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Original Scientific Paper

Zagreb Indices: Extension to Weighted Graphs Representing Molecules Containing Heteroatoms*

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A possible extension of Zagreb indices to weighted graphs representing heterosystems is presented. It is based on the novel definition of the Zagreb indices by way of the here introduced Zagreb matrices. A theorem is given that is valid for the first Zagreb index of strongly weighted graphs.

ORIGINAL DEFINITION OF ZAGREB INDICES

A pair of molecular descriptors, denoted by M_1 and M_2, was introduced 35 years ago.[1] They were originally defined as:

$$M_1 = \sum_{vertices} d(i)\ d(i) \tag{1}$$

$$M_2 = \sum_{edges} d(i)\ d(j) \tag{2}$$

where $d(i)$ is the degree of vertex i and $d(i)\ d(j)$ is the weight of edge i–j.[2] These descriptors were given a variety of names in the literature, *e.g.*,[3,4] but they were most often called the *Zagreb indices*.[5] The Zagreb indices have found extensive applications in the structure-property-activity modeling; for summary see Refs. 3, 5 and 6. These indices are also included in a number of programs for the routine computation of molecular descriptors.[7] Mathematical and computational properties of the Zagreb indices are also continuously reported, *e.g.* Refs. 8 and 9.

DEFINITION OF ZAGREB INDICES *VIA* ZAGREB MATRICES

The Zagreb indices can be also defined in terms of the special graph-theoretical matrices that we have named the *Zagreb matrices*:

$$M_1 = \sum_{i} [\boldsymbol{ZM}]_{ii} \tag{3}$$

$$M_2 = (1/2) \sum_{i \neq j} [\boldsymbol{ZM}]_{ij} \tag{4}$$

where $\boldsymbol{ZM}$ is the Zagreb matrix defined as:

* Dedicated to Professor Nikola Kallay on the occasion of his 65[th] birthday.

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$$\left[\boldsymbol{ZM} \right]_{ij} = \begin{cases} [d(i)\, d(i)] & \text{if } \; i = j \\ [d(i)\, d(j)] & \text{if } \; i \neq j \\ 0 & \text{otherwise} \end{cases} \qquad (5)$$

It should be noted that the Zagreb matrices belong to a class of adjacency matrices.[10] The concept of graph-theoretical matrices as generators of descriptors was initially explored by Randić *et al.*[11] and later by Diudea[12] and others.[5,10]

ZAGREB INDICES FOR HETEROSYSTEMS

To express Zagreb indices *via* Zagreb matrices is a rather convenient way of computing these indices for the molecules with heteroatoms. In the past, the Zagreb indices were applied almost exclusively to hydrocarbons, which are represented by *simple* molecular graphs in chemical graph theory.[2] Molecules containing heteroatoms can be represented by *weighted* graphs.[2] In our case, we use the *vertex-weighted* molecular graphs.[13] We denote the weight of the weighted vertex by w to indicate that this vertex is 'different' from the rest of vertices standing for carbon atoms.

In Figure 1, as an example, we give hydrogen-suppressed 2-methylpentane, the corresponding simple graph (tree) and its vertex-degrees. Likewise in Figure 2, we give the hydrogen-suppressed ethyl isopropyl ether, the corresponding weighted graph (weighted tree – vertex belonging to the oxygen is denoted by a black dot) and its vertex degrees (the degree of the black-labeled vertex is denoted $2w$).

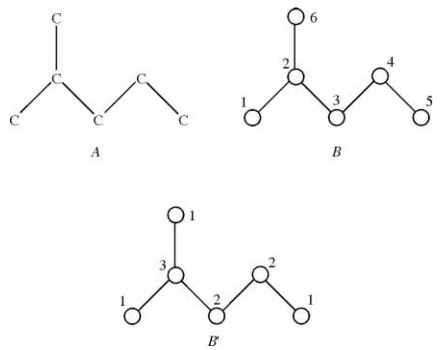


Figure 1. The hydrogen-depleted 2-methylpentane *A*, the corresponding labeled simple graph (tree) *B* and its vertex-degrees *B′*.

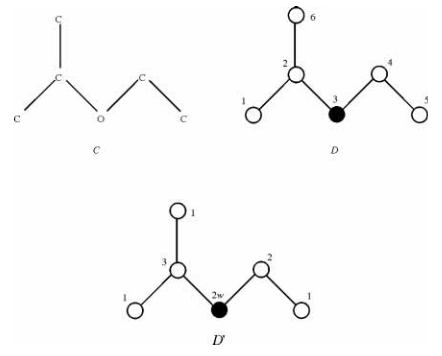


Figure 2. The hydrogen-depleted ethyl isopropyl ether *C*, the corresponding weighted graph (weighted tree – black dot denotes the position of oxygen) *D* and its vertex degrees (the degree of the black-labeled vertex is denoted $2w$) *D′*.

