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Valencies of Property[#]

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Basic topological matrices: the adjacency matrix, $\boldsymbol{A}$, the distance matrix, $\boldsymbol{D}$, the Wiener matrix, $\boldsymbol{W}$, the detour matrix, Δ, the Szeged matrix, $\boldsymbol{SZ}_{\mathbf{u}}$, and the Cluj matrix, $\boldsymbol{CJ}_{\mathbf{u}}$, after application of the walk matrix operator, $\boldsymbol{W}_{(M1,M2,M3)}$, result in matrices whose row sums express the product between a local property of a vertex i and its valency. One of the two variants of these valency-property matrices is derived by a simple graphical method. Non-Cramer matrix algebra involved in the walk matrix is exemplified. Relations of the indices, calculated on these matrices, with the well known indices of Schultz and Dobrynin (valency-distance) indices are discussed. Further use of the obtained matrices is suggested.

Key words: basic topological matrices, walk matrix operator, valency-property matrices

INTRODUCTION

A molecular structure can be represented by different mathematical objects: matrices, polynomials, numeric sequences and single numbers (*i.e.*, topological indices). All these representations are based on the association of a molecule with a graph (actually a molecular graph where vertices represent atoms and edges chemical bonds) and all of them are aimed to be unique.

First identification of an organic molecule with a graph and its representation by a matrix was made by Sylvester,[1] in early 1874. The matrix is

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[#] This work is dedicated to the »TOPO« Group from Novosibirsk, Russia, for their large contribution to the development of chemical graph theory.

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called the adjacency matrix; its (i, j)-entries, $[\boldsymbol{A}]_{ij}$ are 1 if the vertices i and j are connected by an edge and 0, otherwise

$$[\boldsymbol{A}]_{ij} = \begin{cases} 1 \text{ if } i \neq j \text{ and } (i,j) \in E(\mathrm{G}) \\ 0 \text{ if } i = j \text{ or } (i,j) \notin E(\mathrm{G}) \end{cases} \tag{1}$$

where $E(\mathrm{G})$ is the set of edges in a connected graph, G. The diagonal elements are zero. The adjacency matrix is a $\boldsymbol{N} \times \boldsymbol{N}$ array (N being the number of vertices in a connected graph, G), symmetric *vs.* the main diagonal. The row sum, $\mathrm{RS}(\boldsymbol{A})_i$, or column sum, $\mathrm{CS}(\boldsymbol{A})_i$, provides the vertex degree, deg_i, or the *valency*, v_i. Within this paper, the two terms will be used interchangeably. Figure 1 illustrates the adjacency matrix for graph G_1.

A second basic matrix in chemical graph theory is the distance matrix. It came late in the '70s and is due to Harary.[2] It is a square symmetric array whose entries are defined as

$$[\boldsymbol{D}_{\mathrm{e}}]_{ij} = \begin{cases} N_{\mathrm{e},(i,j)}; |(i,j)| = \min, \text{ if } i \neq j \\ 0 \text{ if } i = j \end{cases} \tag{2}$$

where $N_{\mathrm{e},(i,j)}$ is the number of edges separating vertices i and j on the shortest path, (i, j). Entry $[\boldsymbol{D}_{\mathrm{e}}]_{ij}$ is the topological distance, D_{ij}, between vertex i and vertex j. The matrix $\boldsymbol{D}_{\mathbf{e}}$ of graph G_1 is illustrated in Figure 1.

The half sum of all entries in $\boldsymbol{D}_{\mathbf{e}}$ is, according to Hosoya,[3] the famous Wiener index,[4] W

$$W = (1/2)\sum_i \sum_j [\boldsymbol{D}_{\mathrm{e}}]_{ij} = (1/2)\sum_i [\mathrm{RS}(\boldsymbol{D}_{\mathrm{e}})]_i = (1/2)\sum_i [\mathrm{CS}(\boldsymbol{D}_{\mathrm{e}})]_i \,. \tag{3}$$

By using the matrix algebra, W can be calculated by

$$W = (1/2)\boldsymbol{u}\boldsymbol{D}_{\mathrm{e}}\boldsymbol{u}^{\mathrm{T}} \tag{4}$$

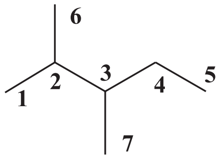
where $\boldsymbol{u}$ and $\boldsymbol{u}^{\mathrm{T}}$ are the unit vector (of order N) and its transpose, respectively. It is easily seen that $\mathrm{RS}(\boldsymbol{M}) = \boldsymbol{M}\boldsymbol{u}^{\mathrm{T}}$ and $\mathrm{CS}(\boldsymbol{M}) = \boldsymbol{u}\boldsymbol{M}$, with $\boldsymbol{M}$ being a square matrix.

The *distance-path* matrix, $\boldsymbol{D}_{\mathrm{p}}$, has been recently proposed.[5,6] This matrix is defined by the expression

$$[\boldsymbol{D}_{\mathrm{p}}]_{ij} = \begin{cases} N_{\mathrm{p},(i,j)}; |(i,j)| = \min, \text{ if } i \neq j \\ 0 \text{ if } i = j \end{cases} \tag{5}$$

where $N_{\mathrm{p},(i,j)}$ is the number of all internal paths of length $1 \leq |p| \leq |(i,j)|$ included in the shortest paths (i,j). $N_{\mathrm{p},(i,j)}$ can be obtained from the classical distance matrix, $\boldsymbol{D}_{\mathrm{e}}$ (*i.e.*, *distance-edge* matrix) by

$$N_{\mathrm{p},(i,j)} = \binom{[D_{\mathrm{e}}]_{ij} + 1}{2}. \tag{6}$$



	A									***CJ***$_u$							
	1	2	3	4	5	6	7	V_i		1	2	3	4	5	6	7	RS(W_e)
1	0	1	0	0	0	0	0	1	1	0	1	1	1	1	1	1	6
2	1	0	1	0	0	1	0	3	2	6	0	3	3	3	6	3	24
3	0	1	0	1	0	0	1	3	3	4	4	0	5	5	4	6	28
4	0	0	1	0	1	0	0	2	4	2	2	2	0	6	2	2	16
5	0	0	0	1	0	0	0	1	5	1	1	1	1	0	1	1	6
6	0	1	0	0	0	0	0	1	6	1	1	1	1	1	0	1	6
7	0	0	1	0	0	0	0	1	7	1	1	1	1	1	1	0	6
	1	3	3	2	1	1	1	12	CS(D_e)	15	10	9	12	17	15	14	92

	D_e									W_e							
	1	2	3	4	5	6	7	RS(D_e)		1	2	3	4	5	6	7	RS(W_e)
1	0	1	2	3	4	2	3	15	1	0	6	0	0	0	0	0	6
2	1	0	1	2	3	1	2	10	2	6	0	12	0	0	6	0	24
3	2	1	0	1	2	2	1	9	3	0	12	0	10	0	0	6	28
4	3	2	1	0	1	3	2	12	4	0	0	10	0	6	0	0	16
5	4	3	2	1	0	4	3	17	5	0	0	0	6	0	0	0	6
6	2	1	2	3	4	0	3	15	6	0	6	0	0	0	0	0	6
7	3	2	1	2	3	3	0	14	7	0	0	6	0	0	0	0	6
	15	10	9	12	17	15	14	92		6	24	28	16	6	6	6	92

