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Cluj Matrix, $\mathbb{CJ}_u$: Source of Various Graph Descriptors

Mircea V. Diudea

Department of Chemistry, "Babes-Bolyai" University, 3400 Cluj, Romania

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Abstract: *The recently proposed unsymmetric square matrix,* $\mathbb{CJ}_u$, *is operated by the more general unsymetric square matrix operator,* $\mathbb{W}_{(M1,M2,M3)}$, *and discussed in the terms of walk numbers . It is shown that* $\mathbb{CJ}_u$ *and the novel distance extended* $\mathbb{D}\_\mathbb{CJ}_u$ *matrix can be used both as sources for graph invariants, such as: Wiener,* ***W****, hyper-Wiener,* ***WW****, Wiener-type numbers of higher rank, and Schultz analogues, and also as partners of other square matrices within the matrix operator,* $\mathbb{W}_{(M1,M2,M3)}$. *On the ground of* the two $\mathbb{CJ}_u$*-type matrices, novel (2D)- and (3D)-Wiener- and Schultz-type numbers are proposed.*

Introduction

Unsymmetric square matrices were introduced in mathematical chemistry since early '40 years, by Balandin [1] . Recently, Randić has proposed unsymmetric matrices based on restricted random walks [2]. In previous works [3-5] we have proposed unsymetric square matrices, constructed on the principle of a single endpoint characterization of paths. Such matrices are easily manipulated by conventional matrix algebra (in opposition to layer matrices [6-8]) and proved [3,9] to bring important additional information, in comparison with the symmetric square matrix descriptors.

One of these matrices, denoted $\mathbb{W}_{(M1,M2,M3)}$, is defined [5] by using walk numbers (*i.e.* row sums, ${}^{e}W_{M,i} = \sum_j[\mathbb{M}^e]_{ij}$, the superscript **e** being the length of walk)

$$[\mathbb{W}_{(M_1,M_2,M_3)}]_{ij} = {}^{[M_2]_{ij}}W_{M_1,i}\,[\mathbb{M}_3]_{ij} \qquad (1)$$

and operates on any square matrices, $\mathbb{M}_1$, $\mathbb{M}_2$ and $\mathbb{M}_3$. It can be used for performing matrix products, based on the following relations [10]

$$\sum_j [\mathbb{W}_{(M1,M2,M3)}]_{ij} = \sum_j ({}^1W_{M1,i}\ [\mathbb{M}_3]_{ij}) = {}^1W_{M1,i} \sum_j [\mathbb{M}_3]_{ij} = {}^1W_{M1,i}\ {}^1W_{M3,i} \qquad (2)$$

where 1 denotes the length of walk and is, at the same time, an entry in the matrix $\mathbb{M}_2$ (actually the matrix $\mathbb{1}$, having its entries $[\mathbb{1}]_{ij} = 1$). Relation **(2)** can be written as

$$ {}^1W_{(M1,1,M3),i} = {}^1W_{M1,i}\ {}^1W_{M3,i} \qquad (3)$$

and by summing over all vertices in graph one obtains

$$\sum_i {}^1W_{(M1,1,M3),i} = \sum_i ({}^1W_{M1,i} * {}^1W_{M3,i}) \qquad (4)$$

or as global walk numbers [5]

$$2\ {}^1W_{(M1,1,M3)} = 2\ {}^2W_{M1,M3} \qquad (5)$$

where ${}^2W_{M1,M3}$ is the mixed walk number of rank 2 (or the half sum of entries of the matrix product $\mathbb{M}_1\mathbb{M}_3$). Note that matrices and related quantities are symbolized by special capital letters whereas numbers (*i.e.* indices) by italics.

In this work, we extend the use of $\mathbb{W}_{(M1,M2,M3)}$ and the involvement of $\mathbb{CJ}_u$ matrix in the construction of several topological indices.

Cluj matrix, $\mathbb{CJ}_u$, and Wiener-Type Indices

In defining the Cluj matrix, $\mathbb{CJ}_u$, we started from the original relation given by Harold Wiener [11] for calculating its "path number", W, (also referred to as the Wiener number) in acyclic structures

$$I = \sum_{e/p} I_{e/p} = \sum_{e/p} N_{i,e/p} N_{j,e/p} \qquad (6)$$

where $N_{i,e/p}$ and $N_{j,e/p}$ denote the number of vertices on the two sides of edge/path, **e/p**, (*i.e.* edge/path **(i,j)** having the vertices **i** and **j** as endpoints). When is defined on edge, ***I*** is just the Wiener number, ***W***; when is defined on path, ***I*** equals the hyper-Wiener number, ***WW***, [12].

