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A NOTE ON TOPOLOGICAL INDICES

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ABSTRACT

A number of topological indices are defined in terms of the higher order adjacency matrices. In this way the similarities and differences between many of the indices may immediately be seen.

1. INTRODUCTION

The revived interest in topological indices is apparent from a number of recent reviews [1-7]. Topological indices are convenient devices for translating chemical constitution into a single number which may be used in quantitative structure-property relationships (QSPR) or in quantitative structure-activity relationships (QSAR). The latter use is especially vigorously exploited in the last few years [1,3-5, 8-13].

We counted 39 topological indices that are presently available in the literature [14]. They are usually classified as topological indices based on the adjacency matrix or on the distance matrix [3-7,15]. Such a large number of topological indices rised a question to what extent are they orthogonal. In other words, is it possible that some topological indices existing in the literature express predominantly the same type of constitutional information: the difference residing in the scaling factor?

Recently the interrelations amongst the topological indices was studied [7,16]. The conclusions reached were that a number of the indices are strongly intercorrelated independently of a way how they were derived. This lead us to look closer at the present classification of topological indices as those based on the adjacency matrix and those based on the distance matrix. It appears that this classification is somewhat artificial. We decided to investigate whether

this variety of topological indices may be derived from the same topological [17] invariant. For this purpose it is natural to select the adjacency matrix of a graph (structure) [18,19] since it can be simply set for any G. In this work we will follow the nomenclature of our book [5,19] and graph theoretical definitions of Harary [20].

2. HIGHER ORDER ADJACENCY MATRICES

Molecules will be represented by chemical graphs [19, 21]. A (chemical) graph G consists of a finite, non-empty set V = V(G) of vertices (atoms), together with a prescribed set E = E(G) of subsets of V with two distinct vertices. The elements of E are called the edges (bonds) of G and denoted as $e = \{u,v\} \epsilon E$. The vertices u and v are said to be adjacent if $\{u,v\} \epsilon E$. Graphs with multiple edges (double, triple bond), weighted vertices (heteroatoms), and weighted edges (heterobonds), are not considered, although this can also be done [22-25].

The adjacency matrix of a labelled graph G, with N vertices, $\underline{A}(G) = \underline{A}$, is the square symmetric matrix which contains information about the internal connectivity of vertices in G. It is defined as

$$(\underline{A})_{ij} = \begin{cases} 1 & \text{if, and only if, } \{i,j\} \epsilon E \\ 0 & \text{otherwise} \end{cases} \qquad (1)$$

The adjacent vertices, i.e. the vertices amongst which the topological distance is unity, are the first neighbours. The vertices amongst which the distance is 2 are the second neighbours. The higher neighbours are defined in an analogous way.

In analogy with the adjacent matrix, $\underline{A} = \underline{A}_1$, one can derive the adjacency matrices of higher orders: second order $\underline{A}_2$, third order $\underline{A}_3$, fourth order $\underline{A}_4$, etc. These matrices are defined as

$$(\underline{A}_k)_{ij} = \begin{cases} 1 & \text{if, and only if, the vertex j is the k-th neighbour of the vertex i} \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

The diagonal elements of the square powers of the higher order adjacency matrices $\underline{A}_k$ ($k = 2,3,4,5,\ldots$), $(\underline{A}_k^2)_{ii}$, give the number of k-th neighbours of the vertex i. The sum of the matrices $\underline{A}_k$ is equal to the matrix $\underline{B}$.

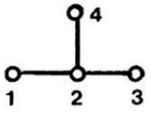
$$\sum_{k=1}^{k_{max}} \underline{A}_k = \underline{B} \qquad (3)$$

where $\underline{B}$ is the (NxN) matrix with entries $(\underline{B})_{ij} = 1$ and $(\underline{B})_{ii} = 0$, respectively.

The example of the first and second order adjacency matrices and their square powers is given in Figure 1.

