Matrix Operator, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$, and Schultz-Type Indices

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Received April 1, 1997⊗

Recently proposed matrix operator, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$, is used to generate the molecular topological index, MTI, and novel Schultz-type descriptors. Matrix algebra involved by this operator is exemplified and discussed in comparison to the Cramer algebra.

INTRODUCTION

Among the modifications of the Wiener index,[1] W, the molecular topological index, MTI, proposed by Schultz,[2] appears to be one of the most studied topological indices.[3−18] It is defined as

$$\mathrm{MTI} = \sum_i [\mathbf{v}(\mathbf{A} + \mathbf{D})]_i \tag{1}$$

where **A** and **D** are the adjacency and the distance matrices, respectively, and $\mathbf{v} = (v_1, v_2, ..., v_N)$ is the vector of the vertex valencies/degrees in a connected graph, G. Recall that the entries in **A** are equal to unity if vertices i and j are adjacent and zero otherwise. The distance matrix collects the number of edges on the shortest path joining the vertices i and j.

By applying the matrix algebra, MTI can be written[8,13,15,19,20] as

$$\mathrm{MTI} = \mathbf{uA}(\mathbf{A} + \mathbf{D})\mathbf{u}^{\mathrm{T}} = S(\mathbf{A}^2) + S(\mathbf{AD}) \tag{2}$$

where

$$S(\mathbf{A}^2) = \mathbf{uA}^2\mathbf{u}^{\mathrm{T}} = \sum_i\sum_j [\mathbf{A}^2]_{ij} = \sum_i (v_i)^2 \tag{3}$$

$$S(\mathbf{AD}) = \mathbf{uADu}^{\mathrm{T}} = \sum_i\sum_j [\mathbf{AD}]_{ij} = \sum_i (v_i d_i) \tag{4}$$

The term $S(\mathbf{A}^2)$ is just the first Zagreb group index, while $S(\mathbf{AD})$ is the true Schultz index (i.e., the nontrivial part of MTI), then reinvented by others.[19,21] The parameter d_i (eq 4) stands for the ith row sum of entries in the distance matrix: $d_i = \sum_i [\mathbf{D}]_{ij}$. In the above relations, **u** and $\mathbf{u}^{\mathrm{T}}$ 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.[19,20] for rejecting the double sum symbol.

In acyclic structures, there exists[12,14,15] a linear correlation between the number $S(\mathbf{AD})$ and the Wiener index

$$S(\mathbf{AD}) = 4W - N(N - 1) \tag{5}$$

S in symbols of the type $S(\mathbf{AD})$ reminds the name of Schultz.

Recall that the Wiener index, in acyclic structures, can be calculated[1] by

$$W = \sum_{(i,j)} N_i N_j \tag{6}$$

where N_i and N_j denote the number of vertices on the two sides of the edge (i,j). The products N_iN_j are just the entries in the Wiener matrix,[22,23] $\mathbf{W}_{\mathrm{e}}$, so that W can be calculated by

$$W = (1/2)\sum_i\sum_j [\mathbf{W}_{\mathrm{e}}]_{ij} = (1/2)\mathbf{uW}_{\mathrm{e}}\mathbf{u}^{\mathrm{T}} \tag{7}$$

In cycle-containing graphs, W can be calculated by means of the **D** matrix[24]

$$W = (1/2)\sum_i\sum_j [\mathbf{D}]_{ij} = (1/2)\mathbf{uDu}^{\mathbf{T}} \tag{8}$$

Gutman[15] has expressed the $S(\mathbf{AD})$ index by analogy to the Wiener index (cf. eq 6)

$$S(\mathbf{AD}) = \sum_{(i,j)} [N_i \sum_{k\in I} v_k + N_j \sum_{k\in J} v_k] \tag{9}$$

where $\sum_{k\in I}$ and $\sum_{k\in J}$ 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.[15,19]

The present paper proposes a joint of the Cramer- and the Hadamard-matrix algebra by means of the $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$ matrix. On this ground an extension of the definition of MTI and $S(\mathbf{AD})$ indices is proposed.

