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THE GRAPH OF ATOMIC ORBITALS AND ITS BASIC PROPERTIES. 2. ZAGREB INDICES

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Abstract

Relations are established between the first and second Zagreb index (M_1 and M_2) of the graph of atomic orbitals (G^*), and of the ordinary hydrogen-depleted (G_C) and hydrogen-filled (G_H) molecular graphs of saturated hydrocarbons. It is shown that $M_1(G^*) = 12\,M_1(G_C) + 9\,M_1(G_H) + 96\,(c-1)$ and $M_2(G^*) = 36\,M_2(G_C) + 15\,M_2(G_H) + 54\,M_1(G_C) + 96\,(c-1)$, where c is the number of (independent) cycles of the underlying molecule.

INTRODUCTION

In this paper we establish connections between the Zagreb indices of the graph of atomic orbitals (GAO) and of the ordinary (hydrogen-depleted and hydrogen-filled) molecular graphs of saturated hydrocarbons. We use the same notation and terminology as in the preceding paper [1], where also the definition of GAO and references to earlier work on this topic are given.

Let G be a graph on n vertices, and let $v_1, v_2, \ldots, v_n$ be its vertices. The degree (number of first neighbors) of the vertex v_r of G is denoted by $\delta_r = \delta_r(G)$.

In the 1970s, within the study of the structure-dependence of total π-electron energy, two graph invariants, M_1 and M_2, were encountered [2], that soon were recognized [3] as measures of the branching of the molecular skeleton, and were eventually named the "*first and second Zagreb indices*" (or Zagreb-group indices) [4, 5]. They are defined as follows

$$M_1 = M_1(G) = \sum_r (\delta_r)^2 \tag{1}$$

$$M_2 = M_2(G) = \sum_{r,s} \delta_r \, \delta_s \, . \tag{2}$$

In Eqs. (1) and (2) the summations go, respectively, over all vertices, and over all pairs of adjacent vertices of the graph G.

After a long period without almost any work on Zagreb indices (see, however, [6]), in recent times these structure-descriptors are again beginning to attract the attention of researchers in chemical graph theory [7–11]. In view of this, and in view of our recent studies of GAOs [1], we got interested in finding connections between the M_1- and M_2-values of GAOs and ordinary molecular graphs.

MOLECULAR GRAPHS OF SATURATED HYDROCARBONS AND THEIR STRUCTURAL FEATURES

Let, as before [1], G_C and G_H denote the hydrogen-depleted and the hydrogen-filled molecular graphs, representing a molecule M, and let G^* be the respective GAO. We shall be concerned with the case when M is a saturated hydrocarbon of the formula $C_n H_{2n+2-2c}$. The parameter c is the cyclomatic number of G_C or G_H,

i. e., the number of (independent) cycles of the underlying molecule M. Thus, acyclic, unicyclic, bicyclic, tricyclic, ... hydrocarbons have $c = 0, 1, 2, 3, \ldots$, respectively.

The n carbon atoms of the considered hydrocarbon are classified into four groups: primary, secondary, tertiary, and quaternary. To each primary (resp. secondary, tertiary, and quaternary) carbon atom three (resp. two, one, and no) hydrogen atoms are attached. If we denote the number of primary, secondary, tertiary, and quaternary carbon atoms by n_1, n_2, n_3, and n_4, respectively, then

$$n_1 + n_2 + n_3 + n_4 = n \tag{3}$$

$$3\,n_1 + 2\,n_2 + n_3 = 2n + 2 - 2c\,. \tag{4}$$

Recall that n_i, $i = 1, 2, 3, 4$, is equal to the number of vertices of degree i in the hydrogen-depleted molecular graph G_C. The number of edges of this graph (equal to the number of carbon–carbon bonds of M) is $n - 1 + c$.

From Eqs. (3) and (4) follows

$$n_1 = n_3 + 2\,n_4 - 2c + 2 \tag{5}$$

$$n_2 = n - 2 + 2c - 2\,n_3 - 3\,n_4\,. \tag{6}$$

Bearing in mind the definition of the Zagreb indices, Eqs. (1) and (2), we now immediately arrive at

$$M_1(G_C) = n_1 + 4\,n_2 + 9\,n_3 + 16\,n_4$$

$$M_1(G_H) = 16\,n + (2n + 2 - 2c)$$

$$M_2(G_H) = 4\,(2n + 2 - 2c) + 16\,(n - 1 + c)$$

which, in view of (5) and (6), become

$$M_1(G_C) = 4n + 6\,(c - 1) + 2\,(n_3 + 3\,n_4) \tag{7}$$

$$M_1(G_H) = 18\,n - 2\,(c - 1) \tag{8}$$

$$M_2(G_H) = 24\,n + 8\,(c - 1)\,. \tag{9}$$

Note that the right-hand sides of the formulas (7)–(9) can be viewed as linear functions of the variables n, $c - 1$, and $n_3 + 3\,n_4$.

THE FIRST ZAGREB INDEX OF GAO

The vertices of the GAO of a saturated hydrocarbon can be classified into five groups: those pertaining to hydrogen atoms, and to primary, secondary, tertiary, and quaternary carbon atoms. Each hydrogen atom is represented by a single vertex. Because a hydrogen atom is adjacent to one carbon atom, and because a carbon atom in the GAO is represented by three vertices, any vertex of the GAO, pertaining to a hydrogen atom, is of degree 3.