Figure 1

The first and second order adjacency matrices and their square powers for a tree-graph G



G

$$\underline{A}_1 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \qquad \underline{A}_1^2 = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 3 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$$

$$\underline{A}_2 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad \underline{A}_2^2 = \begin{bmatrix} 2 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 1 \\ 1 & 0 & 0 & 2 \end{bmatrix}$$

The element $(\underline{A}_k)_{ij} = 1$ means that the distance between the vertices i and j is k. Hence, $(\underline{D})_{ij} = k$, where $\underline{D}$ is the distance matrix [18,19]. Therefore, when all the higher order matrices are known, the elements of the distance matrix are also known.

The matrices $\underline{A}_k$ may be obtained by means of the following procedure based on binary Boolean algebra [16,27,28].

If

$$\underline{S}^k = (\underline{I} + \underline{A}_1)^k \tag{4}$$

where $\underline{I}$ is the unit matrix, and

$$k_{max} = \min k \tag{5}$$

for which

$$(\underline{I} + \underline{A}_1)^k = (\underline{I} + \underline{A}_1)^{k+1} \tag{6}$$

then

$$\underline{S}^o = \underline{I} \tag{7}$$

$$\underline{S}^1 = \underline{I} + \underline{A}_1 \tag{8}$$

$$\underline{S}^2 = (\underline{I} + \underline{A}_1)^2 \tag{9}$$

.....

$$\underline{S}^{k_{max}} = (\underline{I} + \underline{A}_1)^{k_{max}} = (\underline{I} + \underline{A}_1)^{k_{max}+1} \tag{10}$$

and

$$\underline{A}_k = \underline{S}^k - \underline{S}^{k-1} \tag{11}$$

$$(\underline{D})_{ij} = \min k \tag{12}$$

for which

$$k \leqslant k_{max} \tag{13}$$

and

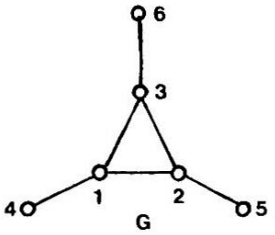
$$(\underline{S}^{(\underline{D})_{ij}})_{ij} = 1 \tag{14}$$

$$\underline{S}^{k_{max}} - \underline{I} = \underline{B} \tag{15}$$

Example is given in Figure 2.

Figure 2

$\underline{S}^k$ and $\underline{A}_k$ matrices of a given graph G



$$\underline{A} = \underline{A}_1 = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

$$\underline{S}^0 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\underline{S}^1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

$$\underline{S}^2 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 \end{bmatrix} \quad \underline{A}_2 = \underline{S}^2 - \underline{S}^1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\underline{S}^3 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad \underline{A}_3 = \underline{S}^3 - \underline{S}^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

$$\underline{S}^4 = \underline{S}^3$$

$$\underline{S}^5 = \underline{S}^4 = \underline{S}^3$$

$$\underline{S}^6 = \underline{S}^5 = \underline{S}^4 = \underline{S}^3$$

We developed a computer program for generating the $\underline{A}_k$ matrices of complex graphs using the above procedure [29].

3. TOPOLOGICAL INDICES DEFINED IN TERMS OF THE HIGHER ORDER ADJACENCY MATRICES

The adjacency matrix appear to be a very convenient basis for defining, and computing a number topological indices. We list several of them below.

(a) Total adjacency index [30,31]

$$A = \frac{1}{2} \sum_{i=1}^{N} A_i \qquad (16)$$

where $A_i = (\underline{A}_1^2)_{ii}$ is the number of all first neighbours of the vertex i and N is the number of vertices. This index is equal to the total number of edges (i.e. 1-walks) in G.

(b) The Zagreb Group indices [32,33]

$$M_1 = \sum_{i=1}^{N} A_i \, A_i \qquad (17)$$

$$M_2 = \sum_{\substack{\text{all} \\ \text{edges}}} A_i \, A_j \qquad (18)$$

(c) Randić's connectivity index [34]

$$\chi_R = \sum_{\substack{\text{all} \\ \text{edges}}} (A_i \, A_j)^{-1/2} \qquad (19)$$

This index is used abundantly in QSAR works.