The Cluj matrix, $\mathbb{CJ}_u$, is defined by following the principle of a single endpoint characterization of paths [5] (see also [2])

$$[\mathbb{CJ}_u]_{ij} = N_{i,(ij)} \qquad (7)$$

$$N_{i,(ij)} = \max \left| \{u \mid u \in V(G);\ [\mathbb{D}_e]_{iu} < [\mathbb{D}_e]_{ju};\ (i,u) \cap (i,j) = \max \{i\};\ |(i,j)| = \min\} \right.$$

$\mathbb{CJ}_u$ is a square matrix, of dimension **N*N**, usually unsymmetric (except for some symmetric regular graphs). It collects all "external" paths, on the left of vertex i, which include the path **p** = **(i,j)**. Definition **(7)** holds both for acyclic [3] and cyclic structures [4]. We limit here to acyclic structures, for which Figure **1** gives an example. Also illustrated are the matrices: $\mathbb{D}_e$ (distance-edge), $\mathbb{W}_e$ (Wiener-edge), $\mathbb{W}_p$ (Wiener-path), $\mathbb{D}\_\mathbb{CJ}_u$ (distance extended unsymmetric Cluj matrix) and the derived Wiener-type indices, for the graph **1** (2,3-dimethylpentane). As can be seen from Figure 1, $\mathbb{CJ}_u$ matrix is a "chimera" between $\mathbb{D}_e$ (*i.e.* the classical $\mathbb{D}$ matrix) and $\mathbb{W}_e$ matrices. Its row sums are identical to the corresponding row sums in the Wiener matrix, $\mathbb{W}_e$

$$RS(\mathbb{CJ}_u)_i = RS(\mathbb{W}_e)_i \qquad (8)$$

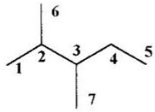
Conversely, their column sums equal to the corresponding column sums in the distance matrix $\mathbb{D}_e$

$$CS(\mathbb{CJ}_u)_j = CS(\mathbb{D}_e)_j \qquad (9)$$

and combining eqs **8** and **9** one can write

$$\textstyle\sum_i RS(\mathbb{CJ}_u)_i = \sum_i RS(\mathbb{W}_e)_i = \sum_j CS(\mathbb{CJ}_u)_j = \sum_j CS(\mathbb{D}_e)_j = 2W \qquad (10)$$

Figure 1. Distance-, Wiener- and Cluj-type matrices and derived Wiener-type indices for the graph 1



1

$\mathbb{D}_e$

	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

$W = D_e = (1/2)\sum_i \sum_j [\mathbb{D}_e]_{ij} = 46$

$\mathbb{W}_e$

	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

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

$\mathbb{D}_p$

	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

$WW = D_p = (1/2)\sum_i \sum_j [\mathbb{D}_p]_{ij} = 83$

$\mathbb{W}_p$

	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

$WW = W_p = (1/2)\sum_i \sum_j [\mathbb{W}_p]_{ij} = 83$

$\mathbb{CJ}_u$

	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	

$W = W_e = (1/2)\sum_i \sum_j [\mathbb{CJ}_u]_{ij} = 46$

$W = D_e = (1/2)\sum_j \sum_i [\mathbb{CJ}_u]_{ij} = 46$

$WW = \sum_{i<j} [\mathbb{CJ}_u]_{ij} [\mathbb{CJ}_u]_{ji} = 83$

$\mathbb{D}\_\mathbb{CJ}_u$

	1	2	3	4	5	6	7	
1	0	1	2	3	4	2	3	15
2	6	0	3	6	9	6	6	36
3	8	4	0	5	10	8	6	41
4	6	4	2	0	6	6	4	28
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
	29	15	12	20	36	29	25	

$WW = W_p = (1/2)\sum_i \sum_j [\mathbb{D}\_\mathbb{CJ}_u]_{ij} = 83$

$WW = D_p = (1/2)\sum_j \sum_i [\mathbb{D}\_\mathbb{CJ}_u]_{ij} = 83$

$D^2\_CJ_u = \sum_{i<j} [\mathbb{D}\_\mathbb{CJ}_u]_{ij} [\mathbb{D}\_\mathbb{CJ}_u]_{ji} = 268$