SCHULTZ-TYPE INDICES AND WALK MATRIX, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$

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, can be written (in Cramer matrix algebra) as

$$\mathrm{MTI}(\mathbf{M}_1,\mathbf{A},\mathbf{M}_3) = \mathbf{uM}_1(\mathbf{A} + \mathbf{M}_3)\mathbf{u}^{\mathrm{T}} = \mathbf{u}(\mathbf{M}_1\mathbf{A} + \mathbf{M}_1\mathbf{M}_3)\mathbf{u}^{\mathrm{T}} = S(\mathbf{M}_1\mathbf{A}) + S(\mathbf{M}_1\mathbf{M}_3) \tag{10}$$

It is easily seen that $\mathrm{MTI}(\mathbf{A},\mathbf{A},\mathbf{D})$ is the Schultz original index. Analogue Schultz indices of sequence, $(\mathbf{D},\mathbf{A},\mathbf{D})$,

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⊗ Abstract published in *Advance ACS Abstracts,* October 1, 1997.

Chart 1. Schultz Index by Cramer Matrix Algebra for the Graph G_1

A

	1	2	3	4	5	6	7	
1	0	1	0	0	0	0	0	1
2	1	0	1	0	0	1	0	3
3	0	1	0	1	0	0	1	3
4	0	0	1	0	1	0	0	2
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

$\mathbf{uAu}^T = 12$

D

	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

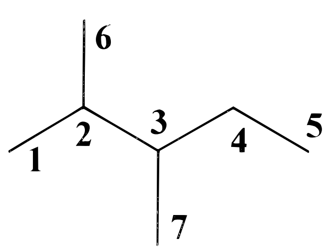
$\mathbf{uDu}^T = 92$

A(A + D)

	1	2	3	4	5	6	7	
1	2	0	2	2	3	2	2	13
2	4	6	4	8	10	4	8	44
3	8	4	6	4	8	8	4	42
4	6	5	2	4	2	6	5	30
5	3	2	2	0	2	3	2	14
6	2	0	2	2	3	2	2	13
7	2	2	0	2	2	2	2	12
	27	19	18	22	30	27	25	

$\mathbf{uA(A+D)u}^T = 168$

(**RD**,**A**,**RD**), and ($\mathbf{W}_p$,**A**,$\mathbf{W}_p$), have been proposed and tested for correlating ability.[16,17,20,25] In the above sequence, **RD** represents the matrix whose nondiagonal entries are $1/[\mathbf{D}]_{ij}$; $\mathbf{W}_p$ is the Wiener-path matrix, i.e., the matrix defined by relation 6 when (i,j) represents a path. Cramer-matrix algebra concerning eqs 2 and 10 ($\mathbf{M}_1 = \mathbf{M}_3$) is illustrated for the graph G_1 (2,3-methylpentane) in the Charts 1 and 2.



$\mathbf{G_1}$

Walk matrix, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$, was defined,[25−27] according to the principle of a single endpoint characterization of a path, as

$$[\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)]_{ij} = {}^{[\mathbf{M}_2]_{ij}}\mathbf{W}_{\mathbf{M}_1,i}[\mathbf{M}_3]_{ij} \qquad (11)$$

where $\mathbf{W}_{\mathbf{M}_1,i}$ is the walk degree[26] of the vertex i, weighted by the property collected in the matrix $\mathbf{M}_1$ (*i.e.*, the ith row

Chart 2. Matrices $\mathbf{W}_e$, **AD**, and $\mathbf{AW}_e$ for the Graph G_1

$\mathbf{W_e}$

	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
	6	24	28	16	6	6	6	

$\mathbf{uW_eu}^T = 92$

AD

	1	2	3	4	5	6	7	
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
	24	14	12	18	28	24	22	

$\mathbf{uADu}^T = 142$

$\mathbf{AW_e}$

	1	2	3	4	5	6	7	
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	25
7	0	12	0	10	0	0	6	28
	18	48	62	36	12	18	18	

$\mathbf{uAW_eu}^T = 212$

sum in the matrix $\mathbf{M}_1$); $[\mathbf{M}_2]_{ij}$ gives the length of the walk, and the factor $[\mathbf{M}_3]_{ij}$ is taken from a third square matrix. Its diagonal entries are zero.

It is a square, (in general) nonsymmetric matrix, of dimension $N \times N$ and was illustrated in refs 26 and 27. In the form $[1/\mathbf{W}(\mathbf{A},\mathbf{D},\mathbf{1})]_{ij}$ (where **1** is the matrix having its (ij)-entries equal to 1 if $i \neq j$ and zero otherwise), it has been defined in connection with the Harary-type indices[28] and proved to be identical to the "restricted random walk matrix" proposed by Randić.[29] In fact, this matrix is a true operator, as will be shown below.

