Molecular Topology. 16. Layer Matrices in Molecular Graphs

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Among the layer matrices,[1,2] the sequence matrices SM and true layer matrices LM are distinguished. These matrices are carefully defined and exemplified. Finally, some applications in construction of topological indices in graph ordering and in graph similarity testing are given.

INTRODUCTION

A molecular graph can be represented by a number, a sequence, a matrix, or a polynomial.[3] All such representations aim to be unique for a given graph. The matrices associated with molecular graphs can be classified in matrices with integers as entries (*e.g.*, the adjacency A and the distance D matrices[4]) and with real numbers as entries (*e.g.*, the reversed distance[5,6] RD, 3D – distance,[7–9] or the topological state matrices[10]). For more details one can consult refs 1 and 8.

In the past few years, some nonsymmetrical matrices were considered (see refs 1, 2, 8, 9, and 11–17) in connection with various particular walk sequences in graphs. These matrices are based on the partition of a graph, G, with respect to its vertices. The i-relative partition of G, $G(i)$, can be written as[1]

$$G(i) = \{G(u)_j;\ j \in [0,\mathrm{ecc}_i] \text{ and } u \in G(u)_j \Leftrightarrow d_{iu} = j\} \quad (1)$$

where $G(u)_j$ are sets of vertices in the i-partition of G, arranged in layers at distance $d_{iu} = j$ from the vertex i (for which $j = 0$) until the maximal one (ecc_i = eccentricity of vertex i). This is consistent with a sequential picture of graph with respect to its vertices, as shown in Figure 1 for the graph **1**.

In this paper we make a distinction between the sequence matrices and true layer matrices, both of them belonging to the nonsymmetrical generic named layer matrices.[1] Each type is rigorously defined and examples given on simple graphs, and some applications in construction of topological indices (TIs) in graph ordering and graph similarity testing are given.

SEQUENCE MATRICES, $SM^{(e)}$

A sequence matrix, $SM^{(e)}$, is a collection of walks (of increasing elongation e) starting from the vertices i to all other $n-1$ vertices in G. The entries in such a matrix, $m_i^{(e)}$ (m being the label for a particular type of walk; d, distance; p, path; srw, self-returning walk, and w, random walk, respectively) represent the number of walks of elongation e emerging from the vertex i. The matrix $SM^{(e)}$ can be written as

$$SM^{(e)} = \{m_i^{(e)},\ i \in [1,n];\ e = 1, 2, ..., \mathrm{esp}\} \quad (2)$$

with n being the number of vertices in G and *esp* (the specified elongation) being ecc_i (for M = D), path-ecc_i (for M = P), and esp $\in (1,\infty)$ (for M = $SRW^{(e)}$ and $W^{(e)}$), respectively. The capitals here are used for labeling the type of walks in sequence matrices. Thus, the rows of $SM^{(e)}$ matrices are just the sequences of walks emerging from the vertex i, *i.e.*, DDS (distance degree sequence[18–21]), PDS (path degree sequence[18–21]), or WS (walk sequence[3]).

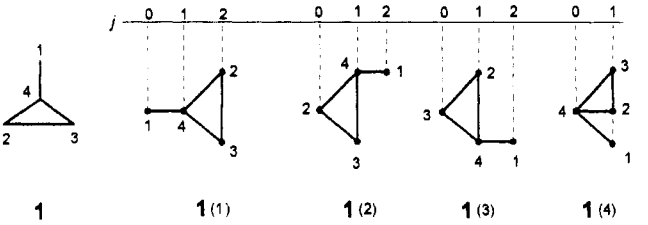

Figure 1. Relative partitions of the graph **1**.

The half sum on columns of the entries in $SM^{(e)}$ offers the global values, $GM^{(e)}$

$$GM^{(e)} = {}^1/_2 \sum_i m_i^{(e)} \quad (3)$$

and hence, the sequence of global values, $SGM^{(e)}$ is

$$SGM^{(e)} = GM^{(e)};\ e = 1, 2, ..., \mathrm{esp} \quad (4)$$

Figure 2 examplifies the $SM^{(e)}$ matrices for the graphs **1** and **2**.

Notice that the SD matrix was called λ in ref 1 and F in ref 11, and the SP matrix was called τ in ref 1.

It is known that the Wiener index,[22] W, equals the sum of all distances (as metrics) in G and the half sum of all entries in the D matrix. Since this index is SD-calculable, we denote by $WM^{(e)}$ an extended Wiener index, which is $SM^{(e)}$-calculable:

$$WM^{(e)} = \sum_e (GM^{(e)} e) = {}^1/_2 \sum_e \sum_i (m_i^{(e)} e) \quad (5)$$

In the case of $SSRW^{(e)}$ and $SW^{(e)}$ matrices, the extended Wiener index counts all the corresponding walks in the graph until the specified elongation, esp. Notice that esp could be unlimited, but $n-1$ is a limit by virtue of Cayley–Hamilton theorem; however, esp is often smaller than $n-1$. For the graphs **1**–**3**, the values $WM^{(e)}$ are given in Figures 2 and 3.

LAYER MATRICES, $LM^{(e)}$

A layer matrix, $LM^{(e)}$, collects the properties (topological and chemical) of vertices u located in concentric shells (layers)

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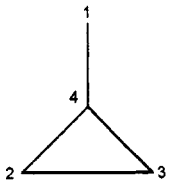
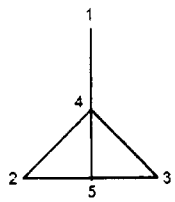


1

	SD		SP			SSRW(3)			SW(3)		
i/e	1	2	1	2	3	1	2	3	1	2	3
1	1	2	1	2	2	0	1	0	1	3	5
2	2	1	2	3	1	0	2	2	2	5	10
3	2	1	2	3	1	0	2	2	2	5	10
4	3	0	3	2	0	0	3	2	3	5	13
SGM(e)	4	2	4	5	2	0	4	3	4	9	19
	WD = 8		WP = 20			WSRW(3) = 17			WW(3) = 79		



2

	SD		SP				SSRW(4)				SW(4)			
i/e	1	2	1	2	3	4	1	2	3	4	1	2	3	4
1	1	3	1	3	4	2	0	1	0	4	1	4	8	26
2	2	2	2	5	5	1	0	2	2	11	2	7	16	48
3	2	2	2	5	5	1	0	2	2	11	2	7	16	48
4	4	0	4	4	2	0	0	4	4	22	4	8	26	62
5	3	1	3	5	4	0	0	3	4	16	3	8	22	58
SGM(e)	6	4	6	11	10	2	0	6	6	32	6	17	44	121
	WD = 14		WP = 66				WSRW(4) = 158				WW(4) = 656			

