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Two theorems on connectivity indices

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Two general cases are pointed out for which the ordering of molecules according to the connectivity index $C(\lambda)$ is the same for all values of the exponent λ.

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INTRODUCTION

The definition of the connectivity index $C(\lambda) = C(\lambda; G) = C(G)$ can be found in the preceding paper[1] where also the ordering of alkanes with regard to $C(\lambda)$ is discussed. It was shown[1] that this ordering is very dependent on the numerical value of the exponent λ. In this paper it will be demonstrated that general classes of molecules (not necessarily alkanes) exist for which the ordering with regard to $C(\lambda)$ is the same for all values of λ.

THE FIRST THEOREM

Consider the molecular graphs G_1 and G_2 shown in Fig. 1, where R and S denote arbitrary fragments. Clearly, G_1 and G_2 represent a pair of consitutional isomers. It is necessary that R consists of more than a single vertex (because otherwise G_1 and G_2 would coincide implying $C(\lambda; G_1) = C(\lambda; G_2)$ for all λ. Therefore, in what follows it is assumed that the degree δ_x of the vertex x is greater than unity.

If $\lambda = 0$ then $C(\lambda, G)$ is equal to the number of edges of the graph G. Consequently, for $\lambda = 0$ all isomers have equal $C(\lambda)$-values. Therefore, in what follows, only the case $\lambda \neq 0$ will be considered.

Theorem 1. For all non-zero values of λ, and for arbitrary R and S, provided $\delta_x > 1$ (*cf.* Fig. 1), the connectivity index G_1 is greater than the connectivity index of G_2.

Proof. Applying the definition of the connectivity index (see Eq. (1) in the preceding paper[1]) to the molecular graphs G_1 and G_2 one obtains:

$$C(\lambda, G_1) = (1 \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot \delta_x)^\lambda + (3 \cdot \delta_y)^\lambda + C(R) + C(S)$$

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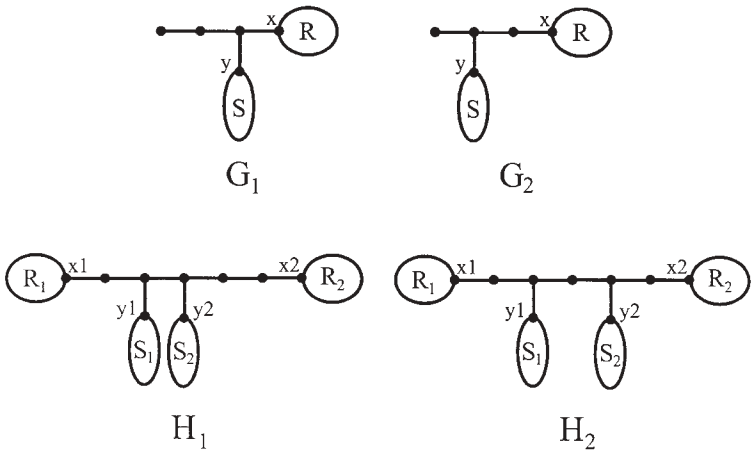

Fig. 1. The structure of the molecular graphs considered in Theorems 1 and 2 and the labeling of their fragments and vertices.

$$C(\lambda, G_2) = (1 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot \delta_x)^\lambda + (3 \cdot \delta_y)^\lambda + C(R) + C(S)$$

from which

$$C(\lambda, G_1) - C(\lambda, G_2) = 2^\lambda + (3\delta_x)^\lambda - 3^\lambda - (2\delta_x)^\lambda = (3^\lambda - 2^\lambda)\,(\delta_x{}^\lambda - 1). \qquad (1)$$

As $\delta_x > 1$, the expression on the right-hand side of (1) is positive for all non-zero values of λ. Indeed, if