Figure 1 (continued)

(3D)D (optimized geometry)

	1	2	3	4	5	6	7
1	0.0000	1.5414	2.5709	3.9411	4.5163	2.5178	3.0305
2	1.5414	0.0000	1.5543	2.5634	3.0891	1.5388	2.5821
3	2.5709	1.5543	0.0000	1.5468	2.5852	2.5930	1.5395
4	3.9411	2.5634	1.5468	0.0000	1.5364	3.0398	2.5461
5	4.5163	3.0891	2.5852	1.5364	0.0000	3.6199	3.9326
6	2.5178	1.5388	2.5930	3.0398	3.6199	0.0000	3.2366
7	3.0305	2.5821	1.5395	2.5461	3.9326	3.2366	0.0000

$$\mathbf{(3D)}W = \mathbf{(3D)}D = (1/2)\sum_i \sum_j [\mathbf{(3D)D}]_{ij} = \mathbf{55.6216}$$

(3D)D_CJ$_u$

	1	2	3	4	5	6	7
1	0.0000	1.5414	2.5709	3.9411	4.5163	2.5178	3.0305
2	9.2484	0.0000	4.6629	7.6902	9.2673	9.2328	7.7463
3	10.2836	6.2172	0.0000	7.7340	12.9260	10.3720	9.2370
4	7.8822	5.1268	3.0936	0.0000	9.2184	6.0796	5.0922
5	4.5163	3.0891	2.5852	1.5364	0.0000	3.6199	3.9326
6	2.5178	1.5388	2.5930	3.0398	3.6199	0.0000	3.2366
7	3.0305	2.5821	1.5395	2.5461	3.9326	3.2366	0.0000

$$\mathbf{(3D)}WW = (1/2)\sum_i \sum_j [\mathbf{(3D)D\_CJ_u}]_{ij} = (1/2)\sum_j \sum_i [\mathbf{(3D)D\_CJ_u}]_{ij} = \mathbf{105.9607}$$

$$\mathbf{(3D)}\ D^2\_CJ_u = \sum_{i<j} [\mathbf{(3D)D\_CJ_u}]_{ij}\ [\mathbf{(3D)D\_CJ_u}]_{ji} = \mathbf{211.0212}$$

where W is the classical Wiener number. Relations **(8)** to **(10)** show the equality of sums of the "external" and "internal" paths of all paths **(i,j)** in graph, as demonstrated by Klein *et al.*[13]. $\mathbb{CJ}_u$ matrix allows the construction of Cluj symmetric matrices, $\mathbb{CJ}_{e/p}$, which in tree graphs are identical to the Wiener matrices, $\mathbb{W}_{e/p}$

$$[\mathbb{CJ}_u]_{ij}\ [\mathbb{CJ}_u]_{ji} = [\mathbb{CJ}_{e/p}]_{ij} = [\mathbb{W}_{e/p}]_{ij} \qquad \mathbf{(11)}$$

From relation **(11)**, the identity of the indices constructed on these matrices is straightforward

$$I = \sum_{i<j} [\mathbb{CJ}_u]_{ij}\ [\mathbb{CJ}_u]_{ji} = (1/2) \sum_i \sum_j [\mathbb{CJ}_{e/p}]_{ij} = (1/2) \sum_i \sum_j [\mathbb{W}_{e/p}]_{ij} \quad (12)$$

Thus, in acyclic structures, the $\mathbb{CJ}_u$ matrix allows the calculation of both W and WW numbers, either directly or by means of symmetric matrices $\mathbb{CJ}_{e/p}$ and $\mathbb{W}_{e/p}$.

Table 1. Wiener , W, hyper-Wiener, WW and the corresponding ^2W_M numbers in octane isomers: M = methyl; E = ethyl.