Figure 2. $SM^{(e)}$ matrices of the graphs **1** and **2**.

at distance j around each vertex $i \in G$. The jth layer of vertex i, $G(u)_j$, can be written as

$$G(u)_j = \{u:\ d_{iu} = j\} \tag{6}$$

and the entries in the layer matrix

$$lm_{i,j}^{(e)} = \sum_{u \in G(u)_j} m_u^{(e)} \tag{7}$$

where m and M are labels for a given property and the corresponding matrix, and e is the elongation. Thus, the layer matrix can be written as

$$LM^{(e)} = \{lm_{i,j}^{(e)};\ i \in [1,n];\ j \in [0,d];\ e \in [1,\text{esp}]\} \tag{8}$$

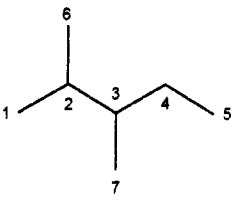
d being the diameter of G, i.e., the largest distance in the graph. The dimensions of such matrices are $n(d+1)$. Some $LM^{(e)}$ matrices are given in Figure 3 (by using vertex-weighted graphs, $G\{m_i^{(e)}\}$).

From Figure 3 one can see that the layer matrices are built on the ground of relative partitions of the graph (see eq 1). The elements of the first column ($j = 0$) in a $LM^{(e)}$ matrix are just the vertex properties. When the property is a topological one it can be

(i) a degree (*i.e.*, the number of walks of elongation e starting from the vertex i—the entry which can just be taken from a $SM^{(e)}$ matrix, $lm_{i,0}^{(e)} = m_i^{(e)}$) and

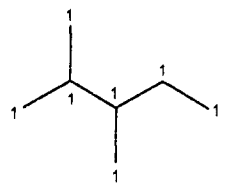
(ii) a metric property, which is $SM^{(e)}$-calculable by

$$lm_{i,0}^{(e)} = \sum_e (m_i^{(e)} e) \tag{9}$$



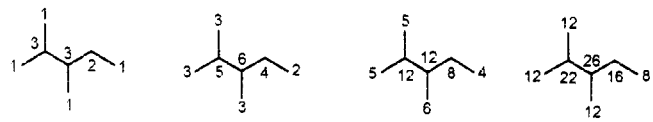
3

	SD = SP				SSRW(4)				SW(4)			
i/e	1	2	3	4	1	2	3	4	1	2	3	4
1	1	2	2	1	0	1	0	3	1	3	5	12
2	3	2	1	0	0	3	0	11	3	5	12	22
3	3	3	0	0	0	3	0	12	3	6	12	26
4	2	2	2	0	0	2	0	6	2	4	8	16
5	1	1	2	2	0	1	0	2	1	2	4	8
6	1	2	2	1	0	1	0	3	1	3	5	12
7	1	2	3	0	0	1	0	3	1	3	6	12
SGM(e)	6	7	6	2	0	6	0	20	6	13	26	54
	WD = 46 = WP				WSRW(4) = 92				WW(4) = 326			



3 $\{c_i\}$

	LC					LSRW(4)				
i/j	0	1	2	3	4	0	1	2	3	4
1	1	1	2	2	1	3	11	15	9	2
2	1	3	2	1	0	11	18	9	2	0
3	1	3	3	0	0	12	20	8	0	0
4	1	2	2	2	0	6	14	14	6	0
5	1	1	1	2	2	2	6	12	14	6
6	1	1	2	2	1	3	11	15	9	2
7	1	1	2	3	0	3	12	17	8	0
					GM(e) 20					



3 $\{W^{(1)}_i = k_i\}$ **3** $\{W^{(2)}_i\}$ **3** $\{W^{(3)}_i\}$ **3** $\{W^{(4)}_i\}$

	LK = LW(1)					LW(2)					LW(3)					LW(4)				
i/j	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4
1	1	3	4	3	1	3	5	9	7	2	5	12	17	14	4	12	22	38	28	8
2	3	5	3	1	0	5	12	7	2	0	12	22	14	4	0	22	50	28	8	0
3	3	6	3	0	0	6	12	8	0	0	12	26	14	0	0	26	50	32	0	0
4	2	4	4	2	0	4	8	8	6	2	8	16	18	10	0	16	34	34	24	0
5	1	2	3	4	2	2	4	6	8	6	4	8	12	18	10	8	16	26	34	24
6	1	3	4	3	1	3	5	9	7	2	5	12	17	14	4	12	22	38	28	8
7	1	3	5	3	0	3	6	9	8	0	6	12	20	14	0	12	26	38	32	0
GM(e)	6					13					26					54				

	LDS = LPS					LSRW(4)S				
i/j	0	1	2	3	4	0	1	2	3	4
1	15	10	24	26	17	14	50	68	42	10
2	10	39	26	17	0	50	82	42	10	0
3	9	36	47	0	0	54	92	38	0	0
4	12	26	24	30	0	28	64	64	28	0
5	17	12	9	24	30	10	28	54	64	28
6	15	10	24	26	17	14	50	68	42	10
7	14	9	22	47	0	14	54	78	38	0
GM(e)	46					92				

	LW(1)S					LW(2)S					LW(3)S					LW(4)S				
i/j	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4
1	1	3	4	3	1	7	13	22	17	5	22	49	73	59	17	70	137	225	171	49
2	3	5	3	1	0	13	29	17	5	0	49	95	59	17	0	137	295	171	49	0
3	3	6	3	0	0	15	30	19	0	0	51	108	61	0	0	155	308	189	0	0
4	2	4	4	2	0	10	20	20	14	0	34	68	74	44	0	98	204	210	140	0
5	1	2	3	4	2	5	10	15	20	14	17	34	51	74	44	49	98	155	210	140
6	1	3	4	3	1	7	13	22	17	5	22	49	73	59	17	70	137	225	171	49
7	1	3	5	3	0	7	15	23	19	0	25	51	83	61	0	73	155	235	189	0
GM(e)	6					32					110					326				

Figure 3. Matrices of the graph **3**.

According to the above properties, the $LM^{(e)}$ matrices can be partitioned into (i) layer matrices of degrees (*i.e.*, of cardinality, LC; of degrees, LK; of walk degrees, $LW^{(e)}$) and (ii) layer matrices of walk sums (*i.e.*, of distance sums, LDS; of path sums, LPS; of walk sums, $LWS^{(e)}$). A particular observation needs the LC matrix, for which the property $m_i^{(e)}$ equals unity. Notice that the property $m_i^{(e)}$ could be any topological or chemical one (see ref 18).

