,j)$ and where

$$V_{i,\,p_k(i,j)} = \{v\ /v + V(\mathrm{G});\ \mathbb{D}_{iv}<\mathbb{D}_{jv};\ p_h(i,v)\equiv p_k(i,j) = \{i\};\ |p_k(i,j)| = \min\} \tag{30}$$
$$k = 1,\ 2,\ \ldots;\ h = 1,2,\ldots$$

The set $V_{i,\,p_k(i,j)}$ (Eq. (30)), consists of vertices lying *closer* to vertex **i** and *external* with respect to the path $p_k(i,j)$ (condition $p_h(i,v)\equiv p_k(i,j) = \{\mathbf{i}\}$). Since in cycle-containing structures various shortest/longest paths, $p_k(i,j)$, could supply various sets $V_{i,\,p_k(i,j)}$, by definition, the $(ij)$- entries in the Cluj matrices are taken as max $|V_{i,\,p_k(i,j)}|$. The diagonal entries are zero. The above definitions (Eqs. (29) and (30)) hold for any connected graph. Cluj matrices, $\mathbb{CJ}_u$, are square arrays of dimension $N \times N$ and are, in general, unsymmetric with respect to the main diagonal.

The symmetric Cluj matrices $\mathbb{CJ}_e$ and $\mathbb{CJ}_p$ are now defined in full analogy to the symmetric Szeged matrices, $\mathbb{SZ}_e$ and $\mathbb{SZ}_p$:

$$[\mathbb{CJ}_e]_{ij} = \Sigma_e\,[\mathbb{CJ}_u\,]_{ij}\,[\mathbb{CJ}_u\,]_{ji} \tag{31}$$

$$[\mathbb{CJ}_p]_{ij} = \Sigma_p\,[\mathbb{CJ}_u\,]_{ij}\,[\mathbb{CJ}_u]_{ji}\ . \tag{32}$$

Also in this case, $\mathbb{CJ}_e$ is the Hadamard product between $\mathbb{CJ}_p$ and the adjacency matrix.
The respective Cluj indices are calculated in full analogy to the Szeged indices

$$CJ_e\ = (1/2)\ \Sigma_i\ \Sigma_j\,[\mathbb{CJ}_e]_{ij} = \Sigma_e\,[\mathbb{CJ}_u]_{ij}\,[\mathbb{CJ}_u]_{ji} \tag{33}$$

$$CJ_p\ = (1/2)\ \Sigma_i\ \Sigma_j\,[\mathbb{CJ}_p]_{ij} = \Sigma_p\,[\mathbb{CJ}_u]_{ij}\,[\mathbb{CJ}_u]_{ji}\ . \tag{34}$$

When defined on edge, the $CJ_e$, index shows the following relations with the Wiener and Szeged indices: $CJ_e(T) = SZ_e(T) = W_e(T)$ and $CJ_e(C) = SZ_e(C)$ $\surd$ $W_e(C)$, where $T$ and $C$ denote trees and cycle-containing structures, respectively. When defined on path, $CJ_p(T) = W_p(T)$ $\surd$ $SZ_p(T)$ and $CJ_p(C)$ $\surd$ $W_p(C)$ $\surd$ $SZ_p(C)$. Despite formal similarity between $CJ_p$ and $SZ_p$ indices, (Eqs. (34) and (26)), the externality condition ($p_h(i,v) \equiv p_k(i,j) = \{\mathbf{i}\}$, see above) detaches the two hyper-indices (and the corresponding matrices).

Since, in trees, the Cluj indices superimpose over the Wiener indices, values of these indices are given for simple cycles, $C_N$, (Table III). Analytical relations for calculating Cluj indices in some classes of graphs can be found in Refs. 63.

$CJ_p$ index correlates[74] well ($r = 0.920$; $s = 17.29$) with the boiling points, BP, of a set of 45 cyclo-alkanes. The correlation increases ($r = 0.991$; $s = 5.93$) if a logarithmic scale is used for the topological descriptor.

TABLE III

Wiener, Szeged and Cluj indices in simple cycles

| $C_N$ | $W_e$ | $W_p$ | $SZ_e$ | $SZ_p$ | $CJ_e$ | $CJ_p$ |
|---|---|---|---|---|---|---|
| 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| 4 | 8 | 10 | 16 | 18 | 16 | 18 |
| 5 | 15 | 20 | 20 | 40 | 20 | 40 |
| 6 | 27 | 42 | 54 | 105 | 54 | 90 |
| 7 | 42 | 70 | 63 | 189 | 63 | 154 |
| 8 | 64 | 120 | 128 | 364 | 128 | 288 |
| 9 | 90 | 180 | 144 | 576 | 144 | 450 |
| 10 | 125 | 275 | 250 | 945 | 250 | 705 |
| 11 | 165 | 385 | 275 | 1375 | 275 | 1001 |
| 12 | 216 | 546 | 432 | 2046 | 432 | 1470 |

Reciprocal Cluj matrices, $\mathbb{RCJ}_e$, $\mathbb{RCJ}_p$ and $\mathbb{RCJ}_u$, allow calculation of the Harary-type indices,[63] $H_{CJe}$ and $H_{CJp}$

$$H_{CJe} = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{RCJ}_e]_{ij} = \Sigma_e\ [\mathbb{RCJ}_u]_{ij}[\mathbb{RCJ}_u]_{ji} \tag{35}$$

$$H_{CJp} = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{RCJ}_p]_{ij} = \Sigma_p\ [\mathbb{RCJ}_u]_{ij}[\mathbb{RCJ}_u]_{ji}\ . \tag{36}$$

In trees, $H_{CJe} = H_{We}$ and $H_{CJp} = H_{Wp}$. Correlations with the van der Waals areas of octanes were shown above. However, in cycle-containing structures, $H_{CJe/p}$ and $H_{We/p}$ are distinct quantities. Values of these indices, in simple cycles, are listed in Table IV.

