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On a matrix representation of molecular structures

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ABSTRACT. In order to discriminate molecular structures containing multiple bonds and heteroatoms, the paper considers the weighted electronic connectivity matrix (CEP). This matrix is obtained by replacing the classical topological distance by the so called weighted electronic distance ($w.e.d$). The CEP matrix can be then used for obtaining several topological indices [10].

1. INTRODUCTION

It is well known that the molecular graphs can be easily represented by topological matrices $[1-3]$. As far as this is concerned, it is extremely convenient to have two matrices: the adjacency matrix of the graph G, $A = A(G)$, and the distance matrix of G, $D = D(G)$.

The adjacency matrix is the most used one to characterize a graph. The distance matrix is, in many cases, reacher in information than the adjacency matrix, which can be considered a very special distance matrix containing only one unit distances. Both these matrices with their standard formulas are limited, that is, they cannot be applied to molecules with multiple bonds and/or heteroatoms. However, the definition of the adjacency has been expanded in order to include all possible chemical structures [1, 4, 5]. The most important step in this approach has been taken by Balaban for multigraphs [6] and Barysz [7], Estrada [8] and Randić [9] for heteroatoms.

The main merit of the matrix we defined recently [10] is its power of reproducing the information concerning both the adjacencies and distances in the molecules on the one hand, but especially the possibility to apply this model to all chemical structures, on the other hand.

We called this matrix the weighted electronic connectivity matrix, CEP.

2. THE WEIGHTED ELECTRONIC CONNECTIVITY MATRIX

The weighted electronic connectivity matrix, CEP, of a simple graph $G = \{V, E\}$, where V is the vertices set and E is the edges set, is a symmetric and quadratic $N \times N$ matrix whose entries are given by:

$$CEP(G) = \left\{[CEP]_{ij};\ i, j \in V(G)\right\} \tag{2.1}$$

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with:

$$[CEP]_{ij} = \begin{cases} w.e.d.(i,j), & \text{if} \quad i \neq j \quad \text{and} \quad (i,j) \in E(G) \\ 0, & \text{if} \quad i = j \quad \text{or} \quad (i,j) \notin E(G), \end{cases} \tag{2.2}$$

where $w.e.d$ is the weighted electronic distance between the atoms (vertices) i and j.

The weighted electronic distance is computed by means of the following formula, obtained in [13]:

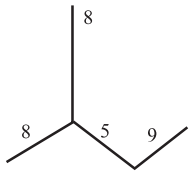
$$w.e.d.(i,j) = \frac{1}{b_r} \cdot \frac{z'_i + z'_j}{v_i \cdot v_j} \tag{2.3}$$

where:

- b_r denotes the bond weight value: 1 for single bond, 2 for double bond, 3 for triple bond and 1,5 for aromatic bond;
- v_j denotes the degree of vertex i;
- z'_idenotes the formal degree of vertex i and is defined by: $z'_i = z_i \cdot v_j$;
- z_i denotes the order number of atom i in Mendeleev's periodic system.

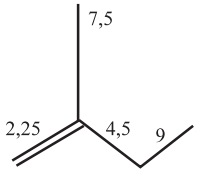
The formal degree z'_i represents a local vertex invariant (LOVI) in the molecular graph, while $w.e.d.(i,j)$ represents a local edge invariant (LOEI). Similar formulas which involve the order numbers as well as the multiplicity order of covalent bonds have been used, but in a different context, by Barysz and collaborators [7] and Balaban [6].

In Figure 1 are given the CEP matrices for five compounds which have the same adjacency matrix. The sum of all entries on the row/column i is denoted by SEP_i and is a local vertex invariant.



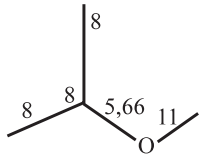
G.1
(2-Methyl-butane)

$$CEP(G.1) = \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{matrix} SEP_i \end{matrix} \\ \begin{bmatrix} 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 5 & 0 & 8 \\ 0 & 5 & 0 & 9 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} \\ 8 \\ 21 \\ 14 \\ 9 \\ 8 \end{array}$$



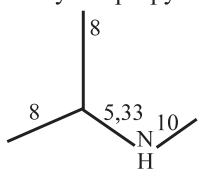
G.2
(2-Methyl-1-butene)

$$CEP(G.2) = \begin{array}{c} \\ \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{matrix} SEP_i \end{matrix} \\ \begin{bmatrix} 0 & 2,25 & 0 & 0 & 0 \\ 2,25 & 0 & 4,5 & 0 & 7,5 \\ 0 & 4,5 & 0 & 9 & 0 \\ 0 & 0 & 9 & 0 & 0 \\ 0 & 7,5 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{array}{c} \\ 2,25 \\ 14,25 \\ 13,5 \\ 9 \\ 7,5 \end{array}$$