Let, first, the combination ($\mathbf{M}_1$,$\mathbf{M}_2$,$\mathbf{M}_3$) be ($\mathbf{M}_1$,**1**,**1**). In this case, each column in the matrix $\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{1})$ is identical to the vector RS($\mathbf{M}_1$) (*i.e.*, the product $\mathbf{M}_1\mathbf{u}^T = \mathbf{u}\mathbf{M}_1^T$) except the (ii)-entries which are zero. Next, consider the combination ($\mathbf{M}_1$,**1**,$\mathbf{M}_3$); the corresponding walk matrix results as a Hadamard (pairwise) product[30] (*i.e.*, $[\mathbf{M}_a\bullet\mathbf{M}_b]_{ij} = [\mathbf{M}_a]_{ij}[\mathbf{M}_b]_{ij}$)

$$\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3) = \mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{1})\bullet\mathbf{M}_3 \qquad (12)$$

Recall that the sum of all entries in the Cramer product matrix, $\mathbf{M}_1\mathbf{M}_3$, can be achieved by multiplying their RS and CS vectors (*i.e.*, the sum of entries on rows and columns, respectively)

$$\sum_i\sum_j[\mathbf{M}_1\mathbf{M}_3]_{ij} = \mathrm{CS}(\mathbf{M}_1)\ \mathrm{RS}(\mathbf{M}_3) = \mathbf{u}\mathbf{M}_1\mathbf{M}_3\mathbf{u}^T \qquad (13)$$

Between $\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3)$ and the Cramer product $\mathbf{M}_1\mathbf{M}_3$ there exist the following relations

$$\mathrm{CS}(\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)) = \mathbf{u}\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3) = \mathrm{CS}(\mathbf{M}_1\mathbf{M}_3) = \mathbf{u}\mathbf{M}_1\mathbf{M}_3 \quad (14)$$

$$\mathrm{CS}(\mathbf{W}(\mathbf{M}_3,\mathbf{1},\mathbf{M}_1^{\mathrm{T}})) = \mathbf{u}\mathbf{W}(\mathbf{M}_3,\mathbf{1},\mathbf{M}_1^{\mathrm{T}}) = \mathrm{RS}(\mathbf{M}_1\mathbf{M}_3) = \mathbf{M}_1\mathbf{M}_3\mathbf{u}^{\mathrm{T}} \quad (15)$$

$$\mathrm{RS}(\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)) = \mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)\mathbf{u}^{\mathrm{T}} = \mathrm{RS}(\mathbf{M}_1^{\mathrm{T}})\cdot\mathrm{RS}(\mathbf{M}_3) \quad (16)$$

$$\mathrm{RS}(\mathbf{W}(\mathbf{M}_3,\mathbf{1},\mathbf{M}_1^{\mathrm{T}})) = \mathbf{W}(\mathbf{M}_3,\mathbf{1},\mathbf{M}_1^{\mathrm{T}})\mathbf{u}^{\mathrm{T}} = \mathrm{RS}(\mathbf{M}_3)\cdot\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}}) \quad (17)$$

$$\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}})\cdot\mathrm{RS}(\mathbf{M}_3) = \mathrm{RS}(\mathbf{M}_3)\cdot\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}}) \quad (18)$$

From (16) and (13) one can write

$$\mathbf{u}\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)\mathbf{u}^{\mathrm{T}} = \mathbf{u}(\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}})\cdot\mathrm{RS}(\mathbf{M}_3)) = \mathbf{u}\mathbf{M}_1\mathbf{M}_3\mathbf{u}^{\mathrm{T}} = \mathrm{CS}(\mathbf{M}_1)\mathrm{RS}(\mathbf{M}_3) \quad (19)$$

Equations 16−18 show that the product within the matrix $\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)$ is commutative. Equation 19 is the most important among the above six relations: it joins the Hadamard- and the Cramer-matrix algebra by means of the $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$ matrix. Moreover, it suggests that the product matrix, $\mathbf{M}_1\mathbf{M}_3$, can also be viewed as a collection of pairwise products of local properties (encoded as row sums). These relations are illustrated, for the graph G_1, in Chart 3.

