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DESIGN OF TOPOLOGICAL INDICES. PART 9[1]

A NEW RECURRENCE RELATIONSHIP FOR THE HOSOYA Z(Ch) STABILITY INDEX OF A MOLECULAR GRAPH

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A recurrence relationship for the Hosoya **Z(Ch)** stability index of a molecular graph *G* is obtained, by means of which the index **Z(Ch)** is expressed as a linear combination of the **Z(Ch)** indices of certain subgraphs of *G*. The subgraphs are obtained by deleting certain vertices and edges from the molecular graph.

INTRODUCTION

Molecular graph polynomials have important applications in the chemical graph theory:[2] Hückel quantum theory, topological resonance energy (TRE), topological effect on molecular orbitals (TEMO), generation of topological indices.

In this paper we will use the standard graph notation and terminology: *G* will denote a graph with N vertices: $v_1, v_2, ..., v_N$. The edge connecting vertices v_i and v_j is denoted by e_{ij}. The subgraph $G - v_i$ is obtained by deleting from the graph *G* the vertex v_i and its incident edges. The subgraph $G - e_{ij}$ is obtained by deleting from the graph *G* the edge e_{ij}. The number $\mathbf{Deg}(v_i)$ of the first neighbors of the vertex v_i is called the degree of the vertex v_i.

The acyclic (matching) polynomial of a graph *G* is defined as:[3-4]

$$\mathbf{Ac}(G,x) = \sum_{k=0}^{L} (-1)^k \mathbf{M}(G,k) x^{N-2k} = \sum_{n=0}^{L} a_n x^{N-n} \tag{1}$$

where $\mathbf{M}(G, k)$ is the number of *k*-matchings of *G*, i.e. the number of selections of *k* mutually non-adjacent edges in *G*, and L = [N/2], is the smallest integer not exceeding N/2. By definition, $\mathbf{M}(G, 0) = 1$ and $\mathbf{M}(G, 1)$ is equal to the number of edges.

The Hosoya **Z(Ac)** index of a graph *G* is given by:[5-15]

$$\mathbf{Z(Ac)} = \sum_{k=0}^{L} \mathbf{M}(G,k) \tag{2}$$

The Hosoya **Z(Ac)** index was applied to various correlations with theoretical and experimental molecular properties: Coulson and Pauling bond order, boiling point, absolute entropy of acyclic saturated hydrocarbons. Various relations and formulas enabling the computation of the topological index **Z(Ac)** were obtained.[5-15]

THE TOPOLOGICAL INDEX Z(Ch)

The characteristic or spectral polynomial $\mathbf{Ch}(G, x)$ of the molecular graph G is the characteristic polynomial of its adjacency matrix:[16–17]

$$\mathbf{Ch}(G,x) = \det(x\mathbf{I} - \mathbf{A}) = \sum_{n=0}^{L} c_n x^{N-n} \tag{3}$$

where $\mathbf{I}$ is the $N \times N$ unit matrix.

The sum of the absolute values of the coefficients a_{2k} appearing alternatively in the characteristic polynomial (i.e. every second, or even, term) is defined as the stability index, $\mathbf{Z(Ch)}$:[18–20]

$$\mathbf{Z(Ch)} = \sum_{k=0}^{L} |c_{2k}| \tag{4}$$

Another form of the stability index may be expressed as:

$$\mathbf{Z(Ch)} = i^{-N}\mathbf{Ch}(G, i) \tag{5}$$

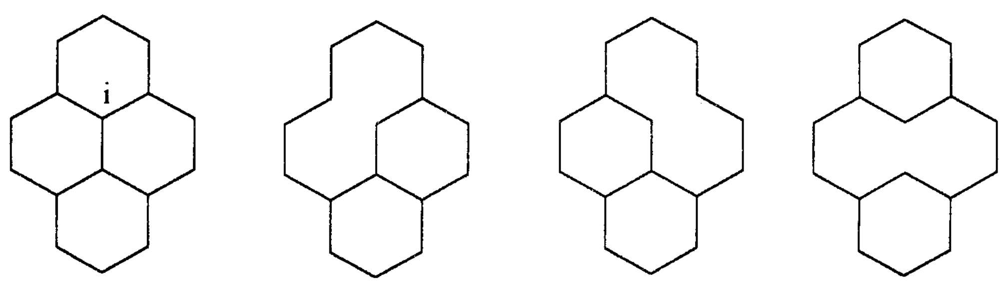
where $i = (-1)^{1/2}$. In the case of benzenoid hydrocarbons, the index $\mathbf{Z(Ch)}$ has been found to be related to the total π-electron energy.