TABLE IV

Harary-type (reciprocal property) indices in simple cycles

| $C_N$ | $H_{De}$ | $H_{Dp}$ | $H_{SZe}$ | $H_{SZp}$ | $H_{CJe}$ | $H_{CJp}$ |
|---|---|---|---|---|---|---|
| 3 | 3.0000 | 3.0000 | 3.0000 | 3.0000 | 3.0000 | 3.0000 |
| 4 | 5.0000 | 4.6667 | 1.0000 | 3.0000 | 1.0000 | 3.0000 |
| 5 | 7.5000 | 6.6667 | 1.2500 | 2.5000 | 1.2500 | 2.5000 |
| 6 | 10.0000 | 8.5000 | 0.6667 | 2.5000 | 0.6667 | 2.9167 |
| 7 | 12.8333 | 10.5000 | 0.7778 | 2.3333 | 0.7778 | 3.3056 |
| 8 | 15.6667 | 12.4000 | 0.5000 | 2.3333 | 0.5000 | 3.2778 |
| 9 | 18.7500 | 14.4000 | 0.5625 | 2.2500 | 0.5625 | 3.1250 |
| 10 | 21.8333 | 16.3333 | 0.4000 | 2.2500 | 0.4000 | 3.3167 |
| 11 | 25.1167 | 18.3333 | 0.4400 | 2.2000 | 0.4400 | 3.4772 |
| 12 | 28.4000 | 20.2857 | 0.3333 | 2.2000 | 0.3333 | 3.4600 |

## DISTANCE EXTENDED INDICES

Tratch *et al.*[77] have recently proposed an *expanded distance matrix*, $\mathbb{E}$, which in this paper will be considered only in the case of trees, and will be denoted by $\mathbb{D}\_\mathbb{W}_p$. On this matrix, a distance-extended Wiener index, $D\_W_p$, was defined

$$D\_W_p = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}\_\mathbb{W}_p]_{ij} = (1/2)\ \Sigma_i\ \Sigma_j\ D_{ij}\, N_i\, N_j \tag{37}$$

where $D_{ij}$ is the distance between vertices **i** and **j** whereas $N_i$, $N_j$ have the same meaning as above. Values of this index for octanes are listed in Table V.

$\mathbb{D}\_\mathbb{W}_p$ matrix results as the Hadamard product[39] $\mathbb{D}_e \bullet \mathbb{W}_p$.

Applying the procedure to other square matrices (*e.g.* $\mathbb{SZ}$, $\mathbb{CJ}$, $\mathbb{W}_{(A,D,1)}$) results in distance-extended matrices: they can be operated either by Eq.

(38) or by the »orthogonal« operator (in fact, the half sum of entries in $\mathbb{M} \bullet \mathbb{M}^{T}$ (Eq. (39)), thus giving two types of distance-extended indices, *D_M* and $D^2$*_M,* respectively:[72]

$$D\_M = (1/2)\ \Sigma_{i\ \Sigma j}\ [\mathbb{D}\_\mathbb{M}]_{ij} \tag{38}$$

$$D^2\_M = \Sigma_{\mathrm{p}}\ [\mathbb{D}\_\mathbb{M}]_{ij}\ [\mathbb{D}\_\mathbb{M}]_{ji} = (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{D}\_\mathbb{M} \bullet (\mathbb{D}\_\mathbb{M})^{\mathrm{T}}]_{ij}\ . \tag{39}$$

Note that the first type operator may operate both on symmetric and unsymmetric square matrices while the second one is valid only on unsymmetric square matrices (*e.g.,* $\mathbb{SZ}_{\mathrm{u}}$, $\mathbb{CJ}_{\mathrm{u}}$ – see below).

Indices $D^2$*_M* involve squared distances (indicated by superscript 2), which are used for calculating the moment of inertia of molecules (see Ref. 77). Values of distance-extended indices in octanes are listed in Table V.

In acyclic structures, the following relations hold[72]

$$D\_CJ_p = (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{D}\_\mathbb{CJ}\ _{\mathrm{p}}]_{ij} = (1/2)\ \Sigma_{i\Sigma j}\ D_{ij}\ N_{i,p}\ N_{j,p} = D\_W_p \tag{40}$$

$$\begin{aligned} D^2\_CJ_u &= \Sigma_{\mathrm{p}}\ [\mathbb{D}\_\mathbb{CJ}\ _{\mathrm{u}}]_{ij}\ [\mathbb{D}\_\mathbb{CJ}\ _{\mathrm{u}}]_{ji} = (1/2)\ \Sigma_{i\Sigma j}\ (D_{ij})^2 N_{i,p} N_{j,p} = \\ &= (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{D}_{\mathrm{e}}]_{ij}\ [\mathbb{D}\_\mathbb{W}_{\mathrm{p}}]_{ij} = (1/2)\ \Sigma_{i\Sigma j} [\mathbb{D}_{\mathrm{e}} \bullet \mathbb{D}_{\mathrm{e}} \bullet \mathbb{W}_{\mathrm{p}}]_{ij}\ . \end{aligned} \tag{41}$$

When Eq. (38) is applied on the $\mathbb{CJ}_{\mathrm{u}}$ matrix, it results in a $D\_CJ_u$ index, which, in acyclic structures, equals the hyper-Wiener index:

$$\begin{aligned} D\_CJ_u &= (1/2)\ \Sigma_{i\Sigma j} [\mathbb{D}\_\mathbb{CJ}_{\mathrm{u}}]_{ij} = (1/2)\ \Sigma_{i\Sigma j}\ D_{ij} N_{i,p} = \\ &= (1/2)\ \Sigma_{i\Sigma j}\ N_{i,p} N_{j,p} = (1/2)\ \Sigma_{i\Sigma j} [\mathbb{W}_{\mathrm{p}}]_{ij} = W_p\ . \end{aligned} \tag{42}$$

Other *D_M* indices, such as $D\_SZ_p$ and $D\_W_{(A,D,1)}$, are distinct quantities.[72] All these indices are distinct in cycle-containing structures.

(3D)*D_M* and (3D)$D^2$*_M* indices are also conceivable,[75] using the (3D)$\mathbb{D}_{\mathrm{e}}$ matrix in the extending procedure.

When the Hadamard multiplication is performed using the reciprocal distance matrix, $\mathbb{RD}_{\mathrm{e}}$ (*i.e.* $\mathbb{RD}_{\mathrm{e}} \bullet \mathbb{M}$), it results in new (reciprocal) distance-extended indices,[63,72] *H_M* and $H^2$*_M*:

$$H\_M = (1/2)\ \Sigma_{i\Sigma j}\ [\mathbb{RD}\_\mathbb{M}]_{ij} \tag{43}$$

$$H^2\_M = \Sigma_{p}\ [\mathbb{RD}\_\mathbb{M}]_{ij}\ [\mathbb{RD}\_\mathbb{M}]_{ji}\ . \tag{44}$$

In acyclic structures, *H_Wp = H_CJp* √ *H_SZp,* relations which come out of: *D_Wp = D_CJp* √ *D_SZp*. Values of these indices, for octanes, are included in Table V.