A condition for identical $\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3)$ matrices (for one and the same graph) can be formulated.

$$\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3) \equiv \mathbf{W}(\mathbf{M'}_1,\mathbf{1},\mathbf{M}_3) \Leftrightarrow \mathrm{RS}(\mathbf{M}_1) \equiv \mathrm{RS}(\mathbf{M'}_1) \quad (20)$$

Examples of identical $\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3)$ matrices will be given below.

A condition for degeneracy (*i.e.*, a single value for two different graphs, G_a and G_b) of the sum of entries in the product matrix $\mathbf{M}_1\mathbf{M}_3$ can be drawn from eqs 18 and 19

$$\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}}(G_a))\cdot\mathrm{RS}(\mathbf{M}_3(G_a)) = \mathrm{RS}(\mathbf{M}_3(G_b))\cdot\mathrm{RS}(\mathbf{M}_1^{\mathrm{T}}(G_b)) \quad (21)$$

From relation 19 it is obvious that the same condition is also true for the degeneracy within the $\mathbf{W}(\mathbf{M}_1,\mathbf{1},\mathbf{M}_3)$ matrix.

The walk matrix, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$, can be related to the Schultz numbers (cf. eq 10) as follows:

$$S(\mathbf{M}_1\mathbf{A}) = \mathbf{u}\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{A})\mathbf{u}^{\mathrm{T}} \quad (22)$$

$$S(\mathbf{M}_1\mathbf{M}_3) = \mathbf{u}\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3)\mathbf{u}^{\mathrm{T}} \quad (23)$$

$$\mathrm{MTI}(\mathbf{M}_1,\mathbf{A},\mathbf{M}_3) = \mathbf{u}(\mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{A}) + \mathbf{W}(\mathbf{M}_1^{\mathrm{T}},\mathbf{1},\mathbf{M}_3))\mathbf{u}^{\mathrm{T}} \quad (24)$$

It is easily seen that eqs 10 and 24 are equivalent.

Equation 23 can be extended for raising at a power $n + 1$ a square matrix $\mathbf{M} = \mathbf{M}_1 = \mathbf{M}_3$ by the aid of the walk matrix

$$\mathbf{u}(\mathbf{M}^{n+1})\mathbf{u}^{\mathrm{T}} = \mathbf{u}\mathbf{W}(\mathbf{M}^{\mathrm{T}},\mathbf{n},\mathbf{M})\mathbf{u}^{\mathrm{T}} = \mathbf{u}\mathbf{W}(\mathbf{M},\mathbf{n},\mathbf{M}^{\mathrm{T}})\mathbf{u}^{\mathrm{T}} \quad (25)$$

Chart 3. Schultz-Type Indices by $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$ Algebra for the Graph G_1

W(A,1,1)

	1	2	3	4	5	6	7	
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

W(A,1,A)

	1	2	3	4	5	6	7	
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	

$\mathrm{u}\mathbf{W}(\mathbf{A},\mathbf{1},\mathbf{A})\mathrm{u}^{\mathrm{T}} = 26$

W(A,1,D)

	1	2	3	4	5	6	7	
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
	24	14	12	18	28	24	22	

$\mathrm{u}\mathbf{W}(\mathbf{A},\mathbf{1},\mathbf{D})\mathrm{u}^{\mathrm{T}} = 142$

W(D,1,1)

	1	2	3	4	5	6	7	
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

W(D,1,A)

	1	2	3	4	5	6	7	
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	

$\mathrm{u}\mathbf{W}(\mathbf{D},\mathbf{1},\mathbf{A})\mathrm{u}^{\mathrm{T}} = 142$

W(D,1,D)

	1	2	3	4	5	6	7	
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	

$\mathrm{u}\mathbf{W}(\mathbf{D},\mathbf{1},\mathbf{D})\mathrm{u}^{\mathrm{T}} = 1260$

where $\mathbf{n}$ is the matrix having the (ij)-entries $[\mathbf{n}]_{ij}$ for $i \neq j$ and zero for $i = j$.

