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Vertex-degree-based molecular structure descriptors of benzenoid systems and phenylenes

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Abstract. Several recently published papers report expressions for various vertex-degree-based molecular structure descriptors of benzenoid systems and phenylenes. Herein, the general expression for these descriptors is deduced, and it is shown that a simple and generally valid relation exists between such structure descriptors of phenylenes and their hexagonal squeezes.

Keywords: molecular structure descriptor; topological index; degree-based molecular structure descriptor; benzenoid system; phenylene; hexagonal squeeze.

INTRODUCTION

Let G be a molecular graph[1] and v its vertex. The *degree* of the vertex v, denoted by $d(v)$, is the number of the first neighbors of v. A large number of molecular structure descriptors (topological indices), defined in terms of vertex degrees, has been considered in the literature.[2,3] The general form of these descriptors is:

$$D = D(G) = \sum_{u \sim v} \psi(d(u), d(v)) \qquad (1)$$

where the summation goes over all pairs of adjacent vertices u,v of the molecular graph G.

In particular, the function ψ in Eq. (1) has the following forms:

$$\psi(p,q) = \frac{1}{\sqrt{pq}}, \text{ for the Randić index,}[4]$$

$$\psi(p,q) = (pq)^{\lambda}, \text{ for the general Randić index,}[5]$$

where λ is an adjustable parameter,

$$\psi(p,q) = pq, \text{ for the second Zagreb index,}[6]$$

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$$\psi(p,q) = \sqrt{\frac{2(p+q-2)}{pq}}$$, for the atom-bond connectivity index,[7]

$$\psi(p,q) = \frac{1}{\sqrt{p+q}}$$, for the sum-connectivity index,[8]

$$\psi(p,q) = (p+q)^{\lambda}$$, for the general sum-connectivity index,[9]

where λ is an adjustable parameter,

$$\psi(p,q) = \frac{\sqrt{pq}}{\frac{1}{2}(p+q)}$$, for the geometric-arithmetic index,[10]

$$\psi(p,q) = \left(\frac{pq}{p+q-2}\right)^3$$, for the augmented Zagreb index,[11]

$$\psi(p,q) = \frac{2}{p+q}$$, for the harmonic index.[12]

In the general case, the calculation of a particular structure descriptor D is not quite easy, and finding molecular graphs possessing extremal (maximal or minimal) values of D is even more difficult. However, in the case of benzenoid systems and phenylenes, this task is much simpler. Namely, the molecular graphs of the latter systems possess only vertices of degree 2 and 3, and therefore there are only three types of contributions $\psi(p,q)$ occurring in the summation on the right-hand side of Eq. (1). Indeed, if m_{22}, m_{23} and m_{33} denote, respectively, the number of edges connecting two vertices of degree 2, the number of edges connecting vertices of degree 2 and 3, and the number of edges connecting two vertices of degree 3, then:

$$D = m_{22}\psi(2,2) + m_{23}\psi(2,3) + m_{33}\psi(3,3) \quad (2)$$

and, moreover, simple expressions for the structure-dependency of the coefficients m_{22}, m_{23}, m_{33} are available (see below). In spite of this, recently a number of papers appeared in which some of the above listed degree-based structure descriptors were studied for benzenoids and phenylenes: general Randić index,[13,14] atom-bond connectivity index,[14–16] general sum-connectivity index,[14,17,18] geometric–arithmetic index.[14,19] All these were preceded by an analogous study of the Randić index, realized more than ten years ago.[20]

It will now be shown how the general solution of this problem can (easily) be achieved. By this, it is hoped that the appearance of additional publications of the same kind as those mentioned above[13–20] will cease.

GENERAL EXPRESSIONS FOR THE INDEX *D* OF BENZENOIDS AND PHENYLENES

The structural features of benzenoid systems are described in detail in the book.[21] The analogous properties of phenylenes and their hexagonal squeezes were established in the paper.[20] Self-explanatory examples of benzenoid systems, phenylenes, and their hexagonal squeezes are provided in Fig. 1.