TABLE V

Distance-extended Wiener-type indices in octanes

| Graph | $D\_W_p$ | $D\_SZ_p$ | $D\_W_{(A,D,1)}$ | $D^2\_CJ_u$ | $D^2\_SZ_u$ | $H\_W_p$ | $H\_SZ_p$ | $H^2\_CJ_u$ | $H^2\_SZ_u$ | $H\_W_{(A,D,1)}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **C8** | 462 | 1068 | 1181 | 1386 | 4440 | 131.4762 | 161.8190 | 103.6704 | 111.36 10 | 70.5833 |
| **2MC7** | 382 | 963 | 1072 | 1056 | 3715 | 120.2333 | 153.7333 | 96.4189 | 105.2822 | 74.7667 |
| **3MC7** | 336 | 891 | 803 | 880 | 3269 | 113.4167 | 149.3667 | 92.0403 | 102.0206 | 68.0917 |
| **4MC7** | 321 | 821 | 783 | 825 | 2877 | 111.1333 | 146.2500 | 90.5767 | 100.5958 | 68.9333 |
| **3EC6** | 275 | 724 | 569 | 649 | 2384 | 104.3167 | 139.0000 | 86.1981 | 96.4500 | 63.3000 |
| **25M2C6** | 309 | 906 | 752 | 775 | 3310 | 109.1333 | 147.1333 | 89.1878 | 99.5044 | 70.4338 |
| **24M2C6** | 269 | 799 | 653 | 635 | 2713 | 102.4833 | 141.5667 | 84.8369 | 96.0856 | 70.1333 |
| **23M2C6** | 259 | 762 | 599 | 605 | 2514 | 100.4000 | 140.5000 | 83.4133 | 95.4083 | 67.0833 |
| **34M2C6** | 234 | 692 | 517 | 520 | 2148 | 96.0333 | 136.5333 | 80.5261 | 93.0844 | 65.2333 |
| **3E2MC5** | 219 | 581 | 471 | 465 | 1643 | 93.7500 | *129.5000* | 79.0625 | 90.5000 | 65.0833 |
| **22M2C6** | 278 | 791 | 721 | 676 | 2779 | 102.9333 | 138.0000 | 84.9394 | 94.7583 | 74.3000 |
| **33M2C6** | 228 | *643* | 553 | 506 | 2011 | 94.2000 | *129.5000* | 79.1650 | 89.9333 | 70.3500 |
| **234M3C5** | 203 | *643* | 482 | 421 | 1869 | 89.8333 | 132.5000 | 76.2778 | 89.8333 | 68.5000 |
| **3E3MC5** | 193 | 508 | 388 | 391 | 1372 | 87.7500 | *121.0000* | 74.8542 | 85.7500 | 63.7500 |
| **224M3C5** | 217 | 664 | 643 | 467 | 2072 | 92.1667 | 129.0000 | 77.7639 | 88.6667 | 80.6667 |
| **223M3C5** | 187 | 589 | 454 | 377 | 1667 | 85.9167 | 126.5000 | 73.4931 | 86.5833 | 70.1667 |
| **233M3C5** | 177 | 556 | 383 | 347 | 1524 | 83.8333 | 124.0000 | 72.0694 | 85.2500 | 66.1667 |
| **2233M4C4** | 145 | 550 | 322 | 259 | 1474 | 76.0000 | *121.0000* | 66.5000 | 81.5000 | 68.5000 |

Indices $D^2\_M$ and $H^2\_M$ show a better discriminating ability than that shown by the $D\_M$ and $H\_M$ indices, as it can be seen from Table VI (degenerate values are shaded).

In correlating tests, $1/D\_W_{(A,D,1)}$ correlates well with the critical pressure of octanes ($r$ = 0.973). The same property is excellently expressed ($r$ = 0.991) in a three variable regression by $H\_W_p$, $W_p$ and $MTI$ indices[72] (see below). Van der Waals areas of these hydrocarbons are correlated up to $r$ = 0.870 with the $H^2\_M$ indices included in Table V.

## WALK NUMBERS, ${}^eW_M$ : WIENER-TYPE INDICES OF HIGHER RANK

The idea of Wiener-type indices of higher rank comes out[44] of the following facts: (*i*) occurrence of degeneracy (since C7 isomers) among the values of classical Wiener indices; (*ii*) the higher rank Wiener indices ${}^kW$, (*i. e.* Wiener numbers counting all paths of length $k$=1, 2, 3, ...), proposed by Randić[37] show no good separating ability (*i.e.* a spectrum of values is necessary for discriminating pairs of isomers like 2,2-dimethylhexane (${}^kW$ sequence: 71, 43, 22, 10, 3) and 2,4-dimethylhexane (${}^kW$ sequence: 71, 43, 22, 9, 2)); and (*iii*) use of higher power distance matrix (*e.g.* in the definition of $W_p$ or in the topographic indices of shape profile).[77]

Walk is a continuous sequence of edges $e_1, e_2, ..., e_l$ traversed so that any two subsequent edges are adjacent.[16] The number of traversed edges is called the length (*i.e.* elongation; rank) of the walk. Revisit of vertices and edges is allowed. Walk numbers (*i.e.,* walk degrees;[79] atomic walk count[80]) can be calculated by raising the adjacency matrix (*i.e.*, the matrix having the nondiagonal entries 1 if two vertices of a graph are connected by an edge, and 0 otherwise) to a power $e$, equaling the requested elongation of walk.

Diudea *et al.* [79] have proposed the so called ${}^eW_M$ algorithm, which eludes the matrix power calculation. It evaluates walk numbers of various ranks, ${}^eW_{M,i}$, on any square matrix, $\mathbb{M}$, by iterative summation of vertex contributions over all first neighbours of vertex **i,** in a graph.