Table 1. Wiener W, Hyper-Cluj CJ_p, Hyper-Szeged, SZ_p, and Some $S(\mathbf{M}^2)$ Indices in Octane Isomers

graph[a]	W	CJ_p	SZ_p	$S(\mathbf{A}^2)$	$S(\mathbf{D}^2)$	$S(\mathbf{CJ}_u{}^2)$	$S(\mathbf{SZ}_u{}^2)$
C8	84	210	340	13	1848	1596	2620
2MC7	79	185	320	14	1628	1396	2430
3MC7	76	170	307	14	1512	1284	2380
4MC7	75	165	294	14	1476	1248	2302
3EC6	72	150	272	14	1360	1136	2142
25M2C6	74	161	308	15	1420	1206	2286
24M2C6	71	147	288	15	1312	1102	2195
23M2C6	70	143	282	15	1280	1072	2154
34M2C6	68	134	268	15	1208	1004	2074
3E2MC5	67	129	242	15	1172	968	1858
22M2C6	71	149	280	16	1316	1112	2089
33M2C6	67	131	250	16	1176	978	1939
234M3C5	65	122	258	16	1096	906	1922
3E3MC5	64	118	220	16	1072	880	1702
224M3C5	66	127	254	17	1128	940	1868
223M3C5	63	115	242	17	1032	850	1784
233M3C5	62	111	234	17	1000	820	1730
2233M4C4	58	97	232	19	868	706	1570

[a] M = methyl; E = ethyl.

Values $S(\mathbf{M}_1\mathbf{M}_3)$, $S(\mathbf{M}_1\mathbf{A})$, and the corresponding indices MTI($\mathbf{M}_1$,$\mathbf{A}$,$\mathbf{M}_3$) ($\mathbf{M}_1 = \mathbf{M}_3$) for octanes are listed in Tables 1 and 2; matrices involved in the calculation of MTI-($\mathbf{M}_1$,$\mathbf{A}$,$\mathbf{M}_3$) indices, for the graph G_1, are illustrated in Charts 3 and 4.

SZEGED AND CLUJ MATRICES IN SCHULTZ-TYPE INDICES

Two unsymmetric matrices, $\mathbf{M}_u$, ($\mathbf{M} = \mathbf{SZ}$, Szeged and $\mathbf{CJ}$, Cluj) have been recently proposed by one of us.[27,31−34] They are defined according to the principle[25−27,31,32] of single endpoint characterization of a path, (i,j) (having its endpoints the vertices i and j)

$$[\mathbf{M}_u]_{ij} = \mathbf{N}_{i,p_k(i,j)} = |V_{i,p_k(i,j)}| \tag{26}$$

$$V_{i,p_k(ij)} = \{v | v \in V(G); [D_e]_{iv} < [D_e]_{jv}\} \tag{27}$$

Chart 4. Schultz Index by $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$ Algebra for the Graph G_1

A+D

	1	2	3	4	5	6	7	
1	0	2	2	3	4	2	3	16
2	2	0	2	2	3	2	2	13
3	2	2	0	2	2	2	2	12
4	3	2	2	0	2	3	2	14
5	4	3	2	2	0	4	3	18
6	2	2	2	3	4	0	3	16
7	3	2	2	2	3	3	0	15
	16	13	12	14	18	16	15	

W(A,1,A) + W(A,1,D)

	1	2	3	4	5	6	7	
1	0	2	2	3	4	2	3	16
2	6	0	6	6	9	6	6	39
3	6	6	0	6	6	6	6	36
4	6	4	4	0	4	6	4	28
5	4	3	2	2	0	4	3	18
6	2	2	2	3	4	0	3	16
7	3	2	2	2	3	3	0	15
	27	19	18	22	30	27	25	

$\mathbf{u}(\mathbf{W}(\mathbf{A},1,\mathbf{A}) + \mathbf{W}(\mathbf{A},1,\mathbf{D}))\mathbf{u}^T = 168$

W((A+D),1,A)

	1	2	3	4	5	6	7	
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	

$\mathbf{u}\mathbf{W}((\mathbf{A}+\mathbf{D}),1,\mathbf{A})\mathbf{u}^T = 168$

$$V_{i,p_k(i,j)} = \{v | v \in V(G); D_{iv} < D_{jv}; p_h(i,v) \cap p_k(i,j) = \{i\}; p_k(i,j)| = \min\} \tag{28}$$

$N_{i,p_k(i,j)} = |V_{i,p_k(i,j)}|$ is the number of elements of the set $V_{i,p_k(i,j)}$, for $\mathbf{CJ}_u$, the maximum value, $\max|V_{i,p_k(i,j)}|$, is taken over all paths $p_k(i,j)$. Diagonal entries are zero. The symbol $N_{i,p_k(i,j)}$ remembers the definition of the Wiener index (cf. eq 6).