	D_p									W_p							
	1	2	3	4	5	6	7	RS(D_p)		1	2	3	4	5	6	7	RS(W_p)
1	0	1	3	6	10	3	6	29	1	0	6	4	2	1	1	1	15
2	1	0	1	3	6	1	3	15	2	6	0	12	6	3	6	3	36
3	3	1	0	1	3	3	1	12	3	4	12	0	10	5	4	6	41
4	6	3	1	0	1	6	3	20	4	2	6	10	0	6	2	2	28
5	10	6	3	1	0	10	6	36	5	1	3	5	6	0	1	1	17
6	3	1	3	6	10	0	6	29	6	1	6	4	2	1	0	1	15
7	6	3	1	3	6	6	0	25	7	1	3	6	2	1	1	0	14
	29	15	12	20	36	29	25	166		15	36	41	28	17	15	14	166

Figure 1. Adjacency, Cluj, Distance and Wiener Matrices for the Graph 1.

Figure 1 illustrates this matrix for graph G_1. The $\boldsymbol{D}_p$ matrix allows direct calculation of the hyper-Wiener index, *WW*, proposed by Randić[7]

$$WW = (1/2)\boldsymbol{u}\boldsymbol{D}_{\mathrm{p}}\boldsymbol{u}^{\mathrm{T}} \ . \tag{7}$$

In fact, Eq. (7) is the matrix form of the general definition of *WW*, proposed by Klein, Lukovits and Gutman.[8]

In full analogy with distance matrices, Eqs. (2) and (5), the *detour matrices*, $\varDelta_{\mathrm{e}}$ and $\varDelta_{\mathrm{p}}$, were introduced.[9–11] The only difference is $|(i, j)| = \max$ (*i.e.*, the longest path joining vertices i and j). Correspondingly, $N_{\mathrm{p},(i,j)}$ is calculated by changing $\boldsymbol{D}_{\mathrm{e}}$ with $\varDelta_{\mathrm{e}}$ in Eq. (6). The indices defined on the detour matrices, the *detour*, w, and the *hyper-detour*, ww, can be calculated according to Eqs. (3), (4) and (7), respectively, by changing the distance matrices with the detour ones.[10–12] Figure 2 illustrates these matrices for 1-ethyl-2-methylcyclopropane, G_2.

Another basic matrix is the Wiener matrix,[13,14] $\boldsymbol{W}$, whose entries are calculated according to the original method given by Wiener[4] to calculate index W

$$[\boldsymbol{W}_{\mathrm{e/p}}]_{ij} = N_{i,(i,j)}\ N_{j,(i,j)} \tag{8}$$

where $N_{i,(i,j)}$ and $N_{j,(i,j)}$ are the numbers of vertices on the two sides of the edge/path (i, j). The $[\boldsymbol{W}_{\mathrm{e/p}}]_{ij}$ entry is the number of (external) paths in G containing the edge/path, e/p, (i, j) The matrix defined on edges, $\boldsymbol{W}_{\mathrm{e}}$, gives W while that defined on paths, $\boldsymbol{W}_{\mathrm{p}}$, leads to WW

$$W = (1/2)\boldsymbol{u}\boldsymbol{W}_{\mathrm{e}}\boldsymbol{u}^{\mathrm{T}} \tag{9}$$

$$WW = (1/2)\boldsymbol{u}\boldsymbol{W}_{\mathrm{p}}\boldsymbol{u}^{\mathrm{T}} \ . \tag{10}$$

Equations (8)–(10) hold only for acyclic graphs. Matrix $\boldsymbol{W}_{\mathrm{e}}$ can be obtained from $\boldsymbol{W}_{\mathrm{p}}$ as the Hadamard product[15] (*i.e.*, $[\boldsymbol{M}_{\mathrm{a}} \bullet \boldsymbol{M}_{\mathrm{b}}]_{ij} = [\boldsymbol{M}_{\mathrm{a}}]_{ij}\ [\boldsymbol{M}_{\mathrm{b}}]_{ij}$) between $\boldsymbol{W}_{\mathrm{p}}$ and $\boldsymbol{A}$

$$\boldsymbol{W}_{\mathrm{e}} = \boldsymbol{W}_{\mathrm{p}} \bullet \boldsymbol{A} \ . \tag{11}$$

Matrices $\boldsymbol{W}_{\mathrm{e}}$ and $\boldsymbol{W}_{\mathrm{p}}$, for graph G_1, are depicted in Figure 1.

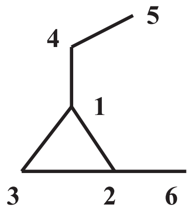
SZEGED AND CLUJ TOPOLOGICAL MATRICES

Two square unsymmetrical matrices, $\boldsymbol{SZ}_{\mathrm{u}}$ (Szeged) and $\boldsymbol{CJ}_{\mathrm{u}}$ (Cluj) have been recently proposed.[16–22] They are defined by a single endpoint characterization of a path, (i, j)

$$[\boldsymbol{SZ}_{\mathrm{u}}]_{ij} = |V_{i,(i,j)}| \tag{12}$$

$\boldsymbol{\Delta}_e$

	1	2	3	4	5	6	RS(Δ_e)
1	0	2	2	1	2	3	10
2	2	0	2	3	4	1	12
3	2	2	0	3	4	3	14
4	1	3	3	0	1	4	12
5	2	4	4	1	0	5	16
6	3	1	3	4	5	0	16
	10	12	14	12	16	16	80



G_2

$\boldsymbol{\Delta}_p$

	1	2	3	4	5	6	RS(Δ_p)
1	0	3	3	1	3	6	16
2	3	0	3	6	10	1	23
3	3	3	0	6	10	6	28
4	1	6	6	0	1	10	24
5	3	10	10	1	0	15	39
6	6	1	6	10	15	0	38
	16	23	28	24	39	38	168

$\boldsymbol{CJ\Delta}_u$

	1	2	3	4	5	6	RS($\boldsymbol{CJ\Delta}_u$)
1	0	3	3	4	4	3	17
2	2	0	2	2	2	5	13
3	1	1	0	1	1	1	5
4	2	2	2	0	5	2	13
5	1	1	1	1	0	1	5
6	1	1	1	1	1	0	5
CS($\boldsymbol{CJ}\Delta_u$)	7	8	9	9	13	12	

$\mathrm{TI}(\boldsymbol{CJ\Delta}_u)_e = \sum_e [\boldsymbol{CJ\Delta}_u]_{ij}\,[\boldsymbol{CJ\Delta}_u]_{ji} = 29$

$\mathrm{TI}(\boldsymbol{CJ\Delta}_u)_p = \sum_p [\boldsymbol{CJ\Delta}_u]_{ij}\,[\boldsymbol{CJ\Delta}_u]_{ji} = 49$

