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Narumi-Katayama index of phenylenes

ŽELJKO TOMOVIĆ[#] and IVAN GUTMAN[#]

Faculty of Science, University of Kragujevac, P.O. Box 60, YU-34000 Kragujevac, Yugoslavia

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The Narumi-Katayama topological indes S of a hydrocarbon is the product of vertex degrees of the respective molecular graph. If PH is a phenylene and HS is its hexagonal squeeze, then the respective Narumi-Katayama indices are related as $S(\mathrm{PH}) = 9^{h-1} S(\mathrm{HS})$, where h is the number of hexagons of PH and HS, or as $S(\mathrm{PH}) = \quad S(\mathrm{HS})$, where $\quad = 0.078$ and $\quad = 1.613$.

Keywords: Narumi-Katayama topological index, phenylenes, hexagonal squeeze, benzenoid hydrocarbons.

INTRODUCTION

Phenylenes are non-benzenoid conjugated -electron systems composed of 6- and 4-membered rings, in which no two 6-membered rings are adjacent, and each 4-membered ring is adjacent to two 6-membered rings. The chemistry of phenylenes is in rapid expansion, mainly due to the work of Peter Vollhardt and his research group; for details see the recent papers[1,2] and the review.[3]

To every phenylene it is possible to associate a catacondensed benzenoid system, obtained so that the 4-membered rings of the phenylene are "squeezed off". This benzenoid system was named[4] the *hexagonal squeeze* of the respective phenylene. The construction of hexagonal squeezes should be evident from the examples depicted in Fig. 1. In the following, a phenylene and its hexagonal squeeze will be denoted by PH and HS, respectively, They possess equal number of hexagons, denoted by h.

In the last few years we established a number of nontrivial relations between the topological properties of phenylenes and their hexagonal squeezes.[4–12] In the present paper one more such connection is reported.

In 1984 Narumi and Katayama[13] put forward a novel toplogical index S defined as:

$$S = S(G) = \sum_{i=1}^{n} \quad i \qquad (1)$$

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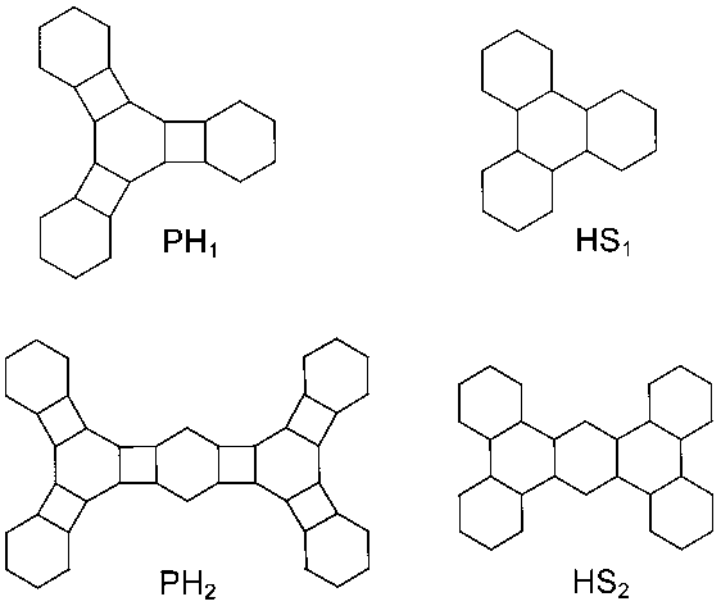

Fig. 1. Two phenylenes (PH_1 and PH_2) and their hexagonal squeezes (HS_1 and HS_2).

where $_i$ is the degree (= number of first neighbors) of the i-th vertex, and n is the number of vertices of the molecular graph G. (Details on graph theory and its applications to chemistry can be found in the books.[14,15])

The quantity S was originally called[13] *simple topological index*, but we shall refer to it as the *Narumi-Katayama index*. More details on its basic properties can be found elsewhere.[15–18]

RELATIONS BETWEEN S(PH) AND S(HS)