Table 2. $S(\mathbf{M}_1\mathbf{A})$ and MTI($\mathbf{M}_1$,$\mathbf{A}$,$\mathbf{M}_3$)[a] Indices in Octane Isomers

graph[b]	$S(\mathbf{AD})$	$S(\mathbf{AW}_e)$	$S(\mathbf{CJ}_u\mathbf{A})$	$S(\mathbf{SZ}_u\mathbf{A})$	(**D**,**A**,**Dq**)	($\mathbf{CJ}_u$,**A**,$\mathbf{CJ}_u$)	($\mathbf{SZ}_u$,**A**,$\mathbf{SZ}_u$)	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

[a] Schultz-type indices, MTI($\mathbf{M}_1$,$\mathbf{A}$,$\mathbf{M}_3$), are written as the sequence ($\mathbf{M}_1$,$\mathbf{A}$,$\mathbf{M}_3$); the original Schultz index is written as MTI. [b] M = methyl; E = ethyl.

Chart 5. Matrices $\mathbf{SZ}_u$ and $\mathbf{CJ}_u$ for the Graph G_1

$\mathbf{SZ_u}$

	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	

$\mathrm{SZ_p} = \sum_{(ij)} [\mathbf{SZ_u}]_{ij}\, [\mathbf{SZ_u}]_{ji} = 151$

$\mathbf{CJ_u}$

	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	

$\mathrm{CJ_p} = \sum_{(ij)} [\mathbf{CJ_u}]_{ij}\, [\mathbf{CJ_u}]_{ji} = 83$

Vertices of the set $V_{i,p_k(i,j)}$ are selected as follows: (i) for $\mathbf{SZ}_u$, they obey the original condition formulated by Gutman[35] for the Szeged index (eq 27). Such vertices lie closer to the vertex i, with respect to the path (ij). (ii) for $\mathbf{CJ}_u$, the set $V_{i,p_k(i,j)}$ consists of the vertices lying *closer* to the vertex i, and *external* with respect to the path $p_k(i,j)$ (condition $p_h(i,v) \cap p_k(i,j) = \{i\}$, eq 28). Since in cycle-containing structures, various shortest 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 $|V_{i,p_k(i,j)}|$ (see above).

Both matrices, $\mathbf{SZ}_u$ and $\mathbf{CJ}_u$, are defined in any connected graph, in contrast to the Wiener matrix, defined only in acyclic graphs. The externality condition (see above) strongly differentiates the two matrices (and their invariants). For the graph G_1 they are illustrated in Chart 5.

The two unsymmetric matrices allow the construction of the corresponding symmetric matrices, $\mathbf{M}_p$ (defined on paths) and $\mathbf{M}_e$ (defined on edges), by

$$\mathbf{M}_p = \mathbf{M}_u \cdot \mathbf{M}_u^{\mathrm{T}} \qquad (29)$$

$$\mathbf{M}_e = \mathbf{M}_p \cdot \mathbf{A} \qquad (30)$$

In acyclic structures, the Cluj matrices, $\mathbf{CJ}_e$ and $\mathbf{CJ}_p$, are identical to the Wiener matrices, $\mathbf{W}_e$ and $\mathbf{W}_p$. In cyclic graphs, $\mathbf{CJ}_e$ superimposes on $\mathbf{SZ}_e$, while $\mathbf{CJ}_p$ is different from $\mathbf{SZ}_p$. In trees, the Cluj matrix obeys the relations[31]

$$\mathrm{RS}(\mathbf{CJ}_u) = \mathrm{RS}(\mathbf{W}_e) \qquad (31)$$

$$\mathrm{CS}(\mathbf{CJ}_u) = \mathrm{CS}(\mathbf{D}) \qquad (32)$$

Thus, $\mathbf{CJ}_u$ is a chimera between $\mathbf{D}$ and $\mathbf{W}_e$ (see below).

Several indices can be calculated[27,31−34] on these matrices, either as the half-sum of their entries (a relation of the type 7) or by

$$I_{e/p} = \sum_{(ij)} [\mathbf{M}_u]_{ij} [\mathbf{M}_u]_{ji} \qquad (33)$$

When defined on edges, I_e is an index (*e.g.*, $\mathrm{SZ_e}$, the classical Szeged index); when defined on paths, I_p is a hyperindex (*e.g.*, $\mathrm{SZ_p}$ and $\mathrm{CJ_p}$). Note that, in acyclic graphs, $\mathrm{SZ_e} = \mathrm{CJ_e} = W$; also note that $\mathrm{SZ_e} = \mathrm{CJ_e}$ in any connected graph. For other relations see ref 34. Values of these indices in octanes are listed in Table 1.