(d) Platt's number [35]

$$F = \sum_{\substack{\text{all} \\ \text{edges}}} (A_i + A_j - 2) \qquad (20)$$

It may be reformulated as follows

$$F = \sum_{i=1}^{N} (A_i \cdot A_i - A_i) \qquad (21)$$

The first formula enables the direct comparison between F and A, whilst the second between F and the Zagreb Group indices, and also between F and $\mathcal{K}_R$.

(e) Gordon-Scantlebury's index [36]

$$S = \frac{1}{2} \sum_{i=1}^{N} A_i \cdot A_i - (N + \mu - 1) \qquad (22)$$

where μ is the cyclomatic number of a graph. The cyclomatic number of G enumerates the number of independent cycles in G and is equal to the minimum cuts (removal of edges) necessary to convert G into a tree (acyclic graph). For the complex graphs μ may be calculated by means of the following formula

$$\mu = M - N + 1 \qquad (23)$$

where M is the number of edges in G.

Substitution of μ in (22) by (23) leads to

$$S = \frac{1}{2} \sum_{i=1}^{N} A_i \cdot A_i - M \qquad (24)$$

Gordon-Scantlebury's index represents the number of all paths of length two in G. It is easily shown that the S index is equal to the half value of F

$$S = \frac{1}{2} F . \qquad (25)$$

(f) Wiener's number [37]

$$W = \frac{1}{2} \sum_{i=1}^{N} W_i \qquad (26)$$

where

$$W_i = \sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii} \cdot k \qquad (27)$$

(g) The polarity number [37]

$$p = \frac{1}{2} \sum_{i=1}^{N} (\underline{A}_3^2)_{ii} \qquad (28)$$

The polarity number represents pairs of vertices three edges apart in G.

(h) The distance sum index [38,39]

$$v_{D,i} = W_i \tag{29}$$

Because of the strong connection between Wiener's number and W_i, and historical continuation of Wiener's ideas [25,40-44], we propose the name Wiener's vertex index for the distance sum index.

(i) Balaban's index [38]

$$J = \frac{q}{\mu+1} \sum_{\substack{\text{all} \\ \text{edges}}} (v_{D,i} \cdot v_{D,j})^{-1/2} \tag{30}$$

where q is the number of edges in G, μ the cyclomatic number of a graph, and $v_{D,i}$, $v_{D,j}$ Wiener's vertex indices. Balaban's index represents an average distance sum connectivity index.

(j) Altenburg's polynomial [45]

$$P_A(G;x) = \frac{1}{2} \sum_{i=1}^{N} P_i \tag{31}$$

where P_i is Altenburg's index

$$P_i = \sum_{k=1}^{k_{max}} x_k \, (\underline{A}_k^2)_{ii} \tag{32}$$

$(\underline{A}_k^2)_{ii}$ is the number of atoms at a distance k from the i-th atom.

(k) Mean square distance topological index [7]

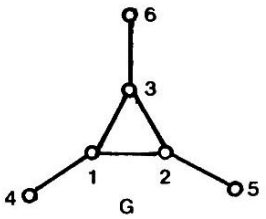
$$D^{(s)} = \left[\frac{\sum_{i=1}^{N} \sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii} \cdot k^s}{\sum_{i=1}^{N} \sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii}} \right]^{1/s} \qquad (33)$$

On testing various exponents s = 1,2,3, or 4 in (33), it was found [38] that for s = 2 afforded for alkanes the smallest degeneracy. For cyclic graphs, however, $D^{(2)}$ has a fairly high degeneracy. $D^{(2)}$ decreases with increasing branching.

In Figure 3 we give as an example the calculations for all listed topological indices.

Figure 3

Calculation of the topological indices presented in this work in terms of the higher order adjacency matrices and their square powers



$$\underline{A}_1 = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix} \qquad \underline{A}_1^2 = \begin{bmatrix} 3 & 1 & 1 & 0 & 1 & 1 \\ 1 & 3 & 1 & 1 & 0 & 1 \\ 1 & 1 & 3 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\underline{A}_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \underline{A}_2^2 = \begin{bmatrix} 2 & 1 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 \\ 1 & 1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 & 2 \end{bmatrix}$$

$$\underline{A}_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \qquad \underline{A}_3^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 & 2 \end{bmatrix}$$

