CROATICA CHEMICA ACTA CCACAA 54 (1) 81—83 (1981)

CCA-1260

YU ISSN 0011-1643
UDC 539.19
*Note*

# On the Characterization of Monocyclic Structures. Hosoya's Index

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Received May 15, 1980

The previous work by Bonchev et al.[3] is complemented by an explicit general topological formula for Hosoya's index of a cycle.

A large number of topological indices which characterize various topological properties of molecules have been proposed in the current chemical literature. (For a recent review see[1].) The main chemical applications of these indices are in bond-additive and other empirical schemes for correlating molecular properties (e. g. boiling point, density, refractive index, surface tension, viscosity, octane number, chromatographic constants, thermodynamic constants, pharmacological activity etc.) with molecular structure[1,2].

In the majority of the papers dealing with topological indices only acyclic structures were considered. However, in recent investigations by Bonchev et al.[3,4] an attempt was made towards the application of topological indices for the characterization of cyclic structures. Monocyclic systems were examined in[3] and polycyclic systems in[4]. In particular, Bonchev et al. considered[3] the following topological indices of the cycle $C_N$: the Wiener number $W$, Randić's connectivity index $\chi_R$, Platt's index $F$, Gordon's and Scantelbury's index $S$, the indices $M_1$ and $M_2$, Hosoya's index $Z$ and the information index $I_D$. They presented explicit analytical expressions for the indices $W$, $\chi_R$, $F$, $S$, $M_1$ and $M_2$, but not the analogous formula for Hosoya's index. In this note we shall solve the problems posed in ref.[3] for the case of Hosoya's index.

Let $G$ be a graph with $N$ vertices and let $N = 2m$ or $N = 2m + 1$. If we denote the number of $k$-matchings of this graph by $p(G, k)$, $k = 1, 2, \ldots$, then Hosoya's index of $G$ is defined as[3,5]

$$Z(G) = \sum_{k=0}^{m} p(G, k)$$

while the matching polynomial of $G$ is given by[6]

$$\alpha(G) = \alpha(G, x) = \sum_{k=0}^{m} (-1)^k p(G, k)\, x^{N-2k}$$

It is immediately seen that

$$Z(G) = i^{-N} \alpha(G, i) \tag{1}$$

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Let $C_N$ denotes the cycle with $N$ vertices. It is well known[7] that

$$p(C_N, k) = \frac{N}{N-k}\binom{N-k}{k}$$

Therefore

$$Z(C_N) = \sum_{k=0}^{m} \frac{N}{N-k}\binom{N-k}{k}$$

is the required topological formula for Hosoya's index of $C_N$. Another, more convenient expression for $Z(C_N)$ is obtained from the relation[8]

$$\alpha(C_N) = x\,\alpha(C_{N-1}) - \alpha(C_{N-2})$$

which together with (1) yields

$$Z(C_N) = Z(C_{N-1}) + Z(C_{N-2}) \tag{2}$$

The solution of the recurrence relation (2) reads[9]

$$Z(C_N) = [(\sqrt{5}+1)/2]^N + (-1)^N [(\sqrt{5}-1)/2]^N \tag{3}$$

where we have used the initial conditions $Z(C_3) = 4$ and $Z(C_4) = 7$.

It is now easy to calculate that

$$\Delta Z(\text{odd} \rightarrow \text{even}) - \Delta Z(\text{even} \rightarrow \text{odd}) =$$
$$= -(\sqrt{5}-2)[(\sqrt{5}+1)/2]^N + (\sqrt{5}+2)[(\sqrt{5}-1)/2]^N \tag{4}$$

where $N$ is the size of the even-membered cycle. The expression on the right side of eq. (4) has negative values for all $N \geqslant 4$ and thus the application of Hosoya's index leads to conclusions about the change in relative cyclicity which are just the opposite to those formulated in Rule 1 in ref.[3].

In ref.[3] it was found that Hosoya's index cannot be normalized by dividing it by the number of carbon atoms. This conclusion is now evident from eq. (3) since we see that $Z(C_N)$ increases exponentially with increasing $N$. We would therefore propose another normalization, namely

$$\overline{Z}(C_N) = \frac{1}{N}\log Z(C_N) \tag{5}$$

which has the advantageous property (6).

$$\Delta\overline{Z}(\text{odd} \rightarrow \text{even}) - \Delta\overline{Z}(\text{even} \rightarrow \text{odd}) > 0 \tag{6}$$

Thus Rule 1 in ref.[3] can also be justified on the basis of the normalized Hosoya's index, eq. (5).

Concluding this note we would like to point out some relations between Hosoya's numbers of a cycle and a path (chain). Let $P_N$ be the path with $N$ vertices. It is long known[5] that

$$Z(P_N) = Z(P_{N-1}) + Z(P_{N-2})$$

and

$$Z(P_N) = \sum_{k=0}^{m}\binom{N-k}{k} = [(\sqrt{5}+1)/2]^{N+1}/\sqrt{5} + (-1)^N [(\sqrt{5}-1)/2]^{N+1}/\sqrt{5}$$

From the following identities between the matching polynomials of paths and cycles[10]

$$\alpha (C_N) = \alpha (P_N) - \alpha (P_{N-2})$$

$$\alpha (C_N) \alpha (P_{N-1}) = \alpha (P_{2N-1})$$

we deduce

$$Z (C_N) = Z (P_N) + Z (P_{N-2}) = Z (P_{2N-1})/Z (P_{N-1})$$

Consequently,

$$Z (\text{chain}) - Z (\text{cycle}) = - Z (P_{N-2}) < 0$$

and

$$\bar{Z} (\text{chain}) - \bar{Z} (\text{cycle}) = - \frac{1}{N} \log [1 + Z (P_{N-2})/Z (P_N)] < 0$$

*Acknowledgement.* — The author thanks the Alexander von Humboldt Foundation for financial support of this research.

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## SAŽETAK

### O karakterizaciji monocikličkih struktura. Hosoyin indeks

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Kao dopuna rada Bončeva i suradnika[3] izvedena je eksplicitna opća topološka formula za Hosoyin indeks monocikličkih struktura.

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Prispjelo 15. svibnja 1980