Coming back to the Schultz-type indices (eq 10), we consider the case of $\mathbf{CJ}_u$ in the sequence $(\mathbf{M}_1,\mathbf{A},\mathbf{M}_3) = (\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u)$. Since the Cramer product is not commutative, and since $\mathbf{CJ}_u$ is an unsymmetric matrix, there exists a strong reason (see eq 13) to write a Schultz-type index as

$$\begin{aligned}\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u) &= (\mathbf{u}(\mathbf{CJ}_u)\mathbf{A}\mathbf{u}^{\mathrm{T}} + \mathbf{u}\mathbf{A}(\mathbf{CJ}_u)\mathbf{u}^{\mathrm{T}})/2 + \mathbf{u}(\mathrm{CJ}_u)^2\mathbf{u}^{\mathrm{T}} \\ &= (\mathbf{u}(\mathbf{CJ}_u)\mathbf{A}\mathbf{u}^{\mathrm{T}} + \mathbf{u}(\mathbf{CJ}_u^{\mathrm{T}})\mathbf{A}\mathbf{u}^{\mathrm{T}})/2 + \mathbf{u}(\mathrm{CJ}_u)^2\mathbf{u}^{\mathrm{T}} = S(\mathbf{CJ}_u\mathbf{A}) + S(\mathbf{CJ}_u^{\,2})\end{aligned} \qquad (34)$$

By virtue of relations 31 and 32, in acyclic structures, relation 34 can be written as

$$\begin{aligned}\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u) &= (\mathbf{uDAu}^{\mathrm{T}} + \mathbf{uAW}_e\mathbf{u}^{\mathrm{T}})/2 + \mathbf{uDW}_e\mathbf{u}^{\mathrm{T}} \\ &= (S(\mathbf{DA}) + S(\mathbf{AW}_e))/2 + S(\mathbf{DW}_e)\end{aligned} \qquad (35)$$

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

Bearing in mind relations 11 and 24, $\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u)$ can be written as

$$\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u) = (\mathbf{uW}(\mathbf{CJ}_u^{\mathrm{T}},\mathbf{1},\mathbf{A})\mathbf{u}^{\mathrm{T}} + \mathbf{uW}(\mathbf{CJ}_u,\mathbf{1},\mathbf{A})\mathbf{u}^{\mathrm{T}})/2 + \mathbf{uW}(\mathbf{CJ}_u^{\mathrm{T}},\mathbf{1},\,\mathbf{CJ}_u)\mathbf{u}^{\mathrm{T}} \qquad (36)$$

which gives the exact result of eq 34 or 35. Relations 34 and 36 allow the calculation of this index in any connected graph. Thus, irrespective of being calculated, by Cramer or Hadamard algebra, the index can be written as in (37). The equivalence of the Schultz-type terms is immediate.

$$\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u) = S(\mathbf{CJ}_u\mathbf{A}) + S(\mathbf{CJ}_u^{\,2}) = (S(\mathbf{DA}) + S(\mathbf{AW}_e))/2 + S(\mathbf{DW}_e) \qquad (37)$$

Equation 37 offers a MTI number which encloses the information of three matrices, as suggested by relation 10. Values $\mathrm{MTI}(\mathbf{CJ}_u,\mathbf{A},\mathbf{CJ}_u)$ (denoted in refs 27 and 34 as $\mathbf{CJ}_u\mathbf{I}$) are given in Table 2.