A simple way to construct a LM matrix is by means of a distance-property matrix, DM, which is the sum of distance matrix D and the diagonal matrix M of vertex properties (see also ref 23). The entries in LM will be

$$lm_{ij} = \sum_{u \in G(u)_j} m_{uu}; \qquad j = d_{iu} \tag{10}$$

For $j = 0$, the entries will be just the diagonal elements in DM (*i.e.*, the property m for the vertex itself). For the graph **1**, the procedure is shown in construction of the layer matrix of degrees, (k_i), LK:

D				M = K				DM				LK		LK		
0	2	2	1	1	0	0	0	1	2	2	1	1 3	2+2	1	3	4
2	0	1	1	0	2	0	0	2	2	1	1	2 2+3	1	2	5	1
2	1	0	1	0	0	2	0	2	1	2	1	2 2+3	1	2	5	1
1	1	1	0	0	0	0	3	1	1	1	3	3 1+2+2	0	3	5	0

(11)

In the following, some additional properties of layer matrices are presented:

$$\text{SD:} \quad \sum_e d_i^{(e)} = n - 1 \tag{12}$$

$$\sum_i d_i^{(1)} = \sum_i k_i = 2q \tag{13}$$

$$\sum_i (d_i^{(1)})^2 - \sum_i d_i^{(2)} = 2q \tag{14}$$

$$\text{LC:} \quad \sum_j lc_{ij} = \sum_i lc_{i0} = n \tag{15}$$

$$\sum_i lc_{i1} = \sum_i k_i = 2q \tag{16}$$

$$\text{LW}^{(e)}: \quad \sum_i (lw_{i0}^{(1)})^2 = \sum_i lw_{i1}^{(1)} = \sum_i lw_{i0}^{(2)} \tag{17}$$

$$lw_{i1}^{(e)} = lw_{i0}^{(e+1)} \tag{18}$$

$$\sum_j lm_{ij}^{(e)} = \sum_i lm_{i0}^{(e)} = 2\text{GM}^{(e)} \tag{19}$$

In the above relations, n stands for the number of vertices in graph and q is the number of edges. Equation 14 holds in graphs without cycles C_3 and C_4 (see ref 17). In eq 19, $GM^{(e)}$ is the global property, which in layer matrices of walk sums equals the corresponding Wiener index, $WM^{(e)}$. For LC, a local property which does not involve edges, eq 19 does not hold.

Of particular attention is eq 18. It shows that the second column in $LW^{(1)}$ becomes the first one in the higher term matrix $LW^{(2)}$. This result holds for $LW^{(e)}$ at any two consecutive elongations in a graph (except for the multigraphs). This represents, in essence, Morgan's extended connectivity algorithm.[24,25]

A computer program TOP facilitated the construction (and comparison—see below) of SM and LM matrices.

Linear Representation of Layer Matrices. Layer matrices can be represented in a line form,[1] which is reminiscent of their walk sequence origins

$$\text{SD}(\mathbf{1}) = \{1(1,2);2(2,1);3(2,1);4(3,0)\} \tag{20}$$

$$\text{LC}(\mathbf{1}) = \{1(1,1,2);2(1,2,1);3(1,2,1);4(1,3,0)\} \tag{21}$$

When the vertex labeling is not important, one can write in a canonical form: the rows are listed in decreasing order of their length and in lexicographic order in the case of equal length. For the graph **1** the canonical form of SD and LC matrices will be

$$\text{SD}(\mathbf{1}) = \{2^*(2,1);(1,2);(3,0)\} \tag{22}$$

$$\text{LC}(\mathbf{1}) = \{2^*(1,2,1);(1,1,2);(1,3,0)\} \tag{23}$$

Another way to order the rows in a layer matrix is to apply the centric criteria of Bonchev et al.,[19,20] which results in a centric ordering and a numbering of a graph.[16]

Applications Based on Layer Matrices. Matrices associated with molecular graphs are themselves invariants, but they represent an additional source of other invariants.[8] Among such invariants, the topological indices, TIs, were widely used in QSPR/QSAR studies[2,8,15,26] or in vertex and graph ordering[9,14,16,27,28] or also in vertex equivalence perception.[3,11,14,16]

Distance and path sequences were used in metric analysis of graphs[1] and in graph ordering.[7,9,18,27] The problem of molecular similarity was quantitatively approached by using path sequences[7] or TIs[29] in the calculation of interstructure Euclidian distances.

1. Topological Indices and Graph Ordering. We defined[2,9,14-16] two types of LOVIs (local vertex invariants) on LM matrices: a centrocomplexity, $x(\text{LM})_i$, and a centric invariant, $c(\text{LM})_i$, according to eqs 24 and 25

$$x(\text{LM})_i = [1/\rho_i \sum_{j=0}^{\text{ecc}_i} lm_{ij} 10^{-zj}]^{\pm 1} \tag{24}$$

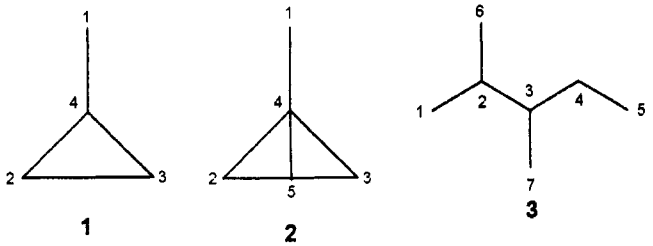
$$c(\text{LM})_i = [\sum_{j=1}^{\text{ecc}_i} (lm_{ij})^{j/\text{dsp}}]^{-1} \tag{25}$$

where z is the number of digits of the *max* lm_{ij}—value in graph, ρ_i is a topological property (*i.e.*, vertex degree k_i, but in this work $\rho_i = 1$ and the exponent is +1), and dsp is a specified topological distance, usually larger than the diameter of graph (here dsp = 10, unless otherwise specified).

Summation of LOVIs over all vertices in G will provide the corresponding TIs, designed by capitals.

(a) Centrocomplexity Ordering. The "x"-type invariants consider first the "more important" vertex in the graph (*i.e.*, one of higher degree), and the remaining ones are ordered according to their increasing distance from that vertex. If there is more than one "important" vertex in the graph, they are ordered in decreasing order of their centricity. This is the meaning of the term *centrocomplexity*. Figure 4 offers $x(\text{LW}^{(e)})_i$ values (in decreasing order) for graphs **1**–**3**.