(a) Total adjacency index

$$A = \frac{1}{2} \sum_{i=1}^{N} \underline{A}_i = \frac{1}{2} \sum_{i=1}^{N} (\underline{A}_1^2)_{ii} =$$

$$= \frac{1}{2} \left[(\underline{A}_1^2)_{11} + (\underline{A}_1^2)_{22} + \ldots + (\underline{A}_1^2)_{66} \right] =$$

$$= 6$$

(b) The Zagreb Group indices

$$M_1 = \sum_{i=1}^{N} A_i \cdot A_i = \sum_{i=1}^{N} (\underline{A}_1^2)_{ii} \cdot (\underline{A}_1^2)_{ii} =$$

$$= (\underline{A}_1^2)_{11} \cdot (\underline{A}_1^2)_{11} + (\underline{A}_1^2)_{22} \cdot (\underline{A}_1^2)_{22} + \ldots +$$

$$+ (\underline{A}_1^2)_{66} \cdot (\underline{A}_1^2)_{66} =$$

$$= 30$$

$$M_2 = \sum_{\substack{\text{all} \\ \text{edges}}} A_i \cdot A_j = \sum_{\substack{\text{all} \\ \text{edges}}} (\underline{A}_1^2)_{ii} \cdot (\underline{A}_1^2)_{jj} =$$

$$= (\underline{A}_1^2)_{11} \cdot (\underline{A}_1^2)_{22} + (\underline{A}_1^2)_{11} \cdot (\underline{A}_1^2)_{33} +$$

$$+ (\underline{A}_1^2)_{11} (\underline{A}_1^2)_{44} + \ldots + (\underline{A}_1^2)_{33} \cdot (\underline{A}_1^2)_{66} =$$

$$= 36$$

(c) Randić's connectivity index

$$\chi_R = \sum_{\substack{\text{all} \\ \text{edges}}} (A_i A_j)^{-1/2} = \sum_{\substack{\text{all} \\ \text{edges}}} \left[(\underline{A}_1^2)_{ii} \cdot (\underline{A}_1^2)_{jj} \right]^{-1/2} =$$

$$= \left[(\underline{A}_1^2)_{11} \cdot (\underline{A}_1^2)_{22} \right]^{-1/2} + \ldots + \left[(\underline{A}_1^2)_{33} \cdot (\underline{A}_1^2)_{66} \right]^{-1/2} =$$

$$= 2.73$$

(d) Platt's number

$$F = \sum_{\substack{\text{all}\\ \text{edges}}} (A_i + A_j - 2) = \sum_{\substack{\text{all}\\ \text{edges}}} (\underline{A}_1^2)_{ii} + (\underline{A}_1^2)_{jj} - 2 =$$

$$= \left[(\underline{A}_1^2)_{11} + (\underline{A}_1^2)_{22} - 2 \right] + \ldots + \left[(\underline{A}_1^2)_{33} + (\underline{A}_1^2)_{66} - 2 \right] =$$

$$= 18$$

(e) Gordon-Scantlebury's index

$$S = \frac{1}{2} \sum_{i=1}^{N} A_i \cdot A_i - M =$$

$$= \frac{1}{2} M_1 - M =$$

$$= 9$$

(f) Wiener's number

$$W = \frac{1}{2} \sum_{i=1}^{N} W_i = \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii} \cdot k =$$

$$= \frac{1}{2} \left\{ \sum_{i=1}^{N} \left[(\underline{A}_1^2)_{ii} \cdot 1 + (\underline{A}_2^2)_{ii} \cdot 2 + (\underline{A}_3^2)_{ii} \cdot 3 \right] \right\} =$$

$$= \frac{1}{2} \left\{ \left[(\underline{A}_1^2)_{11} \cdot 1 + (\underline{A}_1^2)_{22} \cdot 1 + \ldots + (\underline{A}_1^2)_{66} \cdot 1 \right] + \right.$$

$$+\left[(\underline{A}_2^2)_{11} \cdot 2 + (\underline{A}_2^2)_{22} \cdot 2 + \ldots + (\underline{A}_2^2)_{66} \cdot 2 \right] +$$