$\boldsymbol{SZ}_u$

	1	2	3	4	5	6	RS(SZ_u)
1	0	3	3	4	4	4	18
2	2	0	2	3	4	5	16
3	1	1	0	3	4	4	13
4	2	2	2	0	5	3	14
5	1	2	2	1	0	2	8
6	1	1	1	2	3	0	8
CS(SZ_u)	7	9	10	13	20	18	

$\boldsymbol{CJ}_u$

	1	2	3	4	5	6	RS(CJ_u)
1	0	3	3	4	4	4	18
2	2	0	2	3	3	5	15
3	1	1	0	3	3	4	12
4	2	2	2	0	5	2	13
5	1	1	1	1	0	1	5
6	1	1	1	1	1	0	5
CS(CJ_u)	7	8	9	12	16	16	

$\mathrm{TI}(\boldsymbol{SZ}_u)_e = \sum_e [\boldsymbol{SZ}_u]_{ij}\,[\boldsymbol{SZ}_u]_{ji} = 29$

$\mathrm{TI}(\boldsymbol{SZ}_u)_p = \sum_p [\boldsymbol{SZ}_u]_{ij}\,[\boldsymbol{SZ}_u]_{ji} = 81$

$\mathrm{TI}(\boldsymbol{CJ}_u)_e = \sum_e [\boldsymbol{CJ}_u]_{ij}\,[\boldsymbol{CJ}_u]_{ji} = 29$

$\mathrm{TI}(\boldsymbol{CJ}_u)_p = \sum_p [\boldsymbol{CJ}_u]_{ij}\,[\boldsymbol{CJ}_u]_{ji} = 62$

Figure 2. Detour, Detour-Cluj, Szeged and Cluj Matrices for the Graph G_2.

$$V_{i,(i,j)} = \{v|v \in V(\mathrm{G});\ D_{iv} < D_{jv} \tag{13}$$

$$[\boldsymbol{CJX}_u]_{ij} = \max|V_{i,(i,j)_k}| \tag{14}$$

$$V_{\mathrm{i,(i,j)}} = \{v|v \in V(\mathrm{G});\ D_{iv} < D_{jv};\ (i,v)_h \cap (i,j)_k = \{i\};\ |(i,j)_k| = \min/\max\} \tag{15}$$

$k = 1, 2, \ldots;\ h = 1,2,\ldots;\ X = D$ for $|(i,j)_k| = \min$; $X = \Delta$ for $|(i,j)_k| = \max$.

The set $V_{i,(i,j)}$, Eqs. (12) and (13), is defined in the same way as Gutman[23] did in the case of the Szeged index (see also Refs. 24–30). $V_{i,(i,j)}$ consists of vertices being closer to vertex i, with respect to the path (i,j). $V(\mathrm{G})$ in the above equations means the set of vertices in G. All diagonal entries are zero. The Szeged matrix of graph G_2 is shown in Figure 2.

The condition $(i,v)_h \cap (i,j)_k = \{\mathrm{i}\}$ Eq. (15) means that any vertex belonging to the path $(i,v)_h$; h = 1, 2,.. is external with respect to any shortest path $(i,j)_k$. In a cycle-containing structure, various shortest/longest paths $(i,j)_k$, k = 1, 2, ... can generate different sets $V_{i,(i,j)}$. The matrix element, $[\boldsymbol{CJX}_{\mathrm{u}}]_{ij}$, is, by definition, $\max|V_{i,(i,j)_k}|$ (see also Refs. 22 and 29). The diagonal entries are zero. When defined according to the minimum path concept (Eq. (15), $|(i,j)_k|$ = min; $X = D$), the Cluj-Distance matrix is denoted by $\boldsymbol{CJD}_{\mathrm{u}}$. Matrix $\boldsymbol{CJ\Delta}_{\mathrm{u}}$ is the Cluj-Detour matrix,[31] *i.e.*, the matrix based on the maximum path concept Eq. (15), $|(i,j)_k|$ = max; $X = \Delta$).

Both matrices, $\boldsymbol{SZ}_{\mathrm{u}}$ and $\boldsymbol{CJX}_{\mathrm{u}}$, are defined for any connected graph, in contrast to the Wiener matrix, defined Eq. (8) only for acyclic graphs. Matrices $\boldsymbol{CJD}_{\mathrm{u}}$ and $\boldsymbol{CJ\Delta}_{\mathrm{u}}$ are illustrated in Figures 1 and 2. In the present paper, only the $\boldsymbol{CJD}_{\mathrm{u}}$ matrix will be considered. For simplicity, it will be denoted by $\boldsymbol{CJ}_{\mathrm{u}}$.

The unsymmetrical matrices, $\boldsymbol{M}_{\mathrm{u}}$, $\boldsymbol{M} = \boldsymbol{SZ}$; $\boldsymbol{CJ}$ allow construction of the corresponding symmetric matrices, $\boldsymbol{M}_{\mathrm{p}}$ (defined on paths) and $\boldsymbol{M}_{\mathrm{e}}$ (defined by edges) using the relation

$$\boldsymbol{M}_{\mathrm{p}} = \boldsymbol{M}_{\mathrm{u}} \bullet (\boldsymbol{M}_{\mathrm{u}})^{\mathrm{T}} \tag{16}$$

$$\boldsymbol{M}_{\mathrm{e}} = \boldsymbol{M}_{\mathrm{p}} \bullet \boldsymbol{A}\,. \tag{17}$$

Matrices $\boldsymbol{CJ}_{\mathrm{e}}$ and $\boldsymbol{CJ}_{\mathrm{p}}$ are identical to the Wiener matrices, $\boldsymbol{W}_{\mathrm{e}}$ and $\boldsymbol{W}_{\mathrm{p}}$, in acyclic structures. In cyclic graphs, the entries of $\boldsymbol{CJ}_{\mathrm{e}}$ equal those of $\boldsymbol{SZ}_{\mathrm{e}}$ while the entries of $\boldsymbol{CJ}_{\mathrm{p}}$ are different from those of $\boldsymbol{SZ}_{\mathrm{p}}$. In trees, $\boldsymbol{CJ}_{\mathrm{u}}$ obeys the relations[16–18]

$$\mathrm{RS}(\boldsymbol{CJ}_{\mathrm{u}}) = \mathrm{RS}(\boldsymbol{W}_{\mathrm{e}}) \tag{18}$$

$$\mathrm{CS}(\boldsymbol{CJ}_{\mathrm{u}}) = \mathrm{CS}(\boldsymbol{D}_{\mathrm{e}})\,. \tag{19}$$

Thus, $\boldsymbol{CJ}_{\mathrm{u}}$ contains the information collected both in $\boldsymbol{D}_{\mathrm{e}}$ and $\boldsymbol{W}_{\mathrm{e}}$ (see below).

Several topological indices can be devised on these matrices,[29] either as the half sum of their entries (a relation of the type (3)) or by

$$TI_{e/p} = \sum_{(i,j)} [\boldsymbol{M}_u]_{ij}[\boldsymbol{M}_u]_{ji} \ . \tag{20}$$

When defined on edges (*i.e.*, (*ij*) is an edge), TI_e is an index (*e.g.*, SZ_e, the classical Szeged index); when defined on paths, TI_p is a hyper-index (*e.g.*, SZ_p and CJ_p).