If the ordering induced by the vertex degree (*i.e.*, by $x(\text{LW}^{(1)})_i$ index) is satisfactory in a first approximation, the evaluation of vertex walk degrees of higher elongation is needed, especially for the graphs in which pairs of vertices show oscillating walk degree $w^{(e)}$ values (as e increases). Although the ordering induced by the $x(\text{LW}^{(e)})_i$ indices also oscillates, it tends to overlap over that given by the first eigenvector, as shown on the graphs **4** and **5** (Figure 5). It was useful to normalize the local values by dividing by the global values (actually $nx(\text{LW}^{(e)})_i$ values—see Tables 1 and 2). When e tends to be infinite, the "nx" values overlap the vertex weight values ($\rho_i^{(e)} = w_i^{(e)}/2\text{GW}^{(e)}$) proposed by Rücker and



1 **2** **3**

$x(LW^{(1)})_i$

4	3.50	4	4.80	3	3.630 0
3	2.51	5	3.81	2	3.531 0
2	2.51	3	2.73	4	2.442 0
1	1.34	2	2.73	7	1.353 0
		1	1.47	6	1.343 1
				1	1.343 1
				5	1.234 2

$X(LW^{(1)})$

9.86	15.54	14.876 4

$x(LW^{(2)})_i$

4	5.130 0	4	8.260 0	3	6.120 800 00
3	5.100 3	5	8.220 4	2	5.120 702 00
2	5.100 3	3	7.161 1	4	4.080 806 00
1	3.051 0	2	7.161 1	7	3.060 908 00
		1	4.082 2	6	3.050 907 02
				1	3.050 907 02
				5	2.040 608 06

$X(LW^{(2)})$

18.381 6	34.884 8	26.525 638 10

$x(LW^{(3)})_i$

4	13.250 0	4	26.620 0	3	12.261 400 00
3	10.230 5	5	22.580 8	2	12.221 404 00
2	10.230 5	3	16.482 4	4	8.161 810 00
1	5.132 0	2	16.482 4	7	6.122 014 00
		1	8.265 4	6	5.121 714 04
				1	5.121 714 04
				5	4.081 218 10

$X(LW^{(3)})$

38.843 0	90.431 0	53.091 274 18

Figure 4. Some "x" LOVIs (in decreasing order) and corresponding *TIs* for the graphs **1**–**3**.

Rücker[30] and Bonchev *et al.*[31] and also the coefficients of the normalized first eigenvector. Tables 1 and 2 give normalized "nx" values only for even (e) (the ordering which is closer to that of the normalized first eigenvector—see Figure 5), as Bonchev *et al.*[31] suggested by considering the self-returning walks. However, our results show a better correlation (0.995) with the use of random walks (of even e) instead of self-returning walks (0.977).

Since the pairs of vertices 3 and 6′, 6 and 3′, 12 and 12′ in **4** and **5** are isospectral and cannot be discriminated neither by walk degree sequences (see Rücker and Rücker[32]) nor by their weights, we used the $LW^{(e)}$ matrices (see Figure 5), and the "x" indices, which separated these pairs just beginning at the $e = 2$. Other examples about the discriminating capability of $LW^{(e)}$ matrices, along with a simple summation procedure of counting weighted walk degrees are given in ref 25.

(b) Centric Ordering. The "c"-type invariants find the center of a graph in good agreement with the 1D–3D centric criteria of Bonchev *et al.*[19,20] They are as follows:

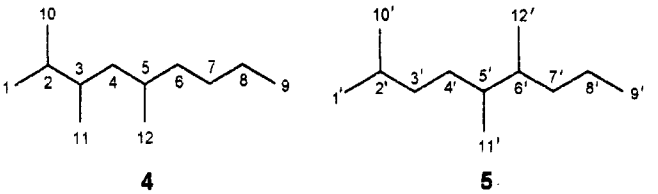
1D: minimal vertex eccentricity, ecc_i = min

2D: minimal vertex distance sum, DS_i = min

3D: minimal number of occurrences of the largest distance (or, when this is identical for two or more vertices, the next largest distance, etc.)

Criteria 1D–3D are applied hierarchically. The 1D criterion is fulfilled by means of the parameter j (the contour of columns), and this is true for any layer matrix. The 2D criterion is obeyed only by the LDS matrix (built up just on DS_i values). The last criterion is sometimes nondecisive, since there are graphs with a pair of degenerate DDS for non-equivalent vertices (see below). As examples two graphs, **6**

(a)



4 **5**

e:	1	2	3	4	5	6	7	8				
2*SGD (**4**):	22,	26,	24,	20,	18,	10,	8,	4				
2*SGD (**5**):	22,	26,	24,	20,	18,	12,	6,	4				
e:	1	2	3	4	5	6	7	8	9	10	11	
2*$SGW^{(e)}$ (**4**;**5**):	22,	48,	98,	212,	444,	958,	2028,	4372,	9302,	20046,	42760	

$LW^{(2)}$ matrices:

	graph **4**									graph **5**								
1	3	5	9	9	5	8	4	3	2	3	4	8	5	6	9	8	3	2
2	5	12	9	5	8	4	3	2	0	4	11	5	6	9	8	3	2	0
3	6	14	11	8	4	3	2	0	0	5	9	12	9	8	3	2	0	0
4	6	11	16	10	3	2	0	0	0	5	11	13	14	3	2	0	0	0
5	5	14	10	11	8	0	0	0	0	6	14	13	7	8	0	0	0	0
6	5	9	12	8	8	6	0	0	0	6	14	11	7	4	6	0	0	0
7	4	8	7	9	6	8	6	0	0	5	9	11	8	5	4	6	0	0
8	3	6	5	5	9	6	8	6	0	3	7	6	9	8	5	4	6	0
9	2	3	4	5	5	9	6	8	6	2	3	5	6	9	8	5	4	6
10	3	5	9	9	5	8	4	3	2	3	4	8	5	6	9	8	3	2
11	3	5	11	10	11	8	0	0	0	3	6	11	13	7	8	0	0	0
12	3	6	11	11	8	4	3	2	0	3	6	11	11	7	4	6	0	0
$X(LW^{(2)})$:	48.991 500 806 636 241 0									48.991 500 806 642 181 0								