Graph	W	WW	$^2W_{De}$	$^2W_{We}$	$^2W_{CJu}$	$^2WW_{Dp}$	$^2WW_{Wp}$	$D^2\_CJ_u$
C8	84	210	1848	2100	1596	12726	12054	1386
2MC7	79	185	1628	2000	1396	9711	9829	1056
3MC7	76	170	1512	1892	1284	8256	8338	880
4MC7	75	165	1476	1848	1248	7830	7815	825
3EC6	72	150	1360	1740	1136	6412	6460	649
25M2C6	74	161	1420	1900	1206	7171	7825	775
24M2C6	71	147	1312	1792	1102	6023	6536	635
23M2C6	70	143	1280	1748	1072	5772	6163	605
34M2C6	68	134	1208	1684	1004	5050	5426	520
3E2MC5	67	129	1172	1640	968	4646	4992	465
22M2C6	71	149	1316	1808	1112	6277	6779	676
33M2C6	67	131	1176	1664	978	4878	5221	506
234M3C5	65	122	1096	1648	906	4076	4700	421
3E3MC5	64	118	1072	1564	880	3916	4222	391
224M3C5	66	127	1128	1708	940	4406	5165	467
223M3C5	63	115	1032	1600	850	3653	4220	377
233M3C5	62	111	1000	1564	820	3402	3917	347
2233M4C	58	97	868	1516	706	2521	3169	259

By raising $\mathbb{CJ}_u$ matrix to the second power results in a walk number of rank 2, $^2W_{CJu}$ which is the mean of the half sum of entries in the matrix product, $\mathbb{D}_e\ \mathbb{W}_e$

$$^2W_{CJu} = (1/2)\sum_i\sum_j [\mathbb{CJ}_u^2]_{ij} = \left\{(\sum_i\sum_j [\mathbb{D}_e\mathbb{W}_e]_{ij})/2 + (\sum_i\sum_j [\mathbb{W}_e\mathbb{D}_e]_{ij})/2\ \right\}/2 \quad (13)$$

which is equivalent to

$$^{2}W_{CJu} = (1/2)\sum_{i} {}^{1}W_{De,i}\,{}^{1}W_{We,i} = (1/2)\sum_{i} {}^{1}W_{We,i}\,{}^{1}W_{De,i} = {}^{2}W_{DeWe} \qquad (14)$$

Eq **14** shows that the product of local walk numbers is commutative. Its half sum, over all vertices in graph, gives just the mean of the half sum of entries in the product, to the left and to the right, of matrices $\mathbb{D}_e$ and $\mathbb{W}_e$.

The walk number $^{2}W_{CJu}$ can be also obtained using eq **5**, by operating the matrix $\mathbb{CJ}_u$ by the operator $\mathbb{W}_{(M1,1,M3)}$. The half sum of entries in such a matrix provides various walk numbers, $^{e}W_{M}$, function of matrix combinations:

$(\mathbb{CJ}_{u}, \mathbb{1}, \mathbb{CJ}_{u})$ and $(\mathbb{W}_e, \mathbb{1}, \mathbb{W}_e)$ $\rightarrow$ $^{2}W_{We}$ (*i.e.* $(1/2)\sum_{i<j}(\mathbb{W}_e)^2$)

$(\mathbb{CJ}_{u}^{T}, \mathbb{1}, \mathbb{CJ}_{u}^{T})$ and $(\mathbb{D}_e, \mathbb{1}, \mathbb{D}_e)$ $\rightarrow$ $^{2}W_{De}$ (*i.e.* $(1/2)\sum_{i<j}(\mathbb{D}_e)^2$)

$(\mathbb{CJ}_{u}, \mathbb{1}, \mathbb{CJ}_{u}^{T})$ and $(\mathbb{W}_e, \mathbb{1}, \mathbb{D}_e)$ $\rightarrow$ $^{2}W_{CJu}$ (*i.e.* $(1/2)(\sum_{i<j}\mathbb{D}_e\mathbb{W}_e + \sum_{i<j}\mathbb{D}_e\mathbb{W}_e)$)

where $\mathbb{CJ}_{u}^{T}$ is the transpose of $\mathbb{CJ}_u$.

As illustrated above, various matrix combinations could give the same walk number. Though the product of local walk numbers is commutative, the inner operation of $\mathbb{W}_{(M1,1,M3)}$ is not. Among the $\mathbb{W}_{(M1,1,M3)}$ matrices giving the same walk number, only those constructed on the same $\mathbf{M}_3$ matrix will be identical. For example,

$$\mathbb{W}_{(We,1,CJu)} \equiv \mathbb{W}_{(CJu,1,CJu)} \neq \mathbb{W}_{(CJu,1,We)} \equiv \mathbb{W}_{(We,1,We)}$$

which all give the same $^{2}W_{We}$ number. As it was shown elsewhere [5], the walk numbers (of higher rank) are true Wiener-type numbers (of higher rank). Table **1** lists walk numbers of rank 2 for the above discussed matrices.