The algorithm ${}^eW_M$ is defined by:

$$\mathbb{M} + {}^e\mathbb{W} = {}^e\mathbb{W}_{\mathbb{M}} \tag{45}$$

$$[{}^{e+1}\mathbb{W}_{\mathrm{M}}]_{ii} = \sum_j([\mathbb{M}]_{ij}\,[{}^{e}\mathbb{W}_{\mathrm{M}}]_{jj}); \quad [{}^{0}\mathbb{W}_{\mathrm{M}}]_{jj} = 1 \tag{46}$$

$$[{}^{e+1}\mathbb{W}_{\mathrm{M}}]_{ij} = [{}^{e}\mathbb{W}_{\mathrm{M}}]_{ij} = [\mathbb{M}]_{ij} \tag{47}$$

where ${}^{e}\mathbb{W}_{M}$ is the walk diagonal matrix. Diagonal elements, $[{}^{e}\mathbb{W}_{M}]_{ii}$ equal the sum, on row **i**, of entries $[\mathbb{M}^{e}]_{ij}$, thus giving the walk degrees (weighted by the property collected in $\mathbb{M}$, specified as a subscript letter), ${}^{e}W_{M,i}$:

$$[{}^{e}\mathbb{W}_{M}]_{ii} = \sum_{j} [\mathbb{M}^{e}]_{ij} = {}^{e}W_{M,i} \ . \tag{48}$$

The algorithm offers *global walk numbers,* ${}^{e}W_{M}$, as the half-sum of local numbers:

$${}^{e}W_{M} = (1/2)\ \Sigma_{i}\ {}^{e}W_{M,i} = (1/2)\ \Sigma_{i}\ {}_{\Sigma j}\, [\mathbb{M}^{e}]_{ij} \ . \tag{49}$$

When $\mathbb{M}$ is the distance matrix (or some other matrix involving distances or paths), ${}^{e}W_{M}$ is just a Wiener-type index of rank $\boldsymbol{e}$: ${}^{e}W_{De}$ denotes the Wiener index as defined by Hosoya; ${}^{e}W_{We}$ represents the Wiener index as defined by Wiener; ${}^{e}W_{Wp}$ denotes the hyper-Wiener index as defined by Randić and so on. Walk numbers of rank 2 are listed in Table VI. for octane isomers. The degenerate values are italicized.

TABLE VI

Walk numbers, ${}^{e}W_{M}$ ; $e$ = 2, in octanes

| Graph | ${}^{2}W_{De}$ | ${}^{2}W_{We}$ | ${}^{2}W_{Dp}$ | ${}^{2}W_{Wp}$ | ${}^{2}W_{CJu}$ | ${}^{2}W_{SZu}$ |
|---|---|---|---|---|---|---|
| **C8** | 1848 | 2100 | 12726 | 12054 | 1596 | 2620 |
| **2MC7** | 1628 | 2000 | 9711 | 9829 | 1396 | 2430 |
| **3MC7** | 1512 | 1892 | 8256 | 8338 | 1284 | 2380 |
| **4MC7** | 1476 | 1848 | 7830 | 7815 | 1248 | 2302 |
| **3EC6** | 1360 | 1740 | 6412 | 6460 | 1136 | 2142 |
| **25M2C6** | 1420 | 1900 | 7171 | 7825 | 1206 | 2286 |
| **24M2C6** | 1312 | 1792 | 6023 | 6536 | 1102 | 2195 |
| **23M2C6** | 1280 | 1748 | 5772 | 6163 | 1072 | 2154 |
| **34M2C6** | 1208 | 1684 | 5050 | 5426 | 1004 | 2074 |
| **3E2MC5** | 1172 | 1640 | 4646 | 4992 | 968 | 1858 |
| **22M2C6** | 1316 | 1808 | 6277 | 6779 | 1112 | 2089 |
| **33M2C6** | 1176 | 1664 | 4878 | 5221 | 978 | 1939 |
| **234M3C5** | 1096 | 1648 | 4076 | 4700 | 906 | 1922 |
| **3E3MC5** | 1072 | *1564* | 3916 | 4222 | 880 | 1702 |
| **224M3C5** | 1128 | 1708 | 4406 | 5165 | 940 | 1868 |
| **223M3C5** | 1032 | 1600 | 3653 | 4220 | 850 | 1784 |
| **233M3C5** | 1000 | *1564* | 3402 | 3917 | 820 | 1730 |
| **2233M4C4** | 868 | 1516 | 2521 | 3169 | 706 | 1570 |

Walk numbers can be calculated by means of the *Walk matrix*[44,48,75] $\mathbb{W}_{(M_1,M_2,M_3)}$, which is defined on the basis of the above presented algorithm, as follows:

$$[\mathbb{W}_{(\mathrm{M}_1,\mathrm{M}_2,\mathrm{M}_3)}]_{ij} = {}^{[M_2]_{ij}} W_{M_1,i} \, [\mathbb{M}_3]_{ij} \tag{50}$$

where: $W_{\mathrm{M}_1,i}$ is the walk number of vertex **i**, weighted by the property collected in matrix $\mathbb{M}_1$ ; $[\mathbb{M}_2]_{ij}$ gives the length of the walk and the factor $[\mathbb{M}_3]_{ij}$ is taken from a third square matrix. Appropriate combinations of $\mathbb{M}_1$, $\mathbb{M}_2$ and $\mathbb{M}_3$ matrices offer various unsymmetric matrices (see Figure VI). Values of $W_{W(A,D,1)}$ in octanes are listed in Table I.

Considering $\mathbb{M}_2$ in (51) as a matrix having all the nondiagonal entries equal to 1 (in general $n$), one can obtain ${}^eW_M$ numbers which represent half sums on the matrix product $\mathbb{M}_{1\mathbb{M}3}$

$$\Sigma_j [\mathbb{W}_{(\mathbb{M}_1,\, 1,\, \mathbb{M}_3)}]_{ij} = \Sigma_j \, ({}^1W_{\mathrm{M}_1,i} \, [\mathbb{M}_3]_{ij}) = {}^1W_{\mathrm{M}_1,i} \, \Sigma_j \, [\mathbb{M}3]_{ij} = {}^1W_{\mathrm{M}_1,i} {}^1W_{\mathrm{M}_3,i} \tag{51}$$

$${}^1W_{W(\mathrm{M}_1,1,\mathrm{M}_3),i} = {}^1W_{\mathrm{M}_1,i} \; {}^1W_{\mathrm{M}_3,i} \tag{52}$$

and by summing over all vertices in the graph, one obtains:

$$\Sigma_i \; {}^1W_{W(\mathrm{M}_1,1,\mathrm{M}_3),i} = \Sigma_i \, ({}^1W_{\mathrm{M}_1,i} \; {}^1W_{\mathrm{M}_3,i}) \tag{53}$$

or as global walk numbers:

$$2 \; {}^1W_{W(\mathrm{M}_1,1,\mathrm{M}_3)} = 2 \; {}^1W_{\mathrm{M}_1,\mathrm{M}_3} \; . \tag{54}$$

When $\mathbb{M}_1 = \mathbb{M}_3$, then ${}^1W_{\mathrm{M}_1,\mathrm{M}_3} = {}^1W_{\mathrm{M}_1,\mathrm{M}_1} = {}^2W_{\mathrm{M}_1}$ . Relation (54) can be extended to:

$$2 \; {}^{n+1}W_M = \Sigma_i \, ({}^nW_{M,i} \; {}^1W_{M,i}) = \Sigma_i \; \mathbb{W}_{(\mathrm{M,n,M}),i} = 2W_{W(M,n,M)} \tag{55}$$

where $\mathbb{n}$ is the matrix having entries $[\mathbb{n}]_{ij}$. Eq. (55) proves that $[\mathbb{W}_{(\mathbb{M}_1,\mathbb{M}_2,\,\mathbb{M}_3)}]_{ij}$ is a true matrix operator.