Below we give the Zagreb matrix of the molecular tree *B* and weighted molecular tree *D*.

$$\boldsymbol{ZM}(B) = \begin{bmatrix} 1 & 3 & 0 & 0 & 0 & 0 \\ 3 & 9 & 6 & 0 & 0 & 3 \\ 0 & 6 & 4 & 4 & 0 & 0 \\ 0 & 0 & 4 & 4 & 2 & 0 \\ 0 & 0 & 0 & 2 & 1 & 0 \\ 0 & 3 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The Zagreb indices of *B* can be obtained straightway from $\boldsymbol{ZM}$ ($M_1(B) = 20$ and $M_2(B) = 18$).

The Zagreb matrix of *D* differs from the one of *B* in the positions that contain the vertex with weight w.

$$\boldsymbol{ZM}(B) = \begin{bmatrix} 1 & 3 & 0 & 0 & 0 & 0 \\ 3 & 9 & 6w & 0 & 0 & 3 \\ 0 & 6w & 4w^2 & 4w & 0 & 0 \\ 0 & 0 & 4w & 4 & 2 & 0 \\ 0 & 0 & 0 & 2 & 1 & 0 \\ 0 & 3 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The corresponding values of the Zagreb indices are $M_1(D) = 16 + 4w^2$ and $M_2(D) = 8 + 10w$; for w = 1, $M_1(D)$ and $M_2(D)$ are reduced, of course, to $M_1(B)$ and $M_2(B)$.

Different schemes for assigning the numerical value to w are available.[14–20] However, there is *no* unique recipe for selecting the numerical value of w. The pragmatic approach is to consider w as the *variable* parameter whose optimal value is the result of the fitted procedure in the structure-property-activity modeling. There is also an additional, still not satisfactorily solved, problem related to assigning the numerical values of the multiple bonds.

A THEOREM FOR THE FIRST ZAGREB INDEX OF WEIGHTED GRAPHS

Theorem

For each $a,b,c \in N$ such that $a,b,c \geq 110$. There is a weighted graph with one set of vertices weighted by 1 and another set of vertices weighted by w such that $M_1(G) = aw^2 + bw + c$.

Proof

Let us start with the weighted thorn graph[21–23] G, shown below (white vertices are weighted by 1 and black vertices by w – edge weights are given beside the edges).

Let $G(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9)$, where $x_1, x_6, x_9 \geq 0$, $x_2, x_3, x_4, x_7, x_8 \in \{0,1\}$ and $x_5 \in \{0,1,2,...,6–2x_4\}$ be a graph obtained by (see the following figure):

1) adding x_1 black vertices to edge v_1v_2 and thus transforming it to a path of length $x_1 + 1$

2) adding x_2 fragments denoted by X_2 to the neighbors of v_3

3) adding x_3 fragments denoted by X_3 to the neighbors of v_3

4) adding x_4 fragments denoted by X_4 to the neighbors of v_4

5) adding x_5 fragments denoted by X_5 to the neighbors of v_4

6) adding x_6 white and x_6 black vertices in the alternating order to edge v_5v_6 and thus transforming it to a path of length $2x_6 + 1$

7) adding x_7 fragments denoted by X_7 to the neighbors of v_7

8) adding x_8 fragments denoted by X_8 to the neighbors of v_7

9) adding x_9 vertices to edge v_8v_9 and thus transforming it to a path of length $2x_9 + 1$

It can be easily seen that:

$$M_1(G) = 66w^2 + 52w + 26$$

and that:

$$M_1(G(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9)) =$$

$$(66 + 4x_1 + 41x_2 + 6x_3)w^2 + (52 + 31x_4 + 10x_5$$

$$+ 8x_6)w + (26 + 41x_7 + 6x_8 + 4x_9)$$

Let us show that with appropriate combination of numbers x_1, x_2 and x_3 one can get any number ≥ 112 (as a factor that multiplies w^2):