Distance Extended Cluj Matrices

Tratch et al. [14] have recently proposed an *extended distance matrix*, E, whose entries whose entries are the product of entries of $\mathbf{D}_e$ matrix and a multiplyer, m_{ij} , which is the number of paths in the graph of which path (i,j) is a subgraph. In acyclic structures, m_{ij} equals the entries in the $\mathbf{W}_p$ matrix, so that E is further referred to as $\mathbf{D\_W}_p$ matrix

$$[\mathbf{D\_W}_p]_{ij} = [\mathbf{D}_e]_{ij}\, m_{ij} = [\mathbf{D}_e]_{ij}\, [\mathbf{W}_p]_{ij} = D_{ij} N_i N_j \tag{15}$$

where D_{ij} is the distance between **i** and **j** and N_i , N_j have the same meaning as above. $\mathbf{D\_W}_p$ matrix is just the Hadamard (pairwise) product [15] of the $\mathbf{D}_e$ and $\mathbf{W}_p$ matrices. It is a square symmetric matrix of dimensions N*N. The half sum of its entries gives an expanded Wiener number [14,16].

Similarly, the Hadamard product $\mathbf{D}_e\mathbf{CJ}_u$ (for acyclic structures) leads to a new unsymmetric matrix, $\mathbf{D\_CJ}_u$

$$[\mathbf{D\_CJ}_u]_{ij} = [\mathbf{D}_e]_{ij}\, [\mathbf{CJ}_u]_{ij} = D_{ij} N_i \tag{16}$$

This matrix (illustrated in Figure **1**) obeys the equalities

$$\Sigma_i[\mathbf{D\_CJ}_u]_{ij} = \Sigma_i[\mathbf{D}_p]_{ij} \tag{17}$$

$$\Sigma_j[\mathbf{D\_CJ}_u]_{ij} = \Sigma_j[\mathbf{W}_p]_{ij} \tag{18}$$

The matrix, $\mathbf{D\_CJ}_u$ offers, in fact, a new definition of the hyper-Wiener number

$$WW = (1/2)\, \Sigma_i\Sigma_j[\mathbf{D\_CJ}_u]_{ij} = (1/2)\, \Sigma_i\Sigma_j\, [\mathbf{D}_e]_{ij}\, [\mathbf{CJ}_u]_{ij} = (1/2)\, \Sigma_i\Sigma_j\, D_{ij} N_{i,p} \tag{19}$$

On this ground, a **(3D)**$\mathbf{D\_CJ}_u$ matrix can be constructed (see Figure **1**) from which a *(3D) hyper-Wiener* number, ***(3D)WW***, is straightforward (for the graph **1** - optimized geometry - ***(3D)WW*** = 105.9607; for the ***(3D)W*** number see [17]).

Another way to build a ***(3D)WW*** is offered by relation $WW = (1/2)(\mathrm{Tr}(\mathbf{D}^2)/2 + W)$ (see [5,13]) when the trace,**Tr**, of squared distance matrix and the Wiener number are calculated on the (3D) distance matrix. In such a case, ***(3D)WW*** = 109.4609.

By operating the $\mathbf{D\_CJ}_u$ matrix analogously to the $\mathbf{CJ}_u$ for calculating the hyper-Wiener number (see eq **12**) a new index is obtained, denoted $D^2\_CJ_u$

$$D^2\_CJ_u = \sum_{i<j}[\mathbb{D}\_\mathbb{CJ}_u]_{ij}\,[\mathbb{D}\_\mathbb{CJ}_u]_{ji} \tag{20}$$

This index can be also calculated by

$$D^2\_CJ_u = \sum_{i<j} N_i N_j\,([\mathbb{D}_e]_{ij})^2 = \sum_{i<j}[\mathbb{W}_p]_{ij}\,([\mathbb{D}_e]_{ij})^2 = \sum_{i<j}[\mathbb{D}\_\mathbb{W}_p]_{ij}\,[\mathbb{D}_e]_{ij} \tag{21}$$

Eq **21** relates the $D^2\_CJ_u$ index to the $\mathbb{W}_p$ and $\mathbb{D}\_\mathbb{W}_p$ matrices. It uses squared distances to multiply the Tratch's m_{ij} parameter. Squared distances are used for calculating the moment of inertia of molecules [18]. Values $D^2\_CJ_u$ for octanes are listed in Table **1**. A *(3D)* $D^2\_CJ_u$ number is also conceivable, as shown in Figure **1**.