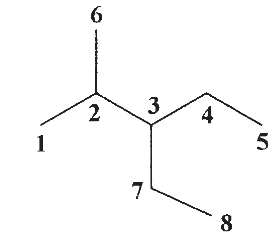
Walk number ${}^2W_{CJu}$ deserves more attention. By raising $\mathbb{CJ}_\mathrm{u}$ matrix to the second power results in the walk number of rank 2, ${}^2W_{CJu}$, which is the mean of the half sum of entries in the matrix product, $\mathbb{D}_\mathrm{e} \, \mathbb{W}_\mathrm{e}$

$${}^2W_{CJu} = (1/2) \; \Sigma_{i\Sigma j} \; [\mathbb{CJ}_\mathrm{u}^2]_{ij} = (1/2) \; \Sigma_{i\Sigma j} \; [\mathbb{D}_\mathrm{e} \, \mathbb{W}_\mathrm{e}]_{ij} \; . \tag{56}$$

In walk number terms, Eq. (56) can be written as:

$${}^2W_{CJu} = (1/2) \; \Sigma_i \; {}^1W_{De,i} \; {}^1W_{We,i} = (1/2) \; \Sigma_i \; {}^1W_{We,i} \; {}^1W_{De,i} = {}^1W_{DeWe} \tag{57}$$

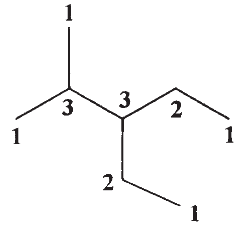
proving that the product of local walk numbers is commutative. $\mathbb{CJ}_\mathrm{u}$ matrix is thus a chimera between the $\mathbb{D}_\mathrm{e}$ and $\mathbb{W}_\mathrm{e}$ matrices.




$G_7$

$(\mathbb{A},\mathbb{D},\mathbb{1})$

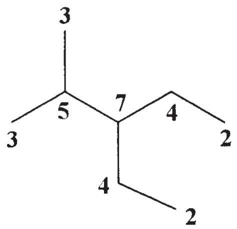
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 3 | 5 | 13 | 3 | 5 | 13 |
| 2 | 3 | 0 | 3 | 5 | 13 | 3 | 5 | 13 |
| 3 | 7 | 3 | 0 | 3 | 7 | 7 | 3 | 7 |
| 4 | 9 | 4 | 2 | 0 | 2 | 9 | 4 | 9 |
| 5 | 9 | 4 | 2 | 1 | 0 | 9 | 4 | 9 |
| 6 | 3 | 1 | 3 | 5 | 13 | 0 | 5 | 13 |
| 7 | 9 | 4 | 2 | 4 | 9 | 9 | 0 | 2 |
| 8 | 9 | 4 | 2 | 4 | 9 | 9 | 1 | 0 |




$G_7\ \{^1W_{A,i}\}$

$(\mathbb{A},\mathbb{D},\mathbb{D})$

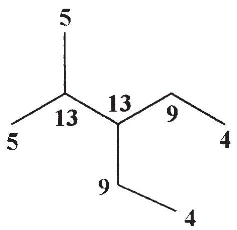
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 6 | 15 | 52 | 6 | 15 | 52 |
| 2 | 3 | 0 | 3 | 10 | 39 | 3 | 10 | 39 |
| 3 | 14 | 3 | 0 | 3 | 14 | 14 | 3 | 14 |
| 4 | 27 | 8 | 2 | 0 | 2 | 27 | 8 | 27 |
| 5 | 36 | 12 | 4 | 1 | 0 | 36 | 12 | 36 |
| 6 | 6 | 1 | 6 | 15 | 52 | 0 | 15 | 52 |
| 7 | 27 | 8 | 2 | 8 | 27 | 27 | 0 | 2 |
| 8 | 36 | 12 | 4 | 12 | 36 | 36 | 1 | 0 |



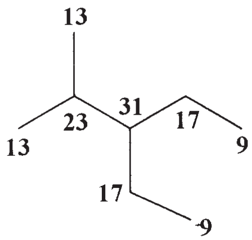

$G_7\ \{^2W_{A,i}\}$

$(\mathbb{A},\mathbb{1},\mathbb{D})$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 2 | 3 | 4 | 2 | 3 | 4 |
| 2 | 3 | 0 | 3 | 6 | 9 | 3 | 6 | 9 |
| 3 | 6 | 3 | 0 | 3 | 6 | 6 | 3 | 6 |
| 4 | 6 | 4 | 2 | 0 | 2 | 6 | 4 | 6 |
| 5 | 4 | 3 | 2 | 1 | 0 | 4 | 3 | 4 |
| 6 | 2 | 1 | 2 | 3 | 4 | 0 | 3 | 4 |
| 7 | 6 | 4 | 2 | 4 | 6 | 6 | 0 | 2 |
| 8 | 4 | 3 | 2 | 3 | 4 | 4 | 1 | 0 |




$G_7\ \{^3W_{A,i}\}$




$G_7\ \{^4W_{A,i}\}$

$(\mathbb{A},\mathbb{2},\mathbb{A})$

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | 5 | 0 | 5 | 0 | 0 | 5 | 0 | 0 |
| 3 | 0 | 7 | 0 | 7 | 0 | 0 | 7 | 0 |
| 4 | 0 | 0 | 4 | 0 | 4 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 |
| 6 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 4 |
| 8 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 0 |

Figure 6. Graph $G_7$ (and its weighted graphs $G_{7\{^eW_{A,i}\}}$) and $\mathbb{W}_{(\mathbb{M}_1,\mathbb{M}_2,\mathbb{M}_3)}$ matrices.

Walk numbers, ${}^{e}W_M$, are useful in discriminating structural isomers. Usually, a rank of two suffices in discriminating *e.g.,* octane isomers.[44] Special graphs, however need, a rank higher than two.