(b) vertex ordering

graph **4**

$x(LW^{(1)})_i$:	3, 5, 2, 4, 6, 7, 8, 12, 11, (1, 10), 9
$x(LW^{(2)})_i$:	3, 4, 5, 2, 6, 7, 12, 8, 11, (1, 10), 9
$x(LW^{(3)})_i$:	3, 5, 2, 4, 6, 7, 12, 8, 11, (1, 10), 9
$x(LW^{(10)})_i$:	3, 4, 5, 2, 6, 12, 11, 7, (1, 10), 8, 9
$x(LW^{(12)})_i$:	3, 4, 2, 5, 6, 12, 11, 7, (1, 10), 8, 9
$x(LW^{(13)})_i$:	3, 5, 4, 2, 6, 12, 7, (1, 10), 11, 8, 9
$x(LW^{(14)})_i$:	3, 4, 2, 5, 6, 12, 11, (1, 10), 7, 8, 9
eigenvector:	3, 4, 5, 2, 6, 12, 11, (1, 10), 7, 8, 9

graph **5**

$x(LW^{(1)})_i$:	5, 6, 2, 4, 3, 7, 8, 11, 12, (1, 10), 9
$x(LW^{(2)})_i$:	5, 6, 4, 3, 7, 2, 8, 11, 12, (1, 10), 9
$x(LW^{(3)})_i$:	5, 6, 4, 2, 3, 7, 8, 11, 12, (1, 10), 9
$x(LW^{(10)})_i$:	5, 6, 4, 7, 3, 2, 12, 11, 8, (1, 10), 9
$x(LW^{(12)})_i$:	5, 6, 4, 7, 3, 12, 2, 11, 8, (1, 10), 9
$x(LW^{(13)})_i$:	6, 5, 4, 7, 3, 2, 11, 12, 8, (1, 10), 9
$x(LW^{(14)})_i$:	5, 6, 4, 7, 3, 12, 11, 2, 8, (1, 10), 9
eigenvector:	5, 6, 4, 7, 3, 11, 12, 2, 8, (1, 10), 9

Figure 5. Sequence of graph distance SGD, sequence of graph walks $SGW^{(e)}$ and $LW^{(2)}$ matrices (a) and vertex ordering (b) in the graphs **4** and **5** according to the normalized $nx(LW^{(e)})_i$ values and normalized first eigenvector (see Tables 1 and 2).

Table 1. Normalized Values of "x" Indices ("nx" and Correlation with the Coefficients of Normalized First Eigenvector in the Graph **4**

	eigenvector	normalized eigenvector $\times 10^{-2}$	$nx(LW^{(e)})_i \times 10^{-2}$			
			e = 10; w	e = 12; w	e = 14; w	e = 12; srw
1	0.1847	5.9903	5.5734	5.6128	5.6477	3.5974
2	0.3966	12.8628	12.5986	12.8050	12.9548	15.7588
3	0.4823	15.6423	14.6547	14.7643	14.8401	21.3600
4	0.4145	13.4434	13.8359	13.8774	13.9006	15.0778
5	0.4078	13.2261	12.7587	12.7736	12.7670	16.1178
6	0.2712	8.7958	9.6846	9.5313	9.4184	8.4983
7	0.1747	5.6660	5.7881	5.6671	5.5935	4.6879
8	0.1039	3.3698	4.0015	3.8479	3.7435	2.3098
9	0.0484	1.5697	1.7165	1.6325	1.5862	0.6503
10	0.1847	5.9903	5.5734	5.6128	5.6477	3.5974
11	0.1899	6.1590	6.6061	6.5539	6.5110	3.6474
12	0.2246	7.2844	7.2298	7.3235	7.3896	4.7207
			r: 0.99351	0.99492	0.99566	0.97727
			s: 0.08678	0.07389	0.19199	0.18375

Table 2. Normalized Values of "x" Indices ("nx") and Correlation with the Coefficients of Normalized First Eigenvector in the Graph 5

	eigenvector	normalized eigenvector $\times 10^{-2}$	$nx(LW^{(e)})_i \times 10^{-2}$			
			e = 10 w	e = 12 w	e = 14 w	e = 12 srw
1	0.1039	3.3699	4.0015	3.8479	3.7435	2.1647
2	0.2230	7.2327	7.3449	7.2302	7.1495	8.3657
3	0.2712	8.7961	9.6846	9.5313	9.4184	8.4982
4	0.3594	11.6567	11.2019	11.2105	11.2110	11.7223
5	0.5005	16.2331	16.4405	16.5834	16.6681	22.0785
6	0.4823	15.6423	14.6547	14.7643	14.8401	21.3601
7	0.3106	10.0739	9.9940	10.0990	10.1873	9.4761
8	0.1847	5.9903	5.5735	5.6128	5.6477	3.7423
9	0.0860	2.7893	2.7642	2.7755	2.7977	0.9095
10	0.1039	3.3699	4.0015	3.8479	3.7435	2.1645
11	0.2331	7.5603	7.1302	7.1759	7.2038	4.8208
12	0.2246	7.2844	7.2298	7.3235	7.3896	4.7207
			r: 0.99351	0.99492	0.99566	0.97211
			s: 0.07084	0.03612	0.11162	1.16896

and **7**, labeled in canonical ordering (according to LDS matrix), are presented in Figure 6.

The graphs **6** and **7** were designed by Ivanciuc[33] to have identical distance degree sequence (in our notation SGD). Moreover, they present a pair of vertices (labeled 15 and 16) which show the same sequence of distances (4,4,2,4,3) in both the graphs. It is obvious that the 3D criterion cannot distinguish between these vertices. Our $c(LDS)_i$ local invariant does it, both intra- and intermolecular, since the LDS matrix is not degenerate in this case. One can see (Figure 6) that the centric ordering induced by the "c"-LOVI reverses the canonical ordering, with a single inversion: vertex 15 before 16, in the graph **6**. An additional mention must be made: despite the matrices SD, LC, and $LW^{(1)}$ degeneration in the graphs **6** and **7**, by increasing the elongation of walks (just from e = 2, see Figure 6), the higher rank layer matrices show low degeneracy (see ref 25). This is also true for the LDS matrix. Only two pairs of nonisomorphic graphs we know of to date show a degenerate LDS matrix and are presented in Figure 7. Since the graphs **8**–**11** in Figure 7 are regular graphs, the counting of walk degrees fails in discriminating their vertices[25] so that all other layer matrices (excepting those constructed on self-returning walks, srw) will be degenerate.

The two types of LOVIs were implemented in algorithms such as MOLCEN[14] and MOLORD[34] and used in vertex equivalence perception.

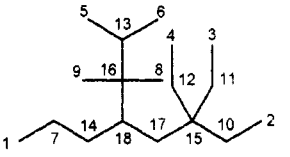
X(LK) global index was tested in QSPR studies[2,15] *vs* van der Waals volumes,[2] boiling points,[2] and octanol–water partition coefficients,[15] with good results. For more details one can consult refs 2, 9, and 14–16.

SP matrices (as global $GP^{(e)}$ values) were used for "x" and "c" ordering of alkane isomers.[7,9,18,27] Table 3 presents our results in the set in heptanes.