THE NEW RECURRENCE RELATIONSHIP

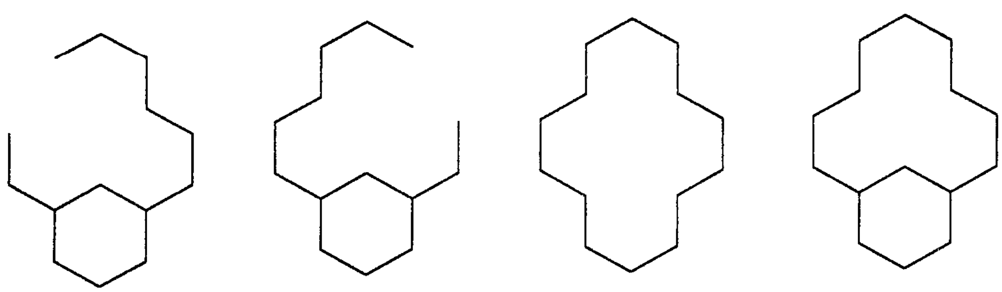
A new recurrence relationship was recently obtained for the characteristic polynomial:[21]

$$\mathbf{Ch}(G) = \frac{1}{\mathbf{Deg}(v_i) - 2}\left[\sum_{v_j} \mathbf{Ch}(G - e_{ij}) + \sum_{v_j} \mathbf{Ch}(G - v_i - v_j) - 2x\mathbf{Ch}(G - v_i)\right] \tag{6}$$

where the summations go over all $\mathbf{Deg}(v_i)$ vertices v_j which are adjacent to the vertex v_i. In Scheme 1 we present an example of application of this recurrence relationship. The vertex where the relationship is applied is indicated on the graph G_1.



G_1 G_2 G_3 G_4



G_5 G_6 G_7 G_8

Scheme 1

The characteristic polynomials of the molecular graphs from Scheme 1 are presented below:

$$\mathbf{Ch}(G_1) = x^{16} - 19x^{14} + 143x^{12} - 555x^{10} + 1208x^8 - 1498x^6 + 1017x^4 - 333x^2 + 36$$

$$\mathbf{Ch}(G_2) = \mathbf{Ch}(G_3) = x^{16} - 18x^{14} + 129x^{12} - 476x^{10} + 974x^8 - 1107x^6 + 659x^4 - 178x^2 + 16$$

$$\mathbf{Ch}(G_4) = x^{16} - 18x^{14} + 129x^{12} - 474x^{10} + 962x^8 - 1084x^6 + 641x^4 - 172x^2 + 16$$

$$\mathbf{Ch}(G_5) = \mathbf{Ch}(G_6) = x^{14} - 14x^{12} + 75x^{10} - 196x^8 + 263x^6 - 174x^4 + 49x^2 - 4$$

$$\mathbf{Ch}(G_7) = x^{14} - 14x^{12} + 77x^{10} - 210x^8 + 294x^6 - 196x^4 + 49x^2 - 4$$

$$\mathbf{Ch}(G_8) = x^{15} - 16x^{13} + 101x^{11} - 322x^9 + 550x^7 - 490x^5 + 199x^3 - 24x$$

Using the values of the characteristic polynomials reported above it is easy to verify the recurrence relationship:

$$\mathbf{Ch}(G_1) = \mathbf{Ch}(G_2) + \mathbf{Ch}(G_3) + \mathbf{Ch}(G_4) + \mathbf{Ch}(G_5) + \mathbf{Ch}(G_6) + \mathbf{Ch}(G_7) - 2x\mathbf{Ch}(G_8)$$

From relationship (5) between the characteristic polynomial and the index **Z(Ch)**, and the recurrence relationship for the characteristic polynomial (6) we obtain a new decomposition formula for **Z(Ch)**, by means of which the index **Z(Ch)** is expressed as a linear combination of the **Z(Ch)** index of certain subgraphs of G:

$$\mathbf{Z}(\mathbf{Ch},G) = \frac{1}{\mathbf{Deg}(v_i) - 2}[\sum_{v_j} \mathbf{Z}(\mathbf{Ch},G - e_{ij}) + \sum_{v_j} \mathbf{Z}(\mathbf{Ch},G - v_i - v_j) - 2\mathbf{Z}(\mathbf{Ch},G - v_i)] \qquad (7)$$

where the summations go over all $\mathbf{Deg}(v_i)$ vertices v_j that are adjacent to the vertex v_i. This recurrence relationship is exemplified for the graph G_1 from Scheme 1 and the indicated vertex v_i. After computing the **Z(Ch)** indices from the coefficients of the characteristic polynomials presented above, we obtain the equality:

$$\mathbf{Z}(\mathbf{Ch}, G_1) = \mathbf{Z}(\mathbf{Ch}, G_2) + \mathbf{Z}(\mathbf{Ch}, G_3) + \mathbf{Z}(\mathbf{Ch}, G_4) - \mathbf{Z}(\mathbf{Ch}, G_5) - \mathbf{Z}(\mathbf{Ch}, G_6) -$$

$$- \mathbf{Z}(\mathbf{Ch}, G_7) - 2\mathbf{Z}(\mathbf{Ch}, G_8) = 3558 + 3558 + 3497 - 776 - 776 - 845 - 2 \cdot 703 = 4810$$

We have to note that for all graphs $G_1 - G_8$ the coefficients c_{2k+1} of the corresponding characteristic polynomial are zero. We will present another example for the new recurrence relationship, where there are characteristic polynomials with some c_{2k+1} coefficients different from zero. The formula is applied to the graph G_9 from Scheme 2, to the vertex v_i indicated in scheme 2.

The characteristic polynomials of the graphs $G_9 - G_{16}$ from Scheme 2 are:

$$\mathbf{Ch}(G_9) = x^7 - 9x^5 - 2x^4 + 19x^3 + 2x^2 - 11x$$

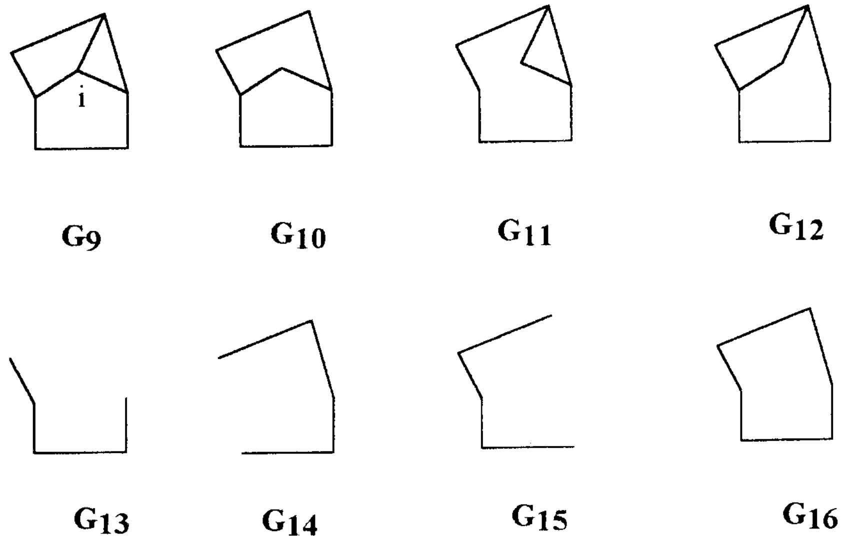
$$\mathbf{Ch}(G_{10}) = x^7 - 8x^5 + 17x^3 - 4x^2 - 10x + 4$$

$$\mathbf{Ch}(G_{11}) = x^7 - 8x^5 - 2x^4 + 17x^3 + 6x^2 - 10x - 4$$

$$\mathbf{Ch}(G_{12}) = x^7 - 8x^5 + 15x^3 - 8x$$

$$\mathbf{Ch}(G_{13}) = \mathbf{Ch}(G_{14}) = \mathbf{Ch}(G_{15}) = x^5 - 4x^3 + 3x$$

$$\mathbf{Ch}(G_{16}) = x^6 - 6x^4 + 9x^2 - 4$$



Scheme 2

From the inspection of the characteristic polynomials of the graphs G_9 – G_{16} we observe that for graphs G_9, G_{10} and G_{11} there are c_{2k+1} non-zero coefficients, which are not considered in the computation of the corresponding **Z(Ch)** indices. After computing the **Z(Ch)** indices, we obtain the following equality:

$$\mathbf{Z(Ch}, G_9) = \mathbf{Z(Ch}, G_{10}) + \mathbf{Z(Ch}, G_{11}) + \mathbf{Z(Ch}, G_{12}) - \mathbf{Z(Ch}, G_{13}) - \mathbf{Z(Ch}, G_{14}) -$$

$$- \mathbf{Z(Ch}, G_{15}) - 2 \cdot \mathbf{Z(Ch}, G_{16}) = 36 + 36 + 32 - 8 - 8 - 8 - 2 \cdot 20 = 40$$

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