By virtue of the above mutual matrix relations, the indices show the following relations: $CJ_e(\mathrm{T}) = SZ_e(\mathrm{T}) = W(\mathrm{T})$ and $CJ_e(\mathrm{C}) = SZ_e(\mathrm{C}) \neq W(\mathrm{C})$; $CJ_p(\mathrm{T}) = WW(\mathrm{T}) \neq SZ_p(\mathrm{T})$ and $CJ_p(\mathrm{C}) \neq WW(\mathrm{C}) \neq SZ_p(\mathrm{C})$ where T and C denote a tree graph and a cycle-containing structure, respectively.

Matrices of reciprocal properties, $\boldsymbol{RM}$, (*i.e.*, matrices having entries $[RM]_{ij} = 1 / [M]_{ij}$ and the diagonal entries zero): $\boldsymbol{M} = \boldsymbol{D}_e$, $\boldsymbol{W}_e$, $\boldsymbol{D}_p$, $\boldsymbol{W}_p$, $\boldsymbol{SZ}_u$, $\boldsymbol{CJ}_u$ and $\boldsymbol{W}_{(A,De,1)}$, (see below) have been considered for deriving the Harary and hyper-Harary type indices.[18] Properties and applications of these indices are described in Ref. 29.

WALK MATRIX, $\boldsymbol{W}_{(M1,M2,M3)}$

Walk matrix, $\boldsymbol{W}_{(M_1,M_2,M_3)}$, is defined[5,6,16,17,32] as

$$[\boldsymbol{W}_{(M_1,M_2,M_3)}]_{ij} = {}^{[\boldsymbol{M}_2]_{ij}}W_{M_1,i}\,[\boldsymbol{M}_3]_{ij} = [\mathrm{RS}((\boldsymbol{M}_1)^{[\boldsymbol{M}_2]_{ij}})]_i[\boldsymbol{M}_3]_{ij} \tag{21}$$

where $W_{M_1,i}$ is the walk degree,[33,34] of elongation $[\boldsymbol{M}_2]_{ij}$, of vertex i, weighted by the property collected in matrix $\boldsymbol{M}_1$ (*i.e.*, the i^{th} row sum of matrix $\boldsymbol{M}_1$, raised to power $[\boldsymbol{M}_2]_{ij}$). The diagonal entries are zero. It is a square, (in general) non-symmetric matrix. This matrix, which mixes three square matrices, is a true matrix operator, as it will be shown below.

Let, first, the combination ($\boldsymbol{M_1}$, $\boldsymbol{M_2}$, $\boldsymbol{M_3}$) be ($\mathbf{M_1}$, $\mathbf{1}$, $\mathbf{1}$), where $\mathbf{1}$ is the matrix with the off-diagonal elements equal to 1. In this case, the elements of matrix $\boldsymbol{W}_{(M_1,1,1)}$ will be

$$[\boldsymbol{W}_{(M_1,1,1)}]_{ij} = [\mathrm{RS}(\boldsymbol{M}_1)]_{\underline{i}} \ . \tag{22}$$

Next, consider the combination ($\boldsymbol{M}_1$, $\mathbf{1}$, $\boldsymbol{M}_3$); the corresponding walk matrix can be expressed as the Hadamard product

$$\boldsymbol{W}_{(M_1,1,M_3)} = \boldsymbol{W}_{(M_1,1,1)} \bullet \boldsymbol{M}_3 \ . \tag{23}$$

Examples are given in Chart 1 for G_1, in case: $\boldsymbol{M}_1 = \mathbf{A}$ and $\boldsymbol{M}_3 = \boldsymbol{D}_\mathbf{e}$.

In this article, the use of the walk matrix in generating two types of valency-property matrices as well as in calculating the Schultz-type indices is presented. Cramer matrix algebra is discussed parallel with the Hadamard algebra, involved in the walk matrix operations.

$\boldsymbol{W}_{(A,1,1)}$

	1	2	3	4	5	6	7	RS
1	0	1	1	1	1	1	1	6
2	3	0	3	3	3	3	3	18
3	3	3	0	3	3	3	3	18
4	2	2	2	0	2	2	2	12
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

$\boldsymbol{W}_{(De,1,1)}$

	1	2	3	4	5	6	7	RS
1	0	15	15	15	15	15	15	90
2	10	0	10	10	10	10	10	60
3	9	9	0	9	9	9	9	54
4	12	12	12	0	12	12	12	72
5	17	17	17	17	0	17	17	102
6	15	15	15	15	15	0	15	90
7	14	14	14	14	14	14	0	84

$\boldsymbol{W}_{(A,1,A)} = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{A}$

	1	2	3	4	5	6	7	RS
1	0	1	0	0	0	0	0	1
2	3	0	3	0	0	3	0	9
3	0	3	0	3	0	0	3	9
4	0	0	2	0	2	0	0	4
5	0	0	0	1	0	0	0	1
6	0	1	0	0	0	0	0	1
7	0	0	1	0	0	0	0	1
	3	5	6	4	2	3	3	26

$\boldsymbol{W}_{(De,1,De)} = \boldsymbol{W}_{(De,1,1)} \bullet \boldsymbol{D}_e$

	1	2	3	4	5	6	7	RS
1	0	15	30	45	60	30	45	225
2	10	0	10	20	30	10	20	100
3	18	9	0	9	18	18	9	81
4	36	24	12	0	12	36	24	144
5	68	51	34	17	0	68	51	289
6	30	15	30	45	60	0	45	225
7	42	28	14	28	42	42	0	196
	204	142	130	164	222	204	194	1260

Chart 1. $\boldsymbol{W}_{(M_1, M_2, M_3)}$ algebra for the graph G_1.

VALENCY-PROPERTY MATRICES

The Cramer matrix product, $\boldsymbol{M}_1\boldsymbol{M}_3$, is related to matrix $\boldsymbol{W}_{(M_1,1,M_3)}$ by the following relations

$$\boldsymbol{u}(\boldsymbol{M}_1\boldsymbol{M}_3)\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}\boldsymbol{W}_{(M_1,1,M_3)}\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}\boldsymbol{W}_{(M_3,1,M_1)}\boldsymbol{u}^{\mathrm{T}} \tag{24}$$

$$\boldsymbol{u}(\boldsymbol{M}_3\boldsymbol{M}_1)\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}\boldsymbol{W}_{(M_1,1,M_3^{\mathrm{T}})}\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}\boldsymbol{W}_{(M_3^{\mathrm{T}},1,M_1)}\boldsymbol{u}^{\mathrm{T}}\,. \tag{25}$$

Recall that, in general, the Cramer product is not commutative, so that

$$\boldsymbol{u}(\boldsymbol{M}_1\boldsymbol{M}_3)\boldsymbol{u}^{\mathrm{T}} \neq \boldsymbol{u}(\boldsymbol{M}_3\boldsymbol{M}_1)\boldsymbol{u}^{\mathrm{T}}\,. \tag{26}$$

In contrast, the Hadamard product is commutative within matrix $\boldsymbol{W}_{(M_1,1,M_3)}$ (see Eqs. 23–25).