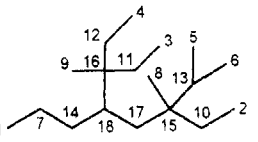
One can see that the increasing lexicographic ordering of global path sequences (X ord in Table 3) superimposes over the ordering given by X(LK) global index and also over that induced by the DM[1] superindex of Balaban *et al.*[35] Application of the 1D–3D criteria of Bonchev *et al.*[19,20] on the global path sequences of heptanes results in a centric ordering of these isomers (C ord in Table 3). For comparison, a "c" index calculated on L3DS matrices (constructed by analogy with LDS by using 3D metric distances instead of the topological ones) of heptanes show a single inversion ($3EC_5$ and $22M_2C_5$) *vs* C ord.

2. Molecular Similarity Testing. The problem of molecular similarity, in quantitative terms, can be approached either by means of interstructure distance calculation[7,29] or in the frame of more sophisticated algorithms, such as the SIBIS model.[36]

(a)



6



7

canonical				LDS (6)					centric	$c(LDS)_i \times 10^2$
1	85	69	55	43	94	240	343	237	18	0.92893
2	79	63	49	171	201	104	260	239	17	0.98765
3	79	63	49	171	201	104	260	239	16	0.98765
4	79	63	49	171	201	104	260	239	15	0.98765
5	77	61	126	173	100	118	274	237	14	0.99034
6	77	61	126	173	100	118	274	237	13	0.99034
7	69	140	43	94	240	343	237	0	12	1.61963
8	65	49	169	254	118	274	237	0	11	1.68283
9	65	49	169	254	118	274	237	0	10	1.68283
10	63	128	171	201	104	260	239	0	9	1.70661
11	63	128	171	201	104	260	239	0	8	1.70661
12	63	128	171	201	104	260	239	0	7	1.70661
13	61	203	173	100	118	274	237	0	6	1.71299
14	55	112	179	240	343	237	0	0	5	2.83069
15	49	234	280	104	260	239	0	0	3	2.98095
16	49	234	254	118	274	237	0	0	4	2.96090
17	45	92	293	497	239	0	0	0	2	4.98333
18	43	149	309	428	237	0	0	0	1	5.03388
									$C(LDS)_i \times 10^2$	36.48041

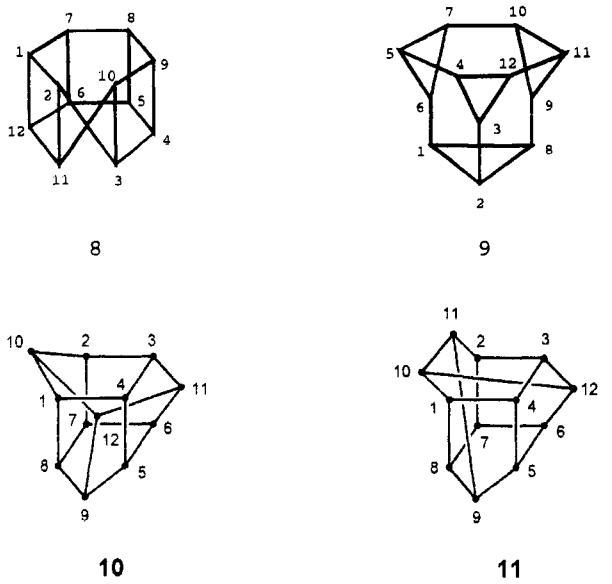
canonical				LDS (7)					centric	$c(LDS)_i \times 10^2$
1	85	69	55	43	94	240	347	233	18	0.93163
2	79	63	49	171	197	104	260	243	17	0.98305
3	79	63	49	171	179	118	274	233	16	0.98405
4	79	63	49	171	179	118	274	233	15	0.98405
5	77	61	126	173	122	104	260	243	14	0.99260
6	77	61	126	173	122	104	260	243	13	0.99260
7	69	140	43	94	240	347	233	0	12	1.62391
8	65	49	169	276	104	260	243	0	11	1.68925
9	65	49	169	258	118	274	233	0	10	1.68981
10	63	128	171	197	104	260	243	0	9	1.69970
11	63	128	171	179	118	274	233	0	8	1.70115
12	63	128	171	179	118	274	233	0	7	1.70115
13	61	203	173	122	104	260	243	0	6	1.71633
14	55	112	179	240	347	233	0	0	5	2.83731
15	49	234	276	104	260	243	0	0	4	2.97033
16	49	234	258	118	274	233	0	0	3	2.97154
17	45	92	293	493	243	0	0	0	2	4.97244
18	43	149	309	432	233	0	0	0	1	5.04486
									$C(LDS)_i \times 10^2$	36.48577

(b)

e:	1	2	3	4	5	6	7	8	9	10 ...
2*SGD (**6**;**7**):	34,	48,	58,	50,	52,	46,	18			
$2*SGW^{(e)}$ (**6**):	34,	82,	188,	452,	1070,	2574,	6136,	14758,	35254,	84756...
$2*SGW^{(e)}$ (**7**):	34,	82,	188,	452,	1070,	2574,	6136,	14750,	35238,	84644...

$LW^{(2)}$ (**6**)									$LW^{(2)}$ (**7**)							
1	2	3	5	8	15	22	21	6	2	3	5	8	15	22	19	8
2	2	5	8	17	12	13	17	8	2	5	8	17	14	13	17	6
3	2	5	8	17	12	13	17	8	2	5	8	17	14	11	17	8
4	2	5	8	17	12	13	17	8	2	5	8	17	14	11	17	8
5	3	6	11	16	12	11	17	6	3	6	11	16	10	13	17	6
6	3	6	11	16	12	11	17	6	3	6	11	16	10	13	17	6
7	3	7	8	15	22	21	6	0	3	7	8	15	22	19	8	0
8	4	8	18	18	11	17	6	0	4	8	18	16	13	17	6	0
9	4	8	18	18	11	17	6	0	4	8	18	16	11	17	8	0
10	5	10	17	12	13	17	8	0	5	10	17	14	13	17	6	0
11	5	10	17	12	13	17	8	0	5	10	17	14	11	17	8	0
12	5	10	17	12	13	17	8	0	5	10	17	14	11	17	8	0
13	6	14	16	12	11	17	6	0	6	14	16	10	13	17	6	0
14	5	11	17	22	21	6	0	0	5	11	17	22	19	8	0	0
15	8	22	14	13	17	8	0	0	8	22	16	13	17	6	0	0
16	8	22	18	11	17	6	0	0	8	22	16	11	17	8	0	0
17	7	16	28	23	8	0	0	0	7	16	28	25	6	0	0	0
18	8	20	25	23	6	0	0	0	8	20	25	21	8	0	0	0

Figure 6. Canonical *vs.* centric ordering, according to *LDS* (and to $c(LDS)_i$): (a) sequence of graph distances SGD and sequence of graph walks $SGW^{(e)}$ and $LW^{(2)}$ matrices (b) for the graphs **6** and **7**.