Walk numbers, as the classical Wiener index, exhibit good correlation with octane numbers: $W_e$ ($r$ = 0.957); ${}^{2}W_{De}$ ($r$ = 0.966); ${}^{2}W_{Dp}$ ($r$ = 0.969) in a single variable regression and in two variables one, $r$ = 0.991 with ${}^{2}W_{D\Delta}$and ${}^{1}W_{W(A,D,D)}$.

## SCHULTZ-TYPE INDICES

Among modifications of the Wiener index, the »molecular topological index«,[81] *MTI,* (or the Schultz number) appears to be one of the most studied (for a complete bibliography see Ref. 82). It is defined as

$$MTI = MTI(\mathrm{G}) = \Sigma_i\,[\mathbb{v}_{(\mathbb{A}\,+\,\mathbb{D}_\mathrm{e})}]_i \tag{58}$$

where $\mathbb{A}$ and $\mathbb{D}_\mathrm{e}$ are the adjacency and the distance matrices, respectively, and $\mathbb{v} = (v_1, v_2, \ldots, v_N)$ is the vector of the vertex valences / degrees of the graph.

By applying the matrix algebra, *MTI* can be written[82–89] as

$$MTI = \boldsymbol{u}(\mathbb{A}(\mathbb{A}+\mathbb{D}_\mathrm{e}))\boldsymbol{u}^\mathrm{T} = S(\mathbb{A}^2) + S(\mathbb{A}\mathbb{D}_\mathrm{e}) \tag{59}$$

where

$$S(\mathbb{A}^2) = \boldsymbol{u}(\mathbb{A}^2)\boldsymbol{u}^\mathrm{T} = \Sigma_i\,\Sigma_j\,[\mathbb{A}^2]_{ij} = \Sigma_i(v_i)^2 \tag{60}$$

$$S(\mathbb{A}\mathbb{D}_\mathrm{e}) = \boldsymbol{u}(\mathbb{A}\mathbb{D}_\mathrm{e})\boldsymbol{u}^\mathrm{T} = \Sigma_i\,\Sigma_j\,[\mathbb{A}\mathbb{D}_\mathrm{e}]_{ij} = \Sigma_i\,(v_i d_i)\,. \tag{61}$$

The term $S(\mathbb{A}^2)$ is just the first Zagreb group index[90,91] while $S(\mathbb{A}\mathbb{D}_\mathrm{e})$ is the true Schultz index (*i.e.*, the non-trivial part of *MTI*), then re-invented by others.[88,92] The parameter $d_i$, (Eq. (61)) stands for the $i^{th}$ row sum of entries in the distance matrix: $d_i = \Sigma_j\,[\mathbb{D}_\mathrm{e}]_{ij}$. In the above relations, $\boldsymbol{u}$ and $\boldsymbol{u}^\mathrm{T}$ are the unit vector (of order $N$, which is the number of vertices in G) and its transpose, respectively, as recently used by Estrada *et al.* [88,89] for rejecting the double sum symbol.

In acyclic structures, there exists[85,93–95] a linear dependency between the number $S(\mathrm{AD}_\mathrm{e})$ and the Wiener index

$$S(\mathbb{A}\mathbb{D}_\mathrm{e}) = 4W - N(N-1)\,. \tag{62}$$

$S$ in symbols of the type $S(\mathbb{A}\mathbb{D}_\mathrm{e})$ reminds of the name of Schultz.

In the formalism of Eq. (59), the Wiener index can be written as

$$W = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{W}_{\mathrm{e}}]_{ij} = (1/2)\boldsymbol{u}\mathbb{W}_{\mathrm{e}}\boldsymbol{u}^{\mathrm{T}} \tag{63}$$

$$W = (1/2)\ \Sigma_i\ \Sigma_j\ [\mathbb{D}_{\mathrm{e}}]_{ij} = (1/2)\boldsymbol{u}\mathbb{D}_{\mathrm{e}}\boldsymbol{u}^{\mathrm{T}} \tag{64}$$

when calculated either from the $\mathbb{W}_{\mathrm{e}}$ or $\mathbb{D}_{\mathrm{e}}$ matrix.

Gutman[85] has expressed the $S(\mathbb{AD}_{\mathrm{e}})$ index by analogy to the Wiener index, *cf.* Eq. (4)),

$$S(\mathbb{AD}_{\mathrm{e}}) = \Sigma_{(i,j)}\ [N_{i\ \Sigma k\in I}\ v_k + N_{j\ \Sigma k\in J}\ v_k] \tag{65}$$

where $\Sigma_{k\in I}$ and $\Sigma_{k\in J}$ denote the summation over all vertices lying on the **i**-side and **j**-side (*i.e.*, to the **I** and **J** fragments, respectively) of the edge **(i,j)**. Other valency-distance indices, composing two or three matrices, have been subsequently proposed.[85,88]

A Schultz-type index, built up on a product of square matrices (of dimension $N\times N$), one of them being obligatory the adjacency matrix, $\mathbb{A}$, can be written as[87]

$$\begin{aligned} MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3) &= \boldsymbol{u}(\mathbb{M}_1(\mathbb{A}+\mathbb{M}_3))\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}(\mathbb{M}_1\mathbb{A} + \mathbb{M}_1\mathbb{M}_3)\boldsymbol{u}^{\mathrm{T}} = \\ &= S(\mathbb{M}_1\mathbb{A}) + S(\mathbb{M}_1\mathbb{M}_3)\ . \end{aligned} \tag{66}$$

It is easily seen that $MTI(\mathbb{A},\mathbb{A},\mathbb{D}_{\mathrm{e}})$ is the Schultz original index. Analogue Schultz indices of sequence: $(\mathbb{D}_{\mathrm{e}},\mathbb{A},\mathbb{D}_{\mathrm{e}})$, $(\mathbb{RD}_{\mathrm{e}},\mathbb{A},\mathbb{RD}_{\mathrm{e}})$, $(\mathbb{W}_{\mathrm{p}},\mathbb{A},\mathbb{W}_{\mathrm{p}})$ have been proposed[82,86,89] and tested for the correlating ability (see below).