The molecular graphs of phenylenes and their hexagonal squeezes possess only vertices of degree two or three. Denote by n(PH) and n(HS) the number of vertices of a phenylene and of its hexagonal squeeze, respectively. Denote by n_2(X), and n_3(X) the number of vertices of degree two and three, respectively of X = PH, HS. Then, for phenylenes one has

$$n(\mathrm{PH}) = 6h \tag{2}$$

$$n_2(\mathrm{PH}) = 2h + 4 \tag{3}$$

$$n_3(\mathrm{PH}) = 4h - 4 \tag{4}$$

and, according to Eq. (1),

$$S(\mathrm{PH}) = 2^{n_2(\mathrm{PH})}\, 3^{n_3(\mathrm{PH})} \tag{5}$$

Substituting Eqs. (3) and (4) back into (5) one arrives at

$$S(\mathrm{PH}) = \frac{16}{81}\ 324^{h} \tag{6}$$

which combined with Eq. (2) yields

$$S(\mathrm{PH}) = \frac{16}{81}\ 18^{n(\mathrm{PH})/3}$$

For the hexagonal squeeze one has:

$$n(\mathrm{HS}) = 4h + 2$$
$$n_2(\mathrm{HS}) = 2h + 4$$
$$n_3(\mathrm{HS}) = 2h - 2$$

which results in

$$S(\mathrm{HS}) = \frac{16}{9}\ 36^{h} \tag{7}$$

and

$$S(\mathrm{HS}) = \frac{8}{27}\ 6^{n(\mathrm{HS})/2}$$

Dividing Eq. (6) by Eq. (7), a simple relation between S(PH) and S(HS) is obtained:

$$S(\mathrm{PH}) = 9^{h-1}\ S(\mathrm{HS}) \tag{8}$$

If it is required that the parameter h be absent from the relation between S(PH) and S(HS), then a somewhat more perplexed expression is obtained:

$$S(\mathrm{PH}) = \quad S(\mathrm{HS}) \tag{9}$$

where

$$= \frac{1}{9}\ \frac{9}{16}^{\ln 9/\ln 36} = 0.078081...$$

$$= 1 \quad \frac{\ln 9}{\ln 36} = 1.613147...$$

ON NARUMI-KATAYAMA TOPOLOGICAL INDEX OF BENZENOID SYSTEMS

Denote by n_i the number of internal vertices in a benzenoid system. A benzenoid system is said to be catacondensed if it does not possess internal vertices ($n_i = 0$). Otherwise, if $n_i > 0$, then the benzenoid system is pericondensed.[19]

As in the case of phenylenes, the molecular graphs of benzenoid systems possess only vertices of degree two and three; their number is denoted by n_2 and n_3, respectively. For a benzenoid system BS with h hexagons and n_i internal vertices, one has[19]

$$n_2 = 2h + 4 - n_i$$

$$n_3 = 2h - 2$$

resulting in

$$S(\mathrm{BS}) = \frac{16}{9}\ 36^h\ 2^{-n_i} \tag{10}$$

If $n_i = 0$ (*i.e.,* if BS is catacondensed), then Eq. (10) reduces to Eq. (7).

DISCUSSION

Formulae (8) and (9) are exact results, valid for all values of h, $h > 1$. They show that the Narumi-Katayama index of a phenylene can be calculated from the Narumi-Katayama index of the corresponding squeeze. In spite of the seemingly simple form of Eq. (8), the actual relation between S(PH) and S(HS), Eq. (9), is far from simple.

The following consequences of our analysis are particularly worth noting:

1. All isomeric phenylenes have equal Narumi-Katayama indices. The S-value of a phenylene is fully determined by the number of hexagons h or by the number of vertices n.

2. The S-value of a phenylene is fully determined by the S-value of its hexagonal squeeze, and *vice versa*.

3. The Narumi-Katayama index of phenylenes is a rapidly (exponentially) increasing function of h or n.

И З В О Д

НАРУМИ-КАТАЈАМИН ТОПОЛОШКИ ИНДЕКС ФЕНИЛЕНА

ЖЕЉКО ТОМОВИЋ и ИВАН ГУТМАН

Природно-математички факултет у Крагујевцу

Наруми-Катајамин тополошки индекс S неког угљоводоника је производ степена чворова одговарајућег молекулског графа. Ако је PH фенилен и HS његова хексагонална основа, онда између одговарајућих Наруми-Катајаминих индекса постоје следеће релације: $S(\mathrm{PH}) = 9^{h-1}\ S(\mathrm{HS})$, где је h број шесточланих прстенова у PH и HS, и $S(\mathrm{PH}) =$ $S(\mathrm{HS})$, где је = 0.078 и = 1.613.

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