Returning to eq 20 and considering again relations 31 and 32, some examples of identical walk matrices are given

$$\mathbf{W}(\mathbf{W}_e,\mathbf{1},\mathbf{A}) \equiv \mathbf{W}(\mathbf{CJ}_u,\mathbf{1},\mathbf{A}); \quad \mathbf{W}(\mathbf{D},\mathbf{1},\mathbf{A}) \equiv \mathbf{W}(\mathbf{CJ}_u^{\mathrm{T}},\mathbf{1},\mathbf{A})$$

$$\mathbf{W}(\mathbf{W}_e,\mathbf{1},\mathbf{CJ}_u) \equiv \mathbf{W}(\mathbf{CJ}_u,\mathbf{1},\mathbf{CJ}_u); \quad \mathbf{W}(\mathbf{D},\mathbf{1},\mathbf{CJ}_u^{\mathrm{T}}) \equiv \mathbf{W}(\mathbf{CJ}_u^{\mathrm{T}},\mathbf{1},\mathbf{CJ}_u^{\mathrm{T}})$$

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

$$\mathrm{MTI}(\mathbf{SZ}_u,\mathbf{A},\mathbf{SZ}_u) = (\mathbf{u}(\mathbf{SZ}_u)\mathbf{A}\mathbf{u}^T + \mathbf{u}\mathbf{A}(\mathbf{SZ}_u)\mathbf{u}^T)/2 + \mathbf{u}(\mathbf{SZ}_u)^2\mathbf{u}^T$$

$$= (\mathbf{u}(\mathbf{SZ}_u)\mathbf{A}\mathbf{u}^T + \mathbf{u}(\mathbf{SZ}_u{}^T)\mathbf{A}\mathbf{u}^T)/2 + \mathbf{u}(\mathbf{SZ}_u)^2\mathbf{u}^T \quad (38)$$

$$\mathrm{MTI}(\mathbf{SZ}_u,\mathbf{A},\mathbf{SZ}_u) = (\mathbf{uW}(\mathbf{SZ}_u{}^T,\mathbf{1},\mathbf{A})\mathbf{u}^T + \mathbf{uW}(\mathbf{SZ}_u,\mathbf{1},\mathbf{A})\mathbf{u}^T)/2 + \mathbf{uW}(\mathbf{SZ}_u{}^T,\mathbf{1}, \mathbf{SZ}_u)\mathbf{u}^T \quad (39)$$

$$\mathrm{MTI}(\mathbf{SZ}_u,\mathbf{A},\mathbf{SZ}_u) = S(\mathbf{SZ}_u\mathbf{A}) + S(\mathbf{SZ}_u{}^2) \quad (40)$$

Values MTI($\mathbf{SZ}_u$,**A**,$\mathbf{SZ}_u$) (denoted in ref 34 as $\mathbf{SZ}_u\mathbf{I}$) are given in Table 2.

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

Conjecture: the sum, over all vertices in a 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*

$$\mathbf{uA}(\mathbf{SZ}_u)\mathbf{u}^T = \mathbf{u}(\mathbf{RS}(\mathbf{A})\cdot\mathrm{RS}(\mathbf{SZ}_u)) = 2\left(2\binom{N}{3} + \binom{N+1}{3}\right) \quad (41)$$

In other words, the sum on the product to the left of the Szeged matrix $\mathbf{SZ}_u$ with the adjacency matrix is a constant. In contrast, the product to the right, $\mathbf{u}(\mathbf{SZ}_u)\mathbf{Au}^T = \mathbf{u}(\mathrm{RS}(\mathbf{A})\cdot\mathrm{CS}(\mathbf{SZ}_u))$ is variable within a set of acyclic isomers.

Schultz-type indices show good correlation[34] with some physicochemical properties of octanes, in two-variable regression: boiling points (MTI(**D**,**A**,**D**) and MTI $= 0.953$), critical pressure (MTI($\mathbf{CJ}_u$,**A**,$\mathbf{CJ}_u$) and MTI $= 0.988$; MTI($\mathbf{SZ}_u$,**A**,$\mathbf{SZ}_u$) and $\chi = 0.967$, χ being the connectivity index[36]), octane number (MTI($\mathbf{CJ}_u$,**A**,$\mathbf{CJ}_u$) and MTI $= 0.987$). Note that the Schultz original index MTI(**A**,**A**,**D**) was written above as simple MTI.

CONCLUSIONS

Walk matrix, $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$, is an interesting operator which works according to the Hadamard-matrix algebra. It offers various global invariants, a function of matrix combinations. Thus, it can be used as an alternative to the Cramer-matrix algebra to calculate Schultz-type indices. Other properties and applications of this operator will be presented in a further study.[37]

ACKNOWLEDGMENT

Many thanks are expressed to Professors Ivan Gutman, University of Kragujevac, Yugoslavia, and Bazil Parv, "Babes-Bolyai" University, Cluj, Romania, for helpful discussions.

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CI970019U