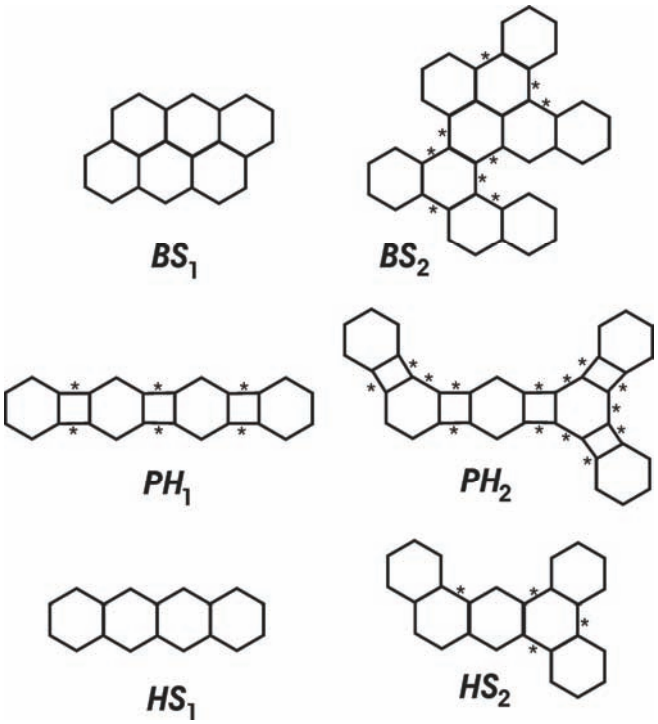

Fig. 1. Examples of benzenoid systems (BS_1 and BS_2), phenylenes (PH_1 and PH_2), and hexagonal squeezes (HS_1 and HS_2). The hexagonal squeeze HS_i corresponds to the phenylene PH_i; i = 1,2. The edges on the perimeter connecting two vertices of degree 3 are indicated by asterisks; their count is b. Thus, $b(BS_1) = 0$, $b(BS_2) = 9$, $b(PH_1) = 6$, $b(PH_2) = 14$, $b(HS_1) = 0$ and $b(HS_2) = 4$.

The basic properties of a benzenoid system are determined[21] by the number of hexagons (h) and internal vertices (n_i). For instance, the formula of the respective benzenoid hydrocarbon is $C_{4h+2-n_i}H_{2h+4-n_i}$. In the examples depicted in Fig. 1, $h(BS_1) = 6$, $h(BS_2) = 10$, $n_i(BS_1) = 4$, $n_i(BS_2) = 2$.

Let b be the number of edges on the perimeter, connecting two vertices of degree 3 (this parameter is usually referred to as the "number of bays"). Then, for a benzenoid system BS, one has:[21]

$$m_{22}(BS) = b + 6$$
$$m_{23}(BS) = 4h - 2b - 2n_i - 4$$
$$m_{33}(BS) = h + b + n_i - 1$$

which combined with Eq. (2) immediately implies:

$$D(BS) = [6\psi(2,2) + (4h - 2n_i - 4)\psi(2,3) + (h + n_i - 1)\psi(3,3)] + \\ + b[\psi(2,2) - 2\psi(2,3) + \psi(3,3)]$$

Phenylenes have no internal vertices, and their structural relations are significantly simpler. One has:[20]

$$m_{22}(PH) = 8 - 2h + b$$
$$m_{23}(PH) = 8h - 2b - 8$$
$$m_{33}(PH) = 2h + b - 2$$

resulting in:

$$D(PH) = [(8 - 2h)\psi(2,2) + (8h - 8)\psi(2,3) + (2h - 2)\psi(3,3)] + \\ + b[\psi(2,2) - 2\psi(2,3) + \psi(3,3)] \quad .$$

Interestingly, the coefficient of the parameter b is same for both *BS* and *PH*. Therefore, if this coefficient, namely $\psi(2,2) - 2\psi(2,3) + \psi(3,3)$, is positive-valued, then the benzenoid system with h hexagons and n_i internal vertices and the phenylene with h hexagons will have maximal (resp. minimal) *D*-index if b is maximal (resp. minimal). If $\psi(2,2) - 2\psi(2,3) + \psi(3,3)$ is negative-valued, the situation is reversed.

Recall that in the case of benzenoid systems, the minimal value of the parameter b is zero (as, for instance, for BS_1), whereas in the case of phenylenes it is $2h–2$ (as, for instance, for PH_1).

By this simple reasoning, the general solution of the problem considered is arrived at, and the benzenoid systems and phenylenes with minimal and maximal *D* index characterized.

RELATING THE INDEX *D* OF PHENYLENES AND THEIR HEXAGONAL SQUEEZES

The concept of "hexagonal squeeze" (*HS*) was introduced[22] in the 1990s, and since then it has played an important role in the theory of phenylenes. The way in which a hexagonal squeeze (which is a catacondensed benzenoid system) is associated with a phenylene is seen from Fig. 1. It is easy to recognize that for a hexagonal squeeze *HS* corresponding to the phenylene *PH* the following identities hold: $m_{22}(HS) = m_{22}(PH)$ and $m_{23}(HS) = m_{23}(PH)$. This means that:

$$D(PH) - D(HS) = [m_{33}(PH) - m_{33}(HS)]\psi(3,3) \, .$$

Because, in addition:

$$m_{33}(HS) = b(HS) + h - 1 = b(PH) - h + 1$$

one arrives at the remarkably simple formula:

$$D(PH) - D(HS) = 3(h-1)\psi(3,3)$$

the special cases of which were reported several times.[13–15,17–20] We hope that this will not be repeated also in the future.

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И З В О Д

НА СТЕПЕНИМА ЧВОРОВА ЗАСНОВАНИ МОЛЕКУЛСКИ СТРУКТУРНИ ДЕСКРИПТОРИ БЕНЗЕНОИДНИХ СИСТЕМА И ФЕНИЛЕНА

ИВАН ГУТМАН и БОРИС ФУРТУЛА

Природно–математички факултет Универзитета у Крагујевцу

Већи број недавно објављених радова наводи формуле за различите, на степенима чворова засноване, молекулске структурне дескрипторе бензеноидних система и фенилена. У овом раду је дат општи израз за ове дескрипторе и показано је да у општем случају постоји једноставна релација између ових дескриптора за фенилене и за њихове хексагоналне основе.

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