$\mathbb{CJ}_u$ *Matrix and Schultz-Type Indices*

Among the modifications of the Wiener number, the Schultz number, ***MTI*** [19], appears to be one of the most studied (see refs in [20]). It is defined as

$$MTI = MTI(G) = \sum_i [\mathbf{v}(\mathbb{A} + \mathbb{D}_e)]_i \tag{22}$$

where $\mathbb{A}$ and $\mathbb{D}_e$ 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 of the graph.

By replacing the valency vector $\mathbf{v}$, by the walk degree vector, ${}^1\mathbb{W}_\mathbb{M}$ and $\mathbb{D}_e$ matrix by the same $\mathbb{M}$ matrix as those used for weighting the walks (*i.e.* the subscript $\mathbb{M}$), ***MTI***, or in general, ***MI*** can be written [20] as

$$MI = MI(G) = \sum_i [{}^1\mathbb{W}_\mathbb{M}(\mathbb{A} + \mathbb{M})]_i \tag{23}$$

By applying matrix algebraic operations, ***MI*** can be decomposed [20-24] as

$$MI = \sum_i \sum_j [\mathbb{M}(\mathbb{A} + \mathbb{M})]_{ij} = S_M + M_2 \tag{24}$$

where

$$S_M = \left(\sum_i \sum_j [\mathbb{M}\mathbb{A}]_{ij} + \sum_i \sum_j [\mathbb{A}\mathbb{M}]_{ij}\right)/2 \tag{25}$$

$$M_2 = \sum_i \sum_j [\mathbb{M}^2]_{ij} \tag{26}$$

In terms of walk numbers (see eqs **3-5**), eq **25** can be written as

$$S_M = \sum_i ({}^1W_{M,i}\ {}^1W_{A,i}) = 2\ {}^2W_{M,A} = 2\ {}^1W_{(M,1,A)} \tag{27}$$

and similarly eq **26** becomes

$$M_2 = 2\ {}^2W_M = 2\ {}^1W_{(M,1,M)} \tag{28}$$

Thus, MI will be

$$MI = 2\ {}^2W_{M,A} + 2\ {}^2W_M \tag{29}$$

which is $\mathbb{W}_{(M1,M2,M3)}$ -calculable, as

$$MI = 2({}^1W_{(M,1,A)} + {}^1W_{(M,1,M)}) \tag{30}$$

In the case $MI = MTI$, $\mathbb{M} = \mathbb{D}$, but $\mathbb{M}$ and $\mathbb{A}$ changes their role in eq **24**, so that one can write

$$MTI = 2({}^1W_{(D,1,A)} + {}^1W_{(A,1,A)}) = S_D + A_2 \tag{31}$$

In the case $MI = Cj_u I$, (a new Schultz analogue index) the parameters of eq **24** will be: $S_M = (1/2)(S_{De} + S_{we})$ and $M_2 = 2^2W_{CJu} = 2^2W_{DeWe}$ (see eq **14**).

In general, S_M means a product between the adjacency matrix $\mathbb{A}$ and other square matrix $\mathbb{M}$ (written as subscript letter). Concerning eq **31**, S_D is considered as the nontrivial part of MTI [23]. However, other M_2 terms (i.e. ${}^2W_M$ numbers) are far more informative than A_2; ${}^2W_M$ are Wiener-type numbers of rank 2 [5], which show interesting correlating and discriminating abilities [24]. Values S_M, ${}^2W_M$, and corresponding MI numbers ($\mathbb{M} = \mathbb{D}_e$, $\mathbb{W}_e$ and $\mathbb{CJ}_u$) for octanes are listed in Table **2**. These indices have shown good correlation with four physico-chemical properties of octanes, in two-variable regression: boiling points (**D_eI & MTI**; 0.953), critical pressure (**CJ_uI & MTI**; 0.988), octane number (**CJ_uI & MTI**; 0.987), and van der Waals surface (**S_{CJu} & S_{We}**; 0.915) [24].