The left hand member of Eq. (24) can be written as

$$\boldsymbol{u}(\boldsymbol{M}_1\boldsymbol{M}_3)\boldsymbol{u}^{\mathrm{T}} = (\boldsymbol{u}\boldsymbol{M}_1)(\boldsymbol{M}_3\boldsymbol{u}^{\mathrm{T}}) = \mathrm{CS}(\boldsymbol{M}_1)\mathrm{RS}(\boldsymbol{M}_3) = \sum_i \sum_j [\boldsymbol{M}_1\boldsymbol{M}_3]_{ij}\,. \tag{27}$$

In other words, the sum of all entries in the matrix product, $\boldsymbol{M}_1\boldsymbol{M}_3$, can be achieved by multiplying the corresponding CS and RS vectors.

On the other hand, the sum of all entries in $\boldsymbol{W}_{(M_1,1,M_3)}$ is obtained by

$$\boldsymbol{u}\boldsymbol{W}_{(M_1,1,M_3)}\boldsymbol{u}^{\mathrm{T}} = \sum_i [\mathrm{RS}(\boldsymbol{W}_{(M_1,1,M_3)})]_i = \sum_i \sum_j [\boldsymbol{W}_{(M_1,1,M_3)}]_{ij} \,. \tag{28}$$

From Eqs. (24), (27) and (28), we obtain

$$[\mathrm{CS}(\boldsymbol{M}_1)]_i[\mathrm{RS}(\boldsymbol{M}_3)]_{\mathrm{i}} = [\mathrm{RS}(\boldsymbol{W}_{(M_1,1,M_3)})]_i \,. \tag{29}$$

In the case of a symmetric matrix, $\mathrm{CS}(\boldsymbol{M}_1) = \boldsymbol{u}\boldsymbol{M}_1 = \boldsymbol{M}_1^{\mathrm{T}}\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{M}_1\boldsymbol{u}^{\mathrm{T}} = \mathrm{RS}(\boldsymbol{M}_1)$, so that Eq. (29) can be written as

$$[\mathrm{RS}(\boldsymbol{M}_1)]_i[\mathrm{RS}(\boldsymbol{M}_3)]_i = [\mathrm{RS}(\boldsymbol{W}_{(M_1,1,M_3)})]_i \,. \tag{30}$$

If $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ are topological square matrices, Eqs. (24), (27)–(30) offer an interesting meaning for the product matrix, $\boldsymbol{M}_1\boldsymbol{M}_3$: it represents a collection of pairwise products of local (topological) properties (encoded as the corresponding row and column sums). Such pairwise products are just entries in the vector $[\mathrm{RS}(\boldsymbol{W}_{(M_1,1,M_3)})]_{\mathrm{i}}$ (Eqs. (29) and (30). Thus, Eq. (24) represents a joint point of Cramer and Hadamard algebra, by means of $\boldsymbol{W}_{(M_1,1,M_3)}$, and proves that this matrix is a true matrix operator.

We introduce here two types of $\boldsymbol{W}_{(M_1,1,M_3)}$ matrices:

(i) $\boldsymbol{V}_M$ (*Valency-Property*), as $\boldsymbol{W}_{(M_1,1,M_3)}$; $\boldsymbol{M}_1 = \boldsymbol{A}$. The pairwise products collected in the row sums $[\mathrm{RS}(\boldsymbol{W}_{(A_1,1,M_3)})]_i$ are just valency-property products, thus justifying the name $\boldsymbol{V}_M$ given to such matrices. Chart 2 illustrates the Cramer product matrix, $\boldsymbol{AM}$, and matrix $\boldsymbol{V}_{\mathrm{M}}$, $\boldsymbol{M} = \boldsymbol{D}_{\mathrm{e}}$, $\boldsymbol{W}_{\mathrm{e}}$, $\boldsymbol{CJ}_{\mathrm{u}}$ and $(\boldsymbol{CJ}_{\mathrm{u}})^{\mathrm{T}}$ for graph G_1. Note that matrices $\boldsymbol{V}_{\mathbf{CJu}}$ and $\boldsymbol{V}_{(\mathbf{CJu})}{}^{\mathrm{T}}$ show the same RS vector as matrices $\boldsymbol{V}_{\boldsymbol{W}e}$ and $\boldsymbol{V}_{\boldsymbol{D}e}$, respectively, proving that $\boldsymbol{CJ}_{\mathrm{u}}$ is, in trees, a chimera between $\boldsymbol{W}_{\mathrm{e}}$ and $\boldsymbol{D}_{\mathrm{e}}$.

(ii) $\boldsymbol{A}_{\mathrm{M}}$ (*Weighted Adjacency*), as $\boldsymbol{W}_{(M_1,1,M_3)}$; $\boldsymbol{M}_3 = \boldsymbol{A}$. In this case, the resulting valency-property matrices are true weighted adjacency matrices. They can be easily built up by a graphical method: (i) draw a graph weighted by the property collected in $\boldsymbol{M}_1$, as $[\mathrm{RS}(\boldsymbol{M}_1)]_i$ (or $[\mathrm{CS}(\boldsymbol{M}_1)]_i$); (ii) write an adjacency matrix of that graph by replacing entries 1 in row i by $[\mathrm{RS}(\boldsymbol{M}_1)]_i$ (or $[\mathrm{CS}(\boldsymbol{M}_1)]_i$). The row sums in such a matrix are just the local valency-property products. $\boldsymbol{A}_{\mathrm{M}}$ matrices for graphs G_1 and G_2 are illustrated in Figures 3 and 4, respectively.

By comparing $\boldsymbol{V}_M$ and $\boldsymbol{A}_M$ with each other and with the Cramer product matrices, $\boldsymbol{AM}$ and $\boldsymbol{MA}$, it comes out that

$$\mathrm{RS}(\boldsymbol{V}_M) = \mathrm{RS}(\boldsymbol{W}_{(A,1,M)}) = \mathrm{RS}(\boldsymbol{A}) \bullet \mathrm{RS}(\boldsymbol{M}) = \mathrm{RS}(\boldsymbol{W}_{(M,1,A)}) = \mathrm{RS}(\boldsymbol{A}_M) \tag{31}$$

$\boldsymbol{AD}_{\mathrm{e}}$

	1	2	3	4	5	6	7	RS
1	1	0	1	2	3	1	2	10
2	4	3	4	7	10	4	7	39
3	7	4	3	4	7	7	4	36
4	6	4	2	2	2	6	4	26
5	3	2	1	0	1	3	2	12
6	1	0	1	2	3	1	2	10
7	2	1	0	1	2	2	1	9
CS	24	14	12	18	28	24	22	142

$\boldsymbol{V}_{De} = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{D}_{\mathrm{e}}$

	1	2	3	4	5	6	7	$V_{\mathrm{i}} \bullet \mathrm{RS}(\boldsymbol{D}_{\mathrm{e}})$
1	0	1	2	3	4	2	3	15
2	3	0	3	6	9	3	6	30
3	6	3	0	3	6	6	3	27
4	6	4	2	0	2	6	4	24
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
CS($\boldsymbol{AD}_{\mathrm{e}}$)	24	14	12	18	28	24	22	142