8 9

10 11

(a)
LDS:
(**8**;**9**): ‖12 × (23, 69, 92, 92)‖
(**10**;**11**): ‖12 × (21, 63, 126, 42)‖
(b)
LSRW$^{(e)}$:
e = 4 **8**: ‖12 × (15, 45, 60, 60)‖
9: ‖12 × (19, 57, 76, 76)‖
e = 5 **10**: ‖9 × (8, 22, 44, 16); 3 × (6, 24, 48, 12)‖
11: ‖4 × (8, 20, 36, 16); 8 × (6, 20, 42, 12)‖
LSRW$^{(e)}$S:
e = 4 **8**: ‖12 × (72, 216, 288, 288)‖
9: ‖12 × (82, 246, 328, 328)‖
e = 5 **10**: ‖9 × (106, 308, 616, 212); 3 × (96, 318, 636, 192)‖
11: ‖4 × (106, 292, 576, 212); 8 × (96, 298, 606, 192)‖

Figure 7. Graphs with degenerate LDS matrices (a) and nondegenerate LSRW$^{(e)}$ and LSRW$^{(e)}$S matrices (b).

Table 3. Path Sequences in Heptanes and the Corresponding "*X*" and "*C*" Intermolecular Ordering Compared with Three TIs: *X*(LK); DM[1], and C(L3DS)

path sequence	*X* ord	*X*(LK)	DM[1 35]	*C* ord	*C*(L3DS)[a]
6 5 4 3 2 1	C_7	14.395 06	13.424 62	C_7	0.589 38
6 6 4 3 2 0	$2MC_6$	14.615 04	14.765 62	$2MC_6$	0.740 61
6 6 5 3 1 0	$3MC_6$	14.636 82	15.082 12	$3MC_6$	0.785 80
6 6 6 3 0 0	$3EC_5$	14.658 60	15.366 58	$24M_2C_5$	0.996 23
6 7 4 4 0 0	$24M_2C_5$	14.836 80	16.363 13	$3EC_5$	1.036 08
6 7 6 2 0 0	$23M_2C_5$	14.876 40	16.949 21	$22M_2C_5$	1.021 87
6 8 4 3 0 0	$22M_2C_5$	15.054 60	17.949 75	$23M_2C_5$	1.068 19
6 8 6 1 0 0	$33M_2C_5$	15.094 20	18.485 28	$33M_2C_5$	1.149 82
6 9 6 0 0 0	$223M_3C_4$	15.312 00	20.547 01	$223M_3C_4$	1.348 05

[a] L3DS is built by analogy with LDS by using 3D metric distances instead of the topological distances; the index is computed on optimized geometry of heptane isomers (see ref 9).

Randić[7] developed the first procedure by using path sequences as a ground for computing Euclidian distances within various sets of compounds. Basak *et al.*[29] performed a PCA (principal component analysis) on a large molecular data base (3692) chemicals) by means of 90 TIs and Euclidian distance for structure similarity measurements.

One defines the generalized Minkowski distance, D_M, as[29,35]

$$D_M = [\sum_{i=1}^{n}(x_i - y_i)^z]^{1/z} \quad (26)$$

with x_i and y_i being the coordinates of two structures and $X(x_1,x_2,...,x_n)$ and $Y(y_1,y_2,...,y_n)$ within an n-dimensional space. For $z = 2$, D_M becomes the Euclidian distance, D_E. For $z = 1$, the Manhattan distance, D_{Mh}, is obtained:

$$D_{Mh} = \sum_{i=1}^{n}|x_i - y_i| \quad (27)$$

We used this last distance, with the specification that x_i and y_i are LOVIs of "*x*" or "*c*" type (cf. eqs 24 and 25), constructed on LM matrices (which arranged in canonical form). Thus, we applied this procedure on a set of four graphs, **12–15** (Figure 8), the first three of them being related by Dobrynin[17] in showing degenerate λ and B matrices (actually SD and LK matrices).

By inspecting the graphs in Figure 8, one can see that these structures can be considered as cycles consisting of two types of half hexes, denoted A and B. Next, one can draw three types of cyclic sequences: (a) ABAB, (b) ABBA, and (c) BAAB. It is easy to prove, by cyclic permutations, that there are only four distinct combinations of AB sequences, a – a, b – a, b – c, and b – b, the last combination corresponding to the additional graph (**15**) included by us in Figure 8. Any other combinations reduce to the above mentioned structures.

The SD and LK (or LW$^{(1)}$) matrices degenerate in the set of graphs **12–15**, so it is expected that they are very similar. Although LW$^{(e)}$ and LW$^{(e)}$S matrices do not degenerate at elongation larger than 2, they differ only in entries corresponding to remote vertices *vs* each *i* vertex in the graph. This is also true in the case of LDS matrix. Indeed, the "*x*" type LOVIs constructed on LW$^{(e)}$S and LDS gave very low values of D_{Mh}, which ranged on five orders of magnitude, as *e* varied between 2 and 6. Better results offered "*c*" type LOVIs, when computed normalized D_{Mh} values, by the following eq:

$$D_{Mh} = \sum_e \sum_i [|c(LM^{(e)})_{i1} - c(LM^{(e)})_{i2}|/(c(LM^{(e)})_{i1} + c(LM^{(e)})_{i2})] \quad (28)$$

Now, the values of D_{Mh} ranges in the domain of 10^{-2}, the results being presented in the distance arrays in Table 4.

From both A_1 and A_2 arrays, one can see that **12** is more similar with **15** and **13** is closer with **14**. The data in A2 (computed on LW$^{(e)}$S) show **13** and **14** to be the most similar structures within the considered set. This result is supported by the sequences of global walk count, SGW$^{(e)}$: they differ, within the set, only starting from $e = 9$ (meaning all structures are very similar), but for **13** and **14** they are still identical (until $e = 13$).

DISCUSSION

Randić claimed some requirements[8] for matrices to become grounds for TIs design: their entries need "to have direct structural interpretation, to represent at least one particular molecular property, to be sensitive to isomeric variations, to be generalized to "higher" analogues, and, if possible, to be easily constructed". We tried to satisfy at least a part of these recommendations.