A carbon atom is represented by three vertices. The vertices corresponding to a primary carbon atom are adjacent to three vertices pertaining to hydrogen atoms and to three vertices pertaining to the (single) adjacent carbon-atom. Thus, the three vertices corresponding to a primary carbon atom have degree 6 each.

Similarly, the vertices corresponding to secondary, tertiary, and quaternary carbon atoms are of degree 8, 10, and 12, respectively. It is easy to see that the degree of a vertex in GAO (pertaining to a carbon atom) and the degree of the corresponding vertex of G_C are related as

$$\delta_r(G^*) = 2\,\delta_r(G_C) + 4\ . \tag{10}$$

The first Zagreb index of the GAO is now easily computed: because there exist $2n + 2 - 2c$ vertices of degree three, $3\,n_1$ vertices of degree six, $3\,n_2$ vertices of degree eight, $3\,n_3$ vertices of degree ten, and $3\,n_4$ vertices of degree twelve,

$$M_1(G^*) = (2n + 2 - 2c)\,3^2 + 3\,n_1\,6^2 + 3\,n_2\,8^2 + 3\,n_3\,10^2 + 3\,n_3\,12^2$$

which by direct calculation and by taking into account (5) and (6), yields:

$$M_1(G^*) = 6\,[35\,n + 25\,(c-1) + 4\,(n_3 + 3\,n_4)]\ . \tag{11}$$

Again, the right-hand side of (11) is a linear function of the variables n, $c-1$, and $n_3 + 3\,n_4$. Taking into account Eqs. (7) and (8), formula (11) can be rewritten as

$$M_1(G^*) = 12\,M_1(G_C) + 9\,M_1(G_H) + 96\,(c-1)\ . \tag{12}$$

As a curiosity, note that the first Zagreb index of the GAO of any saturated hydrocarbon is an integer divisible by 6.

THE SECOND ZAGREB INDEX OF GAO

Denote for brevity $\delta_r(G^*)\,\delta_s(G^*)$ by Δ_{rs}.

The second Zagreb index of the GAO, i. e., the sum of the terms Δ_{rs} over all edges of the GAO can be divided into two parts: the sum over edges corresponding to carbon–hydrogen bonds, denoted by $M_2'(G^*)$, and the sum over edges corresponding to carbon–carbon bonds, denoted by $M_2''(G^*)$, so that $M_2(G^*) = M_2'(G^*) + M_2''(G^*)$.

In order to compute $M_2'(G^*)$ note that each vertex corresponding to a hydrogen atom has degree 3 and thus contributes to $M_2'(G^*)$ by three (mutually equal) summands. For a hydrogen attached to a primary carbon atom, $\Delta_{rs} = 3 \cdot 6$. For a hydrogen attached to a secondary and tertiary carbon atom, $\Delta_{rs} = 3 \cdot 8$ and $\Delta_{rs} = 3 \cdot 10$, respectively. Bearing in mind how many hydrogens are attached to each type of carbon atoms, we get

$$M_2'(G^*) = 3\,[3\,(3 \cdot 6)\,n_1 + 2\,(3 \cdot 8)\,n_2 + (3 \cdot 10)\,n_3]\ .$$

A carbon–carbon bond is represented in the GAO by $3 \cdot 3 = 9$ edges, each having the same Δ_{rs}-value. Then, in view of the relation (10),

$$\begin{aligned} M_2''(G^*) &= 9 \sum_{rs} [2\,\delta_r(G_C) + 4][2\,\delta_s(G_C) + 4] \\ &= 36 \sum_{rs} \delta_r(G_C)\,\delta_s(G_C) + 72 \sum_{rs} [\delta_r(G_C) + \delta_s(G_C)] + 144\,(n - 1 + c) \\ &= 36\,M_2(G_C) + 72\,M_1(G_C) + 144\,(n - 1 + c) \end{aligned}$$

because

$$\sum_{rs} \delta_r(G_C)\,\delta_s(G_C) = M_2(G_C) \quad \text{and} \quad \sum_{rs} [\delta_r(G_C) + \delta_s(G_C)] = M_1(G_C)\ .$$

Summing the above obtained expressions for $M_2'(G^*)$ and $M_2''(G^*)$, and using (5) and (6), we arrive at:

$$M_2(G^*) = 36\,[M_2(G_C) + 16\,n + 15\,(c - 1) + 3\,(n_3 + 3\,n_4)]\ . \tag{13}$$

Eq. (13) reveals that also $M_2(G^*)$ is a linear function of the variables n, $c - 1$, and $n_3 + 3\,n_4$. From it is seen that the second Zagreb index of the GAO of any saturated hydrocarbon is an integer divisible by 36.

Combining (13) with (7) and (9) we obtain:

$$M_2(G^*) = 36\,M_2(G_C) + 15\,M_2(G_H) + 54\,M_1(G_C) + 96\,(c - 1)\ . \tag{14}$$

a result that should be compared with Eq. (12).

Formulas (12) and (14) are our main results. They show that the Zagreb indices of the GAO can be expressed as linear functions of the Zagreb indices of the corresponding ordinary molecular graphs.

The considerations in this work were restricted to saturated hydrocarbons. Analogous, yet significantly more complicated, results can be obtained also in the case of molecules containing atoms different from carbon and hydrogen, and/or containing double and triple bonds.

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