$\boldsymbol{AW}_{\mathrm{e}}$

	1	2	3	4	5	6	7	RS
1	6	0	12	0	0	6	0	24
2	0	24	0	10	0	0	6	40
3	6	0	28	0	6	6	0	46
4	0	12	0	16	0	0	6	34
5	0	0	10	0	6	0	0	16
6	6	0	12	0	0	6	0	24
7	0	12	0	10	0	0	6	28
CS	18	48	62	36	12	18	18	212

$\boldsymbol{V}_{We} = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{W}_{\mathrm{e}}$

	1	2	3	4	5	6	7	$V_{\mathrm{i}} \bullet \mathrm{RS}(\boldsymbol{W}_{\mathrm{e}})$
1	0	6	0	0	0	0	0	6
2	18	0	36	0	0	18	0	72
3	0	36	0	30	0	0	18	84
4	0	0	20	0	12	0	0	32
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
CS($\boldsymbol{AW}_{\mathrm{e}}$)	18	48	62	36	12	18	18	212

$\boldsymbol{ACJ}_{\mathrm{u}}$

	1	2	3	4	5	6	7	RS
1	6	0	3	3	3	6	3	24
2	5	6	2	7	7	5	8	40
3	9	3	6	4	10	9	5	46
4	5	5	1	6	5	5	7	34
5	2	2	2	0	6	2	2	16
6	6	0	3	3	3	6	3	24
7	4	4	0	5	5	4	6	28
CS	37	20	17	28	39	37	34	212

$\boldsymbol{V}_{CJ\mathrm{u}} = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{CJ}_{\mathrm{u}}$

	1	2	3	4	5	6	7	$V_{\mathrm{i}} \bullet \mathrm{RS}(\boldsymbol{W}_{\mathrm{e}})$
1	0	1	1	1	1	1	1	6
2	18	0	9	9	9	18	9	72
3	12	12	0	15	15	12	18	84
4	4	4	4	0	12	4	4	32
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
CS($\boldsymbol{ACJ}_{\mathrm{u}}$)	37	20	17	28	39	37	34	212

$\boldsymbol{ACJ}_{\mathrm{u}}^{\mathrm{T}}$

	1	2	3	4	5	6	7	RS
1	1	0	4	2	1	1	1	10
2	2	15	8	6	3	2	3	39
3	3	6	15	4	3	3	2	36
4	2	6	5	8	1	2	2	26
5	1	3	5	0	1	1	1	12
6	1	0	4	2	1	1	1	10
7	1	3	0	2	1	1	1	9
CS	11	33	41	24	11	11	11	142

$\boldsymbol{V}_{CJ\mathrm{u}}{}^{\mathrm{T}} = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{CJ}_{\mathrm{u}}^{\mathrm{T}}$

	1	2	3	4	5	6	7	$V_{\mathrm{i}} \bullet \mathrm{RS}(\boldsymbol{D}_{\mathrm{e}})$
1	0	6	4	2	1	1	1	15
2	3	0	12	6	3	3	3	30
3	3	9	0	6	3	3	3	27
4	2	6	10	0	2	2	2	24
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
CS($\boldsymbol{ACJ}_{\mathrm{u}}^{\mathrm{T}}$)	11	33	41	24	11	11	11	142

Chart 2. Cramer product $\boldsymbol{AM}$ and $\boldsymbol{V}_{\mathrm{M}}$ (*i.e.*, $\boldsymbol{W}_{(\mathrm{A},1,\mathrm{M})}$) matrices for the graph G_1.

$$\mathrm{RS}(\boldsymbol{V}_{M^{\mathrm{T}}}) = \mathrm{RS}(\boldsymbol{W}_{(A,1,M^{\mathrm{T}})}) = \mathrm{RS}(\boldsymbol{A}) \bullet \mathrm{RS}(\boldsymbol{M}^{\mathrm{T}}) = \mathrm{RS}(\boldsymbol{W}_{(M^{\mathrm{T}},1,A)} = \mathrm{RS}(\boldsymbol{A}_{M^{\mathrm{T}}}) \tag{32}$$

$$\mathrm{CS}(\boldsymbol{AM}) = \mathrm{CS}(\boldsymbol{V}_M);\ \mathrm{CS}(\boldsymbol{MA}) = \mathrm{CS}(\boldsymbol{A}_{M^{\mathrm{T}}}) \tag{33}$$

$$\mathrm{RS}(\boldsymbol{AM}) = \mathrm{CS}(\boldsymbol{A}_{\mathrm{M}});\ \mathrm{RS}(\boldsymbol{MA}) = \mathrm{CS}(\boldsymbol{V}_{M^{\mathrm{T}}}) . \tag{34}$$

Since RS($\boldsymbol{A}$) is just the vector of vertex *valencies*, $\boldsymbol{v}$, the vector product, RS($\boldsymbol{A}$) • RS($\boldsymbol{M}$), reveals just the meaning of the newly proposed valency-property matrices, $\boldsymbol{V}_M$ and $\boldsymbol{A}_M$: they collect valencies weighted by the (topological) property enclosed in matrix $\boldsymbol{M}$.

RELATIONS OF VALENCY-PROPERTY MATRICES WITH SCHULTZ AND DOBRYNIN INDICES

The molecular topological index, *MTI*, or the Schultz index, [35] is defined by

$$MTI = \sum_i [v(\boldsymbol{A}+\boldsymbol{D}_{\mathrm{e}})]_i . \tag{35}$$

By applying matrix algebra, *MTI* may be written as[32]

$$MTI = \boldsymbol{u}(\boldsymbol{A}(\boldsymbol{A}+\boldsymbol{D}_{\mathrm{e}}))\boldsymbol{u}^{\mathrm{T}} = \boldsymbol{u}(\boldsymbol{A}^2)\boldsymbol{u}^{\mathrm{T}} + \boldsymbol{u}(\boldsymbol{AD}_{\mathrm{e}})\boldsymbol{u}^{\mathrm{T}} = S(\boldsymbol{A}^2) + S(\boldsymbol{AD}_{\mathrm{e}}) \tag{36}$$

where

$$S(\boldsymbol{A}^2) = \sum_i [\mathrm{RS}(\boldsymbol{A})]_i[\mathrm{RS}(\boldsymbol{A})]_i = \sum_i (v_i)^2 \tag{37}$$

$$S(\boldsymbol{AD}_{\mathrm{e}}) = \sum_i [\mathrm{RS}(\boldsymbol{A})]_i[\mathrm{RS}(\boldsymbol{D}_{\mathrm{e}})]_i . \tag{38}$$

The term S($\boldsymbol{A}^2$) is just the first Zagreb Group index, while S($\boldsymbol{AD}_{\mathrm{e}}$) is the true Schultz index, reinvented by Dobrynin[36] (the »degree-distance« index) and by Estrada.[37]