Relation **(28)** can be extended to

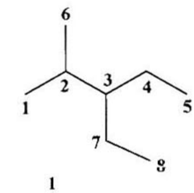
$$2\ {}^{n+1}W_M = \sum_i ({}^{n}W_{M,i}\ {}^{1}W_{M,i}) = \sum_i \mathbf{W}_{(M,,\mathbf{n},M),i} = 2W_{(M,,n,M)} \quad \textbf{(32)}$$

where $\mathbf{n}$ is the matrix having entries $[\mathbf{n}]_{ij}$. Eq **32** proves once again that the unsymmetric $\mathbf{W}_{(M1,M2,M3)}$ is a true matrix operator. Supplementary examples are given in Figure **2**.

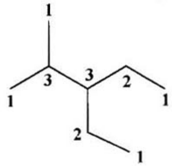
Table 2. S_M and *MI* indices in octane isomers : M = methyl; E = ethyl.

Graph	S_{De}	S_{We}	S_{CJu}	D_eI	W_eI	CJ_uI	*MTI*
C8	280	322	301	3976	4522	3439	306
2MC7	260	324	292	3516	4324	3084	288
3MC7	248	318	283	3272	4102	2851	276
4MC7	244	316	280	3196	4012	2776	272
3EC6	232	306	269	2952	3786	2541	260
25M2C6	240	326	283	3080	4126	2695	270
24M2C6	228	320	274	2852	3904	2478	258
23M2C6	224	318	271	2784	3814	2415	254
34M2C6	216	314	265	2632	3682	2273	246
3E2MC5	212	308	260	2556	3588	2196	242
22M2C6	228	330	279	2860	3946	2503	260
33M2C6	212	322	267	2564	3650	2223	244
234M3C5	204	320	262	2396	3616	2074	236
3E3MC5	200	314	257	2344	3442	2017	232
224M3C5	208	332	270	2464	3748	2150	242
223M3C5	196	326	261	2260	3526	1961	230
233M3C5	192	324	258	2192	3452	1898	226
2233M4C4	176	338	257	1912	3370	1669	214

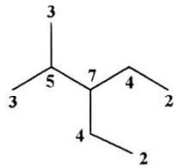
Figure 2 Graph 2 (and its weighted graphs $2\{^{e}W_{A,i}\}$) and $\mathbb{W}_{(M_1,M_2,M_3)}$ matrices.



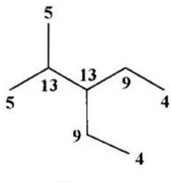
2



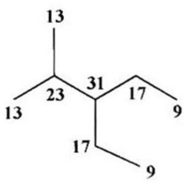
$2\{^{1}W_{A,i}\}$



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



$2\{^{3}W_{A,i}\}$



$2\{^{4}W_{A,i}\}$

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

	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

$$(1/2)\sum_i\sum_j[\mathbb{W}_{(A,D,1)}]_{ij} = 161$$

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

	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

$$(1/2)\sum_i\sum_j[\mathbb{W}_{(A,D,D)}]_{ij} = 471$$

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

	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

$$(1/2)\sum_i\sum_j[\mathbb{W}_{(A,1,D)}]_{ij} = (1/2)[\sum_{ij}[\mathbb{A}\mathbb{D}]_{ij} + \sum_{ij}[\mathbb{D}\mathbb{A}]_{ij}] = 106$$

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

	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

$$(1/2)\sum_i\sum_j[\mathbb{W}_{(A,2,A)}]_{ij} = \sum[\mathbb{A}^3]_{ij} = 31$$

Conclusions

Unsymmetric matrices $\mathbb{CJ}_u$ and $\mathbb{D}\_\mathbb{CJ}_u$ has proved to be sources for various graph invariants: Wiener, hyper-Wiener, Wiener-type numbers of higher rank and Schultz analogues. Distance extended $\mathbb{D}\_\mathbb{CJ}_u$ matrix offer the oportunity of building the first (3D) hyper-Wiener number (cf eq **19**). It also provides the $D^2\_CJ_u$ number which deserves further investigations. Schultz analogues, particularly the newly proposed CJ_uI number, apear to have good correlating ability. Finally, the matrix $\mathbb{W}_{(M1,M2,M3)}$ has proved to be an interesting matrix operator.

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