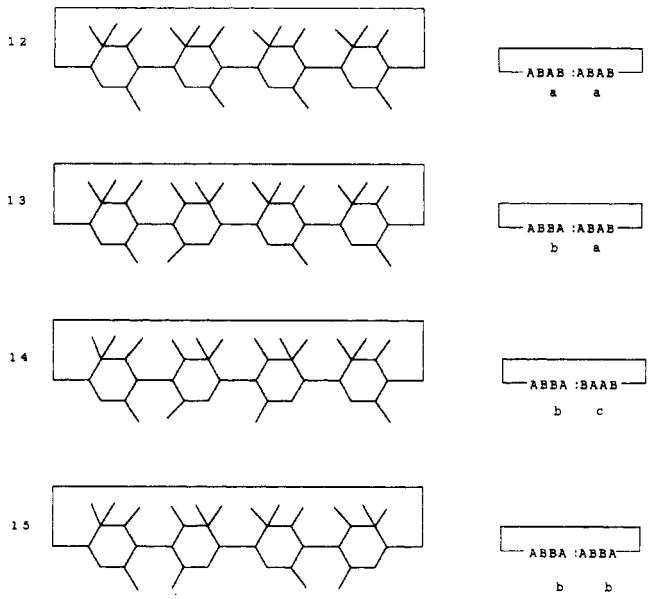
A regard upon the layer matrices enables one some remarks:

1. SM$^{(e)}$, as sequences of degrees (e.g., DDS[18,21]), count the number of walks (of various type and elongation) emerging from a given vertex.

2. LM$^{(e)}$, as matrices of vertex properties, evaluate the property at various shells around the given vertex.

3. Except for SD, the SM matrices do not superimpose over the partitions of the graph and, moreover, SSRW$^{(e)}$ and SW$^{(e)}$ have formally a nonrestricted number of columns (but

(a)



(b)

e:	1	2	3	4	5	6	7	8	9	10
2*SGD(12–15):	88,	152,	200,	216,	248,	224,	168,	136,	96,	32
e:	1	2	3	4	5	6	7	8	9	10
2*SGW$^{(e)}$ (12):	88,	240,	616,	1648,	4312,	11 440,	30 088,	79 592,	209 704,	554 136
2*SGW$^{(e)}$ (13):	88,	240,	616,	1648,	4312,	11 440,	30 088,	79 592,	209 712,	554 136
2*SGW$^{(e)}$ (14):	88,	240,	616,	1648,	4312,	11 440,	30 088,	79 592,	209 712,	554 136
2*SGW$^{(e)}$ (15):	88,	240,	616,	1648,	4312,	11 440,	30 088,	79 592,	209 720,	554 136

Figure 8. Graphs with degenerate SD, LC, and LW$^{(1)}$ matrices (a) and sequences of graph distances SGD and graph walks SGW$^{(e)}$ in the graphs **12–15** (b).

Table 4

A_1: D_{Mh} for the Graphs **12–15**, Computed with $c(LDS)_i \times 10^3$ Values (dsp = 20)

graph	12	13	14	15
12	0	3.3760	5.5463	1.2138
13		0	2.8633	3.4901
14			0	5.8184
15				0

A_2: D_{Mh} for the Graphs **12–15**, computed with $c(LW^{(e)}S)_i \times 10^2$ Values (dsp = 20; e = 2–6)

graph	12	13	14	15
12	0	11.8007	13.8506	11.0244
13		0	6.6727	10.0055
14			0	11.0654
15				0

considering the Cayley–Hamilton theorem, which result states that the nth and all higher rank walks are linear combinations of the lower rank walks, it imposes $e = n - 1$ as a limit).

4. LM$^{(e)}$ matrices follow the partitions of the graph, the number of columns being the graph eccentricity (diameter) plus one.

5. According to the type of graph theoretical property (a degree or a metric property, *i.e.*, a walk sum), LM$^{(e)}$ matrices can be grouped into layer matrices of degrees (LC, LK, LSRW$^{(e)}$, and LW$^{(e)}$) and layer matrices of walk sums (LDS, LPS, LSRW$^{(e)}$S, and LW$^{(e)}$S).

6. Layer degree matrices, such as LW$^{(e)}$, can be derived by "exploding" the SM$^{(e)}$ matrices (the columns of which become the first ones in LM$^{(1)}$ to LM$^{(e)}$ matrices).

7. Layer matrices of walk sums are SM$^{(e)}$-calculable, their first column being $\sum_e(m_i^{(e)}e$.

8. The matrices SD and LC differ only by the lc_{i0} column, which counts the vertex i, itself. If one neglects this column, then the two matrices are identical and represent the common point between SM and LM matrices. The LC matrices just count the vertices in the partitions of the graph. Thus, it is not surprising that Skorobogatov[1] and Dobrynin[17] called their λ matrix a layer matrix. However, in its line form, λ/SD matrice coincides with DDS.[18–21]

9. SD and SP matrices, as global values GM$^{(e)}$, can be used in intermolecular ordering of alkane isomers.

10. The counting of walk degrees is important by virtue of their relation with the spectral properties: the eigenvalues (as shown by Cvetković and Gutman[37] and more recently by Graovac and Babić[38]) and the eigenvectors (as recently demonstrated Rucker and Rucker[30]).

On the other hand, the walk counting offers a set of graph descriptors, of high discriminating power, which are useful both in graph isomorphism testing and in correlating with physicochemical properties (*i.e.*, NMR data[32]). However, in isospectral graphs, or also in regular graphs, single number descriptors based on walk counting fail in differentiating the graphs/subgraphs. In highly similar structures such descriptors need a high rank. In the opposite, our LM$^{(e)}$ matrices (and the indices constructed on them) are efficient at quite a low rank, as we showed in the case of pair isospectral graphs **4** and **5** (and their pairs of isospectral vertices: (3;6′), (6;3′), and (12;12′)) or **6** and **7** (see Figures 5 and 6). For other examples see ref 25.

11. Among the LM$^{(e)}$ matrices, LSRW$^{(e)}$ and LSRW$^{(e)}$S proved to be highly discriminating tools (see examples in Figure 7).

12. Layer matrices, in canonical form, can be taken as a ground for canonical (and centric) numbering of graphs. Thus, they offer the possibility of comparison within a set of isomeric graphs.

CONCLUSIONS

The distinction between sequence matrices SM and (true) layer matrices, LM, we made upon the nonsymmetrical matrices based on the partitions in graphs was proved to be welcome. Once rigorously defined, such matrices, especially LM ones, can be used in various purposes: in design of topological indices (next utilizable in QSPR/QSAR studies), in graph ordering, in topological symmetry perception, and also in molecular similarity testings.

A program TOP (in TURBO PASCAL and operable on IBM PC compatible computers) enabled the computation and comparison of SM and LM matrices within various sets of structures.

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