Diudea and Randić[32] have extended Schultz's definition by using a combination of three square matrices, one of them being obligatory the adjacency matrix. In Cramer matrix algebra, it is defined as

$$\begin{gathered} MTI(M_1,A,M_3) = \boldsymbol{u}(\boldsymbol{M}_1(\boldsymbol{A}+\boldsymbol{M}_3))\boldsymbol{u}^{\mathrm{T}} = \\ \boldsymbol{u}(\boldsymbol{M}_1\boldsymbol{A})\boldsymbol{u}^{\mathrm{T}} + \boldsymbol{u}(\boldsymbol{M}_1\boldsymbol{M}_3)\boldsymbol{u}^{\mathrm{T}} = S(\boldsymbol{M}_1\boldsymbol{A}) + S(\boldsymbol{M}_1\boldsymbol{M}_3) . \end{gathered} \tag{39}$$

It is easily seen that $MTI(A,A,D_{\mathrm{e}})$ is the Schultz original index. Analogue Schultz indices of the sequence: ($\boldsymbol{D}_{\mathrm{e}}$,$\boldsymbol{A}$,$\boldsymbol{D}_{\mathrm{e}}$), ($\boldsymbol{RD}_{\mathrm{e}}$,$\boldsymbol{A}$,$\boldsymbol{RD}_{\mathrm{e}}$) and ($\boldsymbol{W}_{\mathrm{p}}$,$\boldsymbol{A}$,$\boldsymbol{W}_{\mathrm{p}}$) have been proposed and tested for correlating ability.[38–40] In the above sequence, $\boldsymbol{RD}_{\mathrm{e}}$ represents the matrix whose non-diagonal entries are $1/[\boldsymbol{D}_{\mathrm{e}}]_{ij}$.

The walk matrix, $\boldsymbol{W}_{(M_1,M_2,M_3)}$, is related to the Schultz numbers (*cf.* Eq. (30) as

$$S(\boldsymbol{M}_1\boldsymbol{A}) = \boldsymbol{u}\boldsymbol{W}_{(M_1,1,A)}\boldsymbol{u}^{\mathrm{T}} \tag{40}$$

$$S(M_1M_3) = \boldsymbol{u}\boldsymbol{W}_{(M_1,1,M_3)}\boldsymbol{u}^{\mathrm{T}} \tag{41}$$

$$MTI(M_1,A,M_3) = \boldsymbol{u}\boldsymbol{W}_{(M_1,1,A)}\boldsymbol{u}^{\mathrm{T}} + \boldsymbol{u}\boldsymbol{W}_{(M_1,1,M_3)}\boldsymbol{u}^{\mathrm{T}} . \tag{42}$$

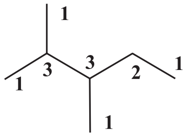
One can see that Eqs. (39) and (42) are equivalent. Values of $S(\boldsymbol{M}_1\boldsymbol{A})$ and of some old and new indices $MTI(\boldsymbol{M}_1,\boldsymbol{A},\boldsymbol{M}_3)$; $\boldsymbol{M}_1 = \boldsymbol{M}_3$ for octanes are listed in

TABLE I

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

Graph	$S(\boldsymbol{D}_e\boldsymbol{A})$	$S(\boldsymbol{W}_e\boldsymbol{A})$	$S(\boldsymbol{CJ}_u\boldsymbol{A})$	$S(\boldsymbol{SZ}_u\boldsymbol{A})$	$(\boldsymbol{D}_e,\boldsymbol{A},\boldsymbol{D}_e)$	$(\boldsymbol{CJ}_u,\boldsymbol{A},\boldsymbol{CJ}_u)$	$(\boldsymbol{SZ}_u,\boldsymbol{A},\boldsymbol{SZ}_u)$	MTI
C8	280	322	301	371	3976	3493	5611	306
2MC7	260	324	292	363	3516	3084	5223	288
3MC7	248	318	283	359	3272	2851	5119	276
4MC7	244	316	280	357	3196	2776	4961	272
3EC6	232	306	269	348	2952	2541	4632	260
25M2C6	240	326	283	355	3080	2695	4927	270
24M2C6	228	320	274	350	2852	2478	4740	258
23M2C6	224	318	271	346	2784	2415	4654	254
34M2C6	216	314	265	341	2632	2273	4489	246
3E2MC5	212	308	260	345	2556	2196	4061	242
22M2C6	228	330	279	347	2860	2503	4525	260
33M2C6	212	322	267	338	2564	2223	4216	244
234M3C5	204	320	262	334	2396	2074	4178	236
3E3MC5	200	314	257	326	2344	2017	3730	232
224M3C5	208	332	270	339	2464	2150	4075	242
223M3C5	196	326	261	327	2260	1961	3895	230
233M3C5	192	324	258	323	2192	1898	3783	226
2233M4C4	176	338	257	311	1912	1669	3451	214

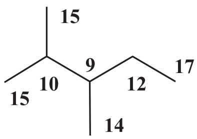
* Schultz-type indices, MTI($\boldsymbol{M}_1$,$\boldsymbol{A}$,$\boldsymbol{M}_3$), are written as the sequence ($\boldsymbol{M}_1$,$\boldsymbol{A}$,$\boldsymbol{M}_3$); the original Schultz index is written as *MTI*.



$G_1\{RS(\boldsymbol{A}) = \boldsymbol{V}_i\}$

$\boldsymbol{A}_A = \boldsymbol{W}_{(A,1,1)} \bullet \boldsymbol{A} = \boldsymbol{W}_{(A,1,A)}$

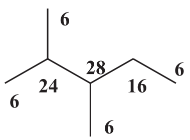
	1	2	3	4	5	6	7	$\boldsymbol{V}_i$ $\boldsymbol{V}_i$
1	0	1	0	0	0	0	0	1
2	3	0	3	0	0	3	0	9
3	0	3	0	3	0	0	3	9
4	0	0	2	0	2	0	0	4
5	0	0	0	1	0	0	0	1
6	0	1	0	0	0	0	0	1
7	0	0	1	0	0	0	0	1
	3	5	6	4	2	3	3	26



$G_1\{RS(\boldsymbol{D}_e)\}$

$\boldsymbol{A}_{De} = \boldsymbol{W}_{(De,1,1)} \bullet \boldsymbol{A} = \boldsymbol{W}_{(De,1,A)}$

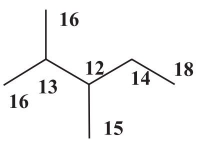
	1	2	3	4	5	6	7	$RS(\boldsymbol{D}_e)$ $\boldsymbol{V}_i$
1	0	15	0	0	0	0	0	15
2	10	0	10	0	0	10	0	30
3	0	9	0	9	0	0	9	27
4	0	0	12	0	12	0	0	24
5	0	0	0	17	0	0	0	17
6	0	15	0	0	0	0	0	15
7	0	0	14	0	0	0	0	14
	10	39	36	26	12	10	9	142



$G_1\{RS(\boldsymbol{W}_e)\}$

$\boldsymbol{A}_{We} = \boldsymbol{W}_{(We,1,1)} \bullet \boldsymbol{A} = \boldsymbol{W}_{(We,1,A)}$

	1	2	3	4	5	6	7	$RS(\boldsymbol{W}_e)$ $\boldsymbol{V}_i$
1	0	6	0	0	0	0	0	6
2	24	0	24	0	0	24	0	72
3	0	28	0	28	0	0	28	84
4	0	0	16	0	16	0	0	32
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
	24	40	46	34	16	24	28	212



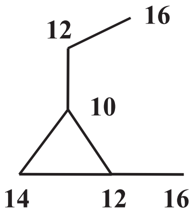
$G_1\{RS(\boldsymbol{D}_e) + \boldsymbol{V}_i\}$

$\boldsymbol{A}_{(A+De)} = \boldsymbol{W}_{((A+De),1,1)} \bullet \boldsymbol{A} = \boldsymbol{W}_{((A+De),1,A)}$

	1	2	3	4	5	6	7	$(RS(\boldsymbol{D}_e)+\boldsymbol{V}_i)$ $\boldsymbol{V}_i$
1	0	16	0	0	0	0	0	16
2	13	0	13	0	0	13	0	39
3	0	12	0	12	0	0	12	36
4	0	0	14	0	14	0	0	28
5	0	0	0	18	0	0	0	18
6	0	16	0	0	0	0	0	16
7	0	0	15	0	0	0	0	15
	13	44	42	30	14	13	12	168

Figure 3. Weighted Adjacency Matrices, $\boldsymbol{A}_M$, for the Graph G_1.