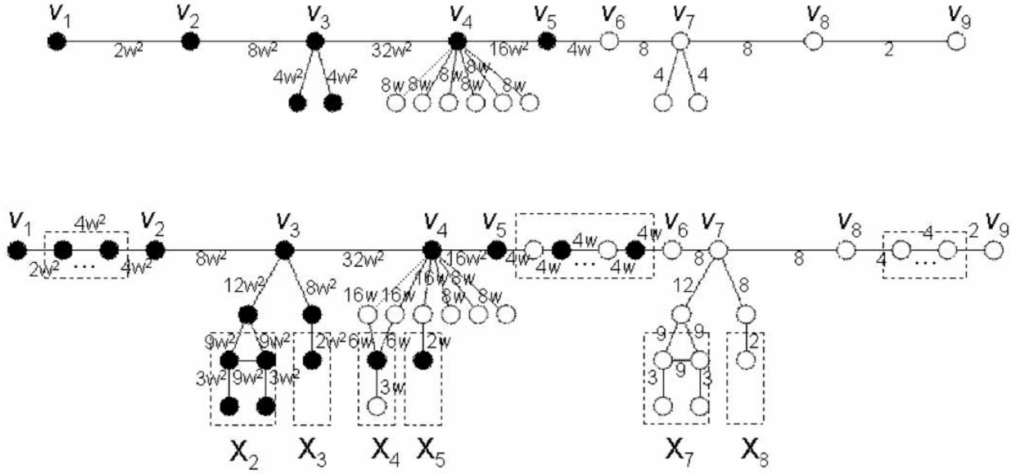
- Choosing values $x_2 = x_3 = 0$ and $x_1 = 11,12,13,...$ one obtains numbers: 110, 114, 118,...
- Choosing values $x_2 = 1$, $x_3 = 0$ and $x_1 = 1,2,3$ one obtains numbers: 111, 115, 119,...
- Choosing values $x_2 = 0$, $x_3 = 1$ and $x_1 = 10,11,12$ one obtains numbers: 112, 116, 120,...
- Choosing values $x_2 = 1$, $x_3 = 1$ and $x_1 = 0,1,2$ one obtains numbers: 113, 117, 121,...

Now, let us show that with appropriate combination of numbers x_4, x_5 and x_6 one can get any number ≥ 106 (as a factor that multiplies w):

- Choosing values $x_4 = 0$, $x_5 = 3$ and $x_6 = 3,4,5,...$ one obtains numbers: 106, 114, 122,…
- Choosing values $x_4 = 1$, $x_5 = 0$ and $x_6 = 3,4,5,...$ one obtains numbers: 107, 115, 123,…
- Choosing values $x_4 = 0$, $x_5 = 0$ and $x_6 = 7,8,9,...$ one obtains numbers: 108, 116, 124,…
- Choosing values $x_4 = 1$, $x_5 = 1$ and $x_6 = 2,3,4,...$ one obtains numbers: 109, 117, 125,…
- Choosing values $x_4 = 0$, $x_5 = 5$ and $x_6 = 1,2,3,...$ one obtains numbers: 110, 118, 126,…
- Choosing values $x_4 = 1$, $x_5 = 2$ and $x_6 = 1,2,3,...$ one obtains numbers: 111, 119, 127,…
- Choosing values $x_4 = 0$, $x_5 = 6$ and $x_6 = 0,1,2,...$ one obtains numbers: 112, 120, 128,…
- Choosing values $x_4 = 1$, $x_5 = 3$ and $x_6 = 0,1,2,...$ one obtains numbers: 113, 121, 129,…

Finally, let us show that with appropriate combination of numbers x_7, x_8 and x_9 one can get any number $\geq$ 70 (as a factor that multiplies w):

- Choosing values $x_7 = 0$, $x_8 = 0$ and $x_9 = 11,12,13,...$ one obtains numbers: 70, 74, 78,…



• Choosing values $x_7 = 1$, $x_8 = 0$ and $x_9 = 1,2,3,...$ one obtains numbers: 71, 75, 79,…

• Choosing values $x_7 = 0$, $x_8 = 1$ and $x_9 = 10,11,12,...$ one obtains numbers: 72, 76, 80,…

• Choosing values $x_7 = 1$, $x_8 = 1$ and $x_9 = 0,1,2,...$ one obtains numbers: 73, 77, 81,…

Hence, all possible polynomials with factors greater or equal to 112 are obtainable.

CONCLUSION

This topic was selected for our report because of an increasing number of publications on the properties and applications of the Zagreb indices in the last couple of years, but not a single one on the Zagreb indices of the weighted graphs, *e.g.* Refs. 24–33.

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SAŽETAK

Zagrebački indeksi: proširenje na utežene grafove koji predstavljaju molekule s heteroatomima

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Razmatrano je moguće proširenje Zagrebačkih indeksa na utežene grafove koji predstavljaju heterosustave. To se proširenje temelji na novoj definiciji Zagrebačkih indeksa pomoću novouvedenih Zagrebačkih matrica. Dan je i teorem za prvi Zagrebački indeks koji vrijedi za jako utežene grafove.