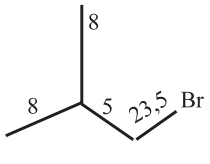
G.3
(Methyl-isopropyl-ether)

$$CEP(G.3) = \begin{bmatrix} 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 5,66 & 0 & 8 \\ 0 & 5,66 & 0 & 11 & 0 \\ 0 & 0 & 11 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 \end{bmatrix} \begin{matrix} SEP_i \\ 8 \\ 21,66 \\ 16,66 \\ 11 \\ 8 \end{matrix}$$



G.4
(Methyl-isopropyl-amine)

$$CEP(G.4) = \begin{bmatrix} 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 5,33 & 0 & 8 \\ 0 & 5,33 & 0 & 10 & 0 \\ 0 & 0 & 10 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 \end{bmatrix} \begin{matrix} SEP_i \\ 8 \\ 21,33 \\ 15,33 \\ 10 \\ 8 \end{matrix}$$



G.5
(3-Methyl-1-bromo-butane)

$$CEP(G.5) = \begin{bmatrix} 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 5 & 0 & 8 \\ 0 & 5 & 0 & 23,5 & 0 \\ 0 & 0 & 23,5 & 0 & 0 \\ 0 & 8 & 0 & 0 & 0 \end{bmatrix} \begin{matrix} SEP_i \\ 8 \\ 21 \\ 28,5 \\ 23,5 \\ 8 \end{matrix}$$

Figure 1. CEP matrices for compounds containing double bonds and heteroatoms

It is easy to see differences between the matrices above, while the adjacency matrix, A, for this five compounds is the same:

$$A(G.1) = A(G.2) = A(G.3) = A(G.4) = A(G.5) = \begin{vmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{vmatrix}. \tag{2.4}$$

Replacing the usual topological distance between two atoms linked covalently by the weighted electronic distance, we obtain a new matricial representation of the molecular structure, which reproduces much more accurately the connectivities between atoms.

Besides the capacity of differentiating the multiple bonds and those containing heteroatoms, *w.e.d.* has the merit of distinguishing even the bonds of the same type between two identical atoms, depending on their connectivities. Thus, the simple bond between two secondary carbon atoms has a *w.e.d.* different from that of a simple covalent bond between a primary and a secondary atom. No other system of representing the chemical bonds has, as for as we know, this power of differentiating the chemical bonds according to the context in which they are in the molecule.

Starting from the CEP matrix some local vertex invariants (SEP_i, formal degree, RS_i, v_i) and three classes of topological indices (ZEP, RZ, V) have been

defined. If we denote:

$$SEP_i = \sum_{j=1}^{n} [CEP]_{ij}, \quad i = 1, n, \tag{2.5}$$

then

$$ZEP = \sum_{i=1}^{n} (SEP_i)^{1/2} \tag{2.6}$$

is a topological index which will be intensively studied [14, 15, 16].

The following index is a Randić type topological index:

$$RZ = \frac{1}{2} \sum_{u=v} (s_u \cdot s_v)^{-\frac{1}{2}}, \tag{2.7}$$

where u, v are adjacent edges and $s_u = w.e.d.(i, j)$, if $u = (i, j)$.

We also consider the topological index

$$V_\gamma = \sum_{i=1}^{n} \frac{SEP_i}{\nu_i} = \sum_{i=1}^{n} V_{\gamma_i} \tag{2.8}$$

where ν_i is the degree of vertex i.

3. Conclusions

If we consider the fact that the matrix of weighted electronic connectivity CEP can be regarded as a matrix of special adjacency from which a distance matrix DEP can be deduced, this means that all the theory in the molecular topology built on the usual adjacency matrix and the usual distance matrix can be rebuilt now, relying on the matrices CEP, respectively DEP. In this manner it is possible to define new topological indices starting from the matrices CEP and DEP and following similar procedures to those by which the common indices have been deduced, starting from the usual adjacency matrix, respectively the usual distance matrix.

From all these directions, we have investigated only one, constructing the index RZ by a procedure similar to the one by which Randić index is defined [11]. But this does not exclude the possibility of obtaining some strong topological indices by means of other procedures by means of other procedures as well, as the index ZEP was obtained, for example [10, 12].

The investigation of these possibilities still remains a theme of open research.

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