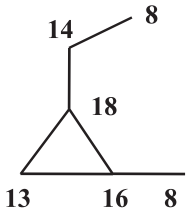
$$A_{\Delta e} = W_{(\Delta e,1,1)} \bullet A = W_{(\Delta e,1,A)}$$



$G_2\{RS(\Delta_e)\}$

	1	2	3	4	5	6	$V_i \bullet RS(\Delta_e)$
1	0	10	10	10	0	0	30
2	12	0	12	0	0	12	36
3	14	14	0	0	0	0	28
4	12	0	0	0	12	0	24
5	0	0	0	16	0	0	16
6	0	16	0	0	0	0	16
CS	38	40	22	26	12	12	150

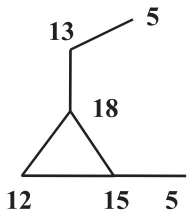
$$A_{SZu} = W_{(SZu,1,1)} \bullet A = W_{(SZu,1,A)}$$



$G_2\{RS(SZ_u)\}$

	1	2	3	4	5	6	$V_i \bullet RS(SZ_u)$
1	0	18	18	18	0	0	54
2	16	0	16	0	0	16	48
3	13	13	0	0	0	0	26
4	14	0	0	0	14	0	28
5	0	0	0	8	0	0	8
6	0	8	0	0	0	0	8
CS	43	39	34	26	14	16	172

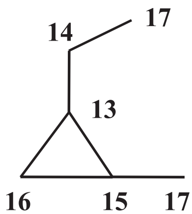
$$A_{CJu} = W_{(CJu,1,1)} \bullet A = W_{(CJu,1,A)}$$



$G_2\{RS(CJ_u)\}$

	1	2	3	4	5	6	$V_i \bullet RS(CJ_u)$
1	0	18	18	18	0	0	54
2	15	0	15	0	0	15	45
3	12	12	0	0	0	0	24
4	13	0	0	0	13	0	26
5	0	0	0	5	0	0	5
6	0	5	0	0	0	0	5
CS	40	35	33	23	13	15	159

$$A_{(A+\Delta e)} = W_{((A+\Delta e,1,1)} \bullet A = W_{(A+\Delta e,1,A)}$$



$G_2\{V_i + RS(\Delta_e)\}$

	1	2	3	4	5	6	$V_i \bullet RS(A+\Delta_e)$
1	0	13	13	13	0	0	39
2	15	0	15	0	0	15	45
3	16	16	0	0	0	0	32
4	14	0	0	0	14	0	28
5	0	0	0	17	0	0	17
6	0	17	0	0	0	0	17
CS	45	46	28	30	14	15	178

Figure 4. Weighted Adjacency Matrices, $\boldsymbol{A}_{\mathbf{M}}$, for the Graph G_2.

Table 1. Matrices $\boldsymbol{W}_{(M_1,M_2,M_3)}$ involved in the calculation of $MTI(\boldsymbol{M}_1,\boldsymbol{A},\boldsymbol{M}_3)$, for graphs G_1 and G_2, are illustrated in Figures 3 and 4.

The novel proposed matrices, $\boldsymbol{V}_M = \boldsymbol{W}_{(A,1,M)}$ and $\boldsymbol{A}_M = \boldsymbol{W}_{(M,1,A)}$ offer just Schultz-Dobrynin-type indices (*e.g.*, $S(\boldsymbol{AD}_\mathrm{e}) = \boldsymbol{u}\boldsymbol{W}_{(A,1,De)}\boldsymbol{u}^\mathrm{T}$). Matrices $\boldsymbol{A}_M$, corresponding to the classical $MTI(\boldsymbol{A},\boldsymbol{A},\Delta_\mathrm{e})$ and to its detour-variant, $MTI(\boldsymbol{A},\boldsymbol{A},\Delta_\mathrm{e})$, are presented in Figures 3 and 4, respectively (last examples).

Use of unsymmetric matrices, such as ***CJ*u**, in construction of *MTI*-type indices, involves, in fact, the information storred in three topological matrices.[34] Other authors have also reported such »three matrix« – *MTI* indices.[37,41]

Matrices $\boldsymbol{V}_M$ and $\boldsymbol{A}_M$ represent a rational basis for the construction of topological indices. In addition, they could offer other molecular descriptors, such as polynomials and eigenvalues, which deserve further investigations.

CONCLUSIONS

A review of basic topological matrices: the adjacency matrix, the distance matrix, the Wiener matrix, the detour matrix, the Szeged matrix and the Cluj matrix has been presented. Walk matrix, $\boldsymbol{W}_{(M_1,M_2,M_3)}$, operating on these matrices by a non-Cramer matrix algebra, offers matrices whose row sums express the product between a local property of a vertex i and its valency. One of the two variants of the newly proposed valency-property matrices is derived by a simple graphical method. Relations of the indices, calculated on these matrices, with the well known Schultz and Dobrynin (valency-distance) indices, as well as with some novel Schultz-type indices have been discussed. Further use of the obtained matrices in calculating polynomials and eigenvalues is suggested.

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SAŽETAK

Valencije svojstava

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Temeljne topološke matrice: matrica susjedstva, $\boldsymbol{A}$, matrica udaljenosti, $\boldsymbol{D}$, Wienerova matrica, $\boldsymbol{W}$, matrica zaobilazaka, Δ, Szegedska matrica, $\boldsymbol{SZ}_{\mathrm{u}}$ i Clujska matrica, $\boldsymbol{CJ}_{\mathrm{u}}$, nakon primjene operatora izraženog matricom šetnji, $\boldsymbol{W}_{(M_1, M_2, M_3)}$, prelaze u matrice čije sume po retcima daju umnožak valencije pripadnog čvora grafa i lokalnog svojstva tog čvora. Te se matrice dadu dobiti jednostavnim grafovskim postupkom. Na primjerima je pokazana primjena pripadne ne-Cramerove matrične algebre. Diskutira se o vezi ovdje uvedenih indeksa s dobro poznatim indeksima Schultza i Dobrynina. Predložena je daljnja primjena ovdje uvedenih matrica i pripadnih topoloških indeksa.