Walk matrix, $\mathbb{W}_{(\mathrm{M}_1,\mathrm{M}_2,\mathrm{M}_3)}$, can be related to the Schultz numbers as follows

$$MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3) = \boldsymbol{u}(\mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{A})} + \mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{M}_3)})\boldsymbol{u}^{\mathrm{T}} = S(\mathbb{M}_1\mathbb{A}) + S(\mathbb{M}_1\mathbb{M}_3) \tag{67}$$

$$S(\mathbb{M}_1\mathbb{A}) = \boldsymbol{u}\mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{A})}\boldsymbol{u}^{\mathrm{T}} \tag{68}$$

$$S(\mathbb{M}_1\mathbb{M}_3) = \boldsymbol{u}\mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{M}_3)}\boldsymbol{u}^{\mathrm{T}}\ . \tag{69}$$

Quantity $\boldsymbol{u}\mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{M}_3)}\boldsymbol{u}^{\mathrm{T}}$ is twice the walk number ${}^1W\mathbb{W}_{(\mathbb{M}_1^{\mathrm{T}},1,\mathbb{M}_3)}$ (compare Eqs. (69) and (54)). Thus, it is not difficult to write a Schultz-type index in terms of walk numbers

$$MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3) = 2({}^1W_{M_1\ A} + {}^1W_{M_1\,M_3}) \tag{70}$$

which is $\mathbb{W}_{(\mathrm{M}_1,\,\mathrm{M}_2,\,\mathrm{M}_3)}$-calculable, as:

$$MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3) = 2({}^1W_{\mathbb{W}_{(\mathbb{M}_1^T,1,\mathbb{A})}} + {}^1W_{\mathbb{W}_{(\mathbb{M}_1^T,1,\mathbb{M}_3)}} . \tag{71}$$

Let us consider the case of $\mathbb{CJ}_u$ in the sequence $(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3) = (\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u)$. Since the Cramer product is not commutative, and since $\mathbb{CJ}_u$ is an unsymmetric matrix, a Schultz-type index can be written as

$$\begin{aligned} MTI(\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u) &= (\boldsymbol{u}(\mathbb{CJ}_{u\mathbb{A}})\boldsymbol{u}^T + \boldsymbol{u}(\mathbb{ACJ}_u)\boldsymbol{u}^T)/2 + \boldsymbol{u}(\mathbb{CJ}_u{}^2)\,\boldsymbol{u}^T = \\ &= (\boldsymbol{u}(\mathbb{CJ}_{u\mathbb{A}})\boldsymbol{u}^T + \boldsymbol{u}(\mathbb{CJ}_u{}^{T\mathbb{A}})\boldsymbol{u}^T)/2 + \boldsymbol{u}(\mathbb{CJ}_u{}^2)\,\boldsymbol{u}^T = \\ &= S(\mathbb{CJ}_{u\mathbb{A}}) + S(\mathbb{CJ}_u{}^2) \end{aligned} \tag{72}$$

and considering that, in acyclic structures, $\mathrm{RS}(\mathbb{CJ}_u) = \mathrm{RS}(\mathbb{W}_e)$ and $\mathrm{CS}(\mathbb{CJ}_u) = \mathrm{CS}(\mathbb{D}_e)$, RS and CS being the row sums and column sums in a matrix, respectively, Eq. (72) becomes

$$\begin{aligned} MTI(\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u) &= (\boldsymbol{u}(\mathbb{D}_{e\mathbb{A}})\boldsymbol{u}^T + \boldsymbol{u}(\mathbb{AW}_e)\boldsymbol{u}^T)/2 + \boldsymbol{u}(\mathbb{D}_{e\mathbb{W}e)}\boldsymbol{u}^T = \\ &= (S(\mathbb{D}_{e\mathbb{A}}) + S(\mathbb{AW}_e))/2 + S(\mathbb{D}_{e\mathbb{W}e}) . \end{aligned} \tag{73}$$

Since $\mathbb{A}$, $\mathbb{D}_e$ and $\mathbb{W}_e$ are symmetric matrices, it is obvious that $S(\mathbb{D}_{e\mathbb{A}}) = S(\mathbb{AD}_e)$ and $S(\mathbb{AW}_e) = S(\mathbb{W}_{e\mathbb{A}})$.

In terms of the $\mathbb{W}_{(\mathbb{M}_1,\mathbb{M}_2,\mathbb{M}_3)}$ matrix, (see Eqs. (50) and (67)), $MTI(\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u)$ can be written as

$$MTI(\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u) = (\boldsymbol{u}\mathbb{W}_{(\mathbb{CJ}_u^T,1,\mathbb{A})}\boldsymbol{u}^T + \boldsymbol{u}\mathbb{W}_{(\mathbb{CJ}_u,1,\mathbb{A})}\boldsymbol{u}^T)/2 + \boldsymbol{u}\mathbb{W}_{(\mathbb{CJ}_u^T,1,\mathbb{CJ}_u)}\boldsymbol{u}^T \tag{74}$$

which gives the exact result of Eq. (72) or (73). Relations (72) and (74) allow the calculation of this index in any connected graph. Relation (73) offers a *MTI* number which encloses the information of three matrices.

Szeged matrix, $\mathbb{SZ}_u$, behaves similarly:

$$\begin{aligned} MTI(\mathbb{SZ}_u,\mathbb{A},\mathbb{SZ}_u) &= (\boldsymbol{u}(\mathbb{SZ}_{u\mathbb{A}})\boldsymbol{u}^T + \boldsymbol{u}(\mathbb{ASZ}_{u)}\boldsymbol{u}^T)/2 + \boldsymbol{u}(\mathbb{SZ}_u{}^2)\mathrm{u}^T = \\ &= (\boldsymbol{u}(\mathbb{SZ}_{u\mathbb{A}})\boldsymbol{u}^T + \boldsymbol{u}(\mathbb{SZ}_u{}^{T\mathbb{A}})\boldsymbol{u}^T)/2 + \boldsymbol{u}(\mathbb{SZ}_u{}^{2)}\boldsymbol{u}^T \end{aligned} \tag{75}$$

$$\begin{aligned} MTI(\mathbb{SZ}_u,\mathbb{A},\mathbb{SZ}_u) &= (\boldsymbol{u}\mathbb{W}_{(\mathbb{SZ}_u^T,1,\mathbb{A})}\boldsymbol{u}^T + \boldsymbol{u}\mathbb{W}_{(\mathbb{SZ}_u,1,\mathbb{A})}\boldsymbol{u}^T)/2 + \\ &+ \boldsymbol{u}\mathbb{W}_{(\mathbb{SZ}_u^T,1,\mathbb{SZ}_u)}\boldsymbol{u}^T \end{aligned} \tag{76}$$

$$MTI(\mathbb{SZ}_u,\mathbb{A},\mathbb{SZ}_u) = S(\mathbb{SZ}_{u\mathbb{A}}) + S(\mathbb{SZ}_u{}^2)\,. \tag{77}$$