$$+\left[(\underline{A}_3^2)_{11} \cdot 3 + (\underline{A}_3^2)_{22} \cdot 3 + \ldots + (\underline{A}_3^2)_{66} \cdot 3 \right] \Bigg\} =$$

$$= 27$$

(g) The polarity number

$$p = \frac{1}{2} \sum_{i=1}^{N} (\underline{A}_3^2)_{ii} = \frac{1}{2} \left[(\underline{A}_3^2)_{11} + (\underline{A}_3^2)_{22} + \ldots + \right.$$

$$\left. + (\underline{A}_3^2)_{66} \right] =$$

$$= 3$$

(h) Wiener's vertex index

$$v_{D,i} = W_i; \; i = 1,2,\ldots,6$$

$$W_i = \sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii} \cdot k$$

$$W_1 = (\underline{A}_1^2)_{11} \cdot 1 + (\underline{A}_2^2)_{11} \cdot 2 + (\underline{A}_3^2)_{11} \cdot 3 =$$

$$= 7$$

$$W_2 = (\underline{A}_1^2)_{22} \cdot 1 + (\underline{A}_2^2)_{22} \cdot 2 + (\underline{A}_3^2)_{22} \cdot 3 =$$

$$= 7$$

.
.
.

$$W_6 = (\underline{A}_1^2)_{66} \cdot 1 + (\underline{A}_2^2)_{66} \cdot 2 + (\underline{A}_3^2)_{66} \cdot 3 =$$

$$= 11$$

(i) Balaban's index

$$J = \frac{q}{\mu+1} \sum_{\substack{\text{all} \\ \text{edges}}} (W_i W_j)^{-1/2} =$$

$$= \frac{6}{1+1} \left[(W_1 \cdot W_2)^{-1/2} + (W_1 \cdot W_3)^{-1/2} + (W_1 \cdot W_4)^{-1/2} + \right.$$

$$\left. + (W_2 \cdot W_3)^{-1/2} + (W_2 \cdot W_5)^{-1/2} + (W_3 \cdot W_6)^{-1/2} \right] =$$

$$= 3 \left[(7 \cdot 7)^{-1/2} + (7 \cdot 7)^{-1/2} + (7 \cdot 11)^{-1/2} + \right.$$

$$\left. + (7 \cdot 7)^{-1/2} + (7 \cdot 11)^{-1/2} + (7 \cdot 11)^{-1/2} \right] =$$

$$= 2.315$$

(j) Altenburg's polynomial

$$P_A(G;x) = \frac{1}{2} \sum_{i=1}^{N} P_i = \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{k_{max}} x_k \, (\underline{A}_k^2)_{ii} =$$

$$= \frac{1}{2} \sum_{i=1}^{N} \left[x_1 (\underline{A}_1^2)_{ii} + x_2 (\underline{A}_2^2)_{ii} + x_3 (\underline{A}_3^2)_{ii} \right] =$$

$$= \frac{1}{2}\left\{\left[x_1(\underline{A}_1^2)_{11} + x_1(\underline{A}_1^2)_{22} + \ldots + x_1(\underline{A}_1^2)_{66}\right] + \right.$$

$$+ \left[x_2(\underline{A}_2^2)_{11} + x_2(\underline{A}_2^2)_{22} + \ldots + x_2(\underline{A}_2^2)_{66}\right] +$$

$$\left. + \left[x_3(\underline{A}_3^2)_{11} + x_3(\underline{A}_3^2)_{22} + \ldots + x_3(\underline{A}_3^2)_{66}\right]\right\} =$$

$$= 6x_1 + 6x_2 + 3x_3$$

(k) Mean Square Distance Topological Index

$$D^{(s)} = \left[\frac{\sum_{i=1}^{N}\sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii} \cdot k^s}{\sum_{i=1}^{N}\sum_{k=1}^{k_{max}} (\underline{A}_k^2)_{ii}}\right]^{1/s}$$

$$D^{(1)} = \left[\frac{\sum_{i=1}^{N} (\underline{A}_1^2)_{ii}\cdot 1^1 + (\underline{A}_2^2)_{ii}\cdot 2^1 + (\underline{A}_3^2)_{ii}\cdot 3^1}{\sum_{i=1}^{N} (\underline{A}_1^2)_{ii} + (\underline{A}_2^2)_{ii} + (\underline{A}_3^2)_{ii}}\right]^{1/1} =$$