Within a set of acyclic isomers, a very interesting property comes from the definition of $\mathbb{SZ}_u$, which is presented as follows

TABLE VII

$S(\mathbb{M}_1\mathbb{A})$ and $MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3)$ indices in octane isomers

| Graph | $S(\mathbb{M}_1\mathbb{A})$ | | | | $MTI(\mathbb{M}_1,\mathrm{A},\mathbb{M}_3)$ | | | |
|---|---|---|---|---|---|---|---|---|
| | $(\mathbb{D}_e\mathbb{A})$ | $(\mathbb{W}_e\mathbb{A})$ | $(\mathbb{CJ}_u\mathbb{A})$ | $(\mathbb{SZ}_u\mathbb{A})$ | $(\mathbb{D}_e,\mathbb{A},\mathbb{D}_e)$ | $(\mathbb{W}_e,\mathbb{A},\mathbb{W}_e)$ | $(\mathbb{CJ}_u,\mathbb{A},\mathbb{CJ}_u)$ | $(\mathbb{SZ}_u,\mathbb{A},\mathbb{SZ}_u)$ |
| **C8** | 280 | 322 | 301 | 371 | 3976 | 4522 | 3493 | 5611 |
| **2MC7** | 260 | 324 | 292 | 363 | 3516 | 4324 | 3084 | 5223 |
| **3MC7** | 248 | 318 | 283 | 359 | 3272 | 4102 | 2851 | 5119 |
| **4MC7** | 244 | 316 | 280 | 357 | 3196 | 4012 | 2776 | 4961 |
| **3EC6** | 232 | 306 | 269 | 348 | 2952 | 3786 | 2541 | 4632 |
| **25M2C6** | 240 | 326 | 283 | 355 | 3080 | 4126 | 2695 | 4927 |
| **24M2C6** | *228* | 320 | 274 | 350 | 2852 | 3904 | 2478 | 4740 |
| **23M2C6** | 224 | 318 | 271 | 346 | 2784 | 3814 | 2415 | 4654 |
| **34M2C6** | 216 | 314 | 265 | 341 | 2632 | 3682 | 2273 | 4489 |
| **3E2MC5** | *212* | 308 | 260 | 345 | 2556 | 3588 | 2196 | 4061 |
| **22M2C6** | *228* | 330 | 279 | 347 | 2860 | 3946 | 2503 | 4525 |
| **33M2C6** | *212* | 322 | 267 | 338 | 2564 | 3650 | 2223 | 4216 |
| **234M3C5** | 204 | 320 | 262 | 334 | 2396 | 3616 | 2074 | 4178 |
| **3E3MC5** | 200 | 314 | 257 | 326 | 2344 | 3442 | 2017 | 3730 |
| **224M3C5** | 208 | 332 | 270 | 339 | 2464 | 3748 | 2150 | 4075 |
| **223M3C5** | 196 | 326 | 261 | 327 | 2260 | 3526 | 1961 | 3895 |
| **233M3C5** | 192 | 324 | 258 | 323 | 2192 | 3452 | 1898 | 3783 |
| **2233M4C4** | 176 | 338 | 257 | 311 | 1912 | 3370 | 1669 | 3451 |

**Conjecture:** the sum, over all vertices in the graph, of the products between the valency of a vertex **i** and the number of vertices closer to **i** (than to any other vertex **j**) is a constant[87]

$$\boldsymbol{u}(\mathbb{A}\mathbb{S}\mathbb{Z}_{\mathrm{u}})\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}(\mathrm{RS}(\mathbb{A}) \bullet \mathrm{RS}(\mathbb{S}\mathbb{Z}_{\mathrm{u}})) = 2\left[2\binom{N}{3}+\binom{N+1}{3}\right]. \tag{78}$$

In other words, the sum on the product to the left of the Szeged matrix $\mathrm{SZ}_{\mathrm{u}}$ with the adjacency matrix is a constant. In contrast, the product to the right, $\boldsymbol{u}(\mathbb{S}\mathbb{Z}_{\mathrm{u}\mathbb{A}})\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}(\mathrm{RS}(\mathbb{A}) \square \mathrm{CS}(\mathbb{S}\mathbb{Z}_{\mathrm{u}}))$, is variable within a set of acyclic isomers. Values $S(\mathbb{M}_{1\mathbb{A}})$ and the corresponding $MTI(\mathbb{M}_1,\mathbb{A},\mathbb{M}_3)$ indices ($\mathbb{M}_1 = \mathbb{M}_3 = \mathbb{D}\mathrm{e}$, $\mathbb{W}\mathrm{e}$, $\mathbb{C}\mathbb{J}_{\mathrm{u}}$ and $\mathbb{S}\mathbb{Z}_{\mathrm{u}}$) are listed in Table VII.

Schultz-type indices show good correlation[72] with some physico-chemical properties of octanes, in two-variables regression: boiling points ($MTI(\mathbb{D}_{\mathrm{e}},\mathbb{A},\mathbb{D}_{\mathrm{e}})$ & $MTI$ : $r = 0.953$), critical pressure ($MTI(\mathbb{C}\mathbb{J}_{\mathrm{u}},\mathbb{A},\mathbb{C}\mathbb{J}_{\mathrm{u}})$ & $MTI$ : $r = 0.988$; $MTI(\mathbb{S}\mathbb{Z}_{\mathrm{u}},\mathbb{A},\mathbb{S}\mathbb{Z}_{\mathrm{u}})$ & $\chi$: $r = 0.967$ – $\chi$ being the connectivity index[96], octane number ($MTI(\mathbb{C}\mathbb{J}_{\mathrm{u}},\mathbb{A},\mathbb{C}\mathbb{J}_{\mathrm{u}})$& $MTI$ : $r = 0.987$). Note that the Schultz original index $MTI(\mathbb{A},\mathbb{A},\mathbb{D})$ was written above as simple $MTI$.

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## SAŽETAK

### Topologijski indeksi Wienerova tipa

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Prikazan je unificiran pristup Wienerovu topologijskom indeksu i njegovim inačicama. Osobita pozornost obraćena je Kirchoffovu, Harareyevu, Cluj-skom i Shultzovu indeksu te njihovim brojnim varijantama i poopćenjima. Razmotreni su odnosi između tih indeksa i metoda njihova računanja. Izražene su korelacije tih topologijskih indeksa s fizikalnim i kemijskim svojstvima molekula.