$$= \frac{(\underline{A}_1^2)_{11}\cdot 1 + (\underline{A}_1^2)_{22}\cdot 1 + \ldots + (\underline{A}_3^2)_{66}\cdot 3}{(\underline{A}_1^2)_{11} + (\underline{A}_1^2)_{22} + \ldots + (\underline{A}_3^2)66} =$$

$$= 1.8$$

$$D^{(2)} = \left\{ \frac{\sum_{i=1}^{N} \left[(\underline{A}_1^2)_{ii} \cdot 1^2 + (\underline{A}_2^2)_{ii} \cdot 2^2 + (\underline{A}_3^2)_{ii} \cdot 3^2 \right]}{\sum_{i=1}^{N} \left[(\underline{A}_1^2)_{ii} + (\underline{A}_2^2)_{ii} + (\underline{A}_3^2)_{ii} \right]} \right\}^{1/2} =$$

$$= \left[\frac{(\underline{A}_1^2)_{11} \cdot 1 + (\underline{A}_1^2)_{22} \cdot 1 + \ldots + (\underline{A}_3^2)_{66} \cdot 3^2}{(\underline{A}_1^2)_{11} + (\underline{A}_1^2)_{22} + \ldots + (\underline{A}_3^2)_{66}} \right]^{1/2} =$$

$$= 1.95$$

4. CONCLUDING REMARKS

Higher order adjacency matrices provide a way for the uniform definition of many topological indices. The comparison between indices (a)-(e) (these are topological inidices earlier classified as those based on the adjacency matrix [46]) and (f)-(k) (these are topological indices earlier classified as those based on the distance matrix) reveals that the first set of indices is based on the number of first neighbours, whereas the indices in the second set are based on the number of second, third, and higher order neighbours, respectively. However, all these indices are related through the adjacency matrix. The strong intercorrelation between M_1 and S (the correlation coefficient is 0.98 for alkanes, 0.99 for alkylbenzenes, and 0.97 for cyclic structures [16]) is not sur-

prising, because these two indices differ for a given graph for the number of bonds only

$$2S - M_1 = 2M . \tag{34}$$

Interesting finding by Motoc et al. [16] is the high correlation between Randić's connectivity index and Wiener's number (the correlation coefficient 0.98 for alkanes, 0.99 for alkylbenzenes, and 0.98 cyclic structures [16]). The only reason for the strong intercorrelation we see in the fact that at the root of both indices is the adjacency matrix. The above result justifies the use of Wiener's number in QSPR and QSAR studies on equal footing to highly successful Randić's connectivity index [13,40,41,47].

A fairly high correlation is also found between M_1 index and Wiener's number (the correlation coefficient is 0.80 for alkanes, 0.88 for alkylbenzenes, and 0.84 for cyclic structure [16]). This leads to the idea that the Zagreb Group indices may be redefined in terms of the distance sum indices

$$M_1' = \sum_{i=1}^{N} W_i \cdot W_i \tag{35}$$

$$M_2' = \sum_{\substack{\text{all} \\ \text{edges}}} W_i \cdot W_j \tag{36}$$

It is well known that the indices M_1 and χ_R are related through the adjacency matrix. Thus, the high interrelationship between them is not surprising (the correlation coefficient is 0.78 for alkanes, 0.89 for alkylbenzenes, and 0.81 for cyclic structures [16]).

Our present work in progress [48] is aimed to detailed study of the intercorrelation between topological indices for alkane-trees and polyhexes.

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[28] Rules of Boolean Algebra

Two operations, addition (+) and multiplication (·), are presented, and the following laws of arithmetic are used:

(1) $0 \cdot 0 = 0$

$$1 + 1 = 1$$

(2) $1 \cdot 1 = 1$

$$0 + 0 = 0$$

(3) $1 \cdot 0 = 0 \cdot 1 = 0$

$$0 + 1 = 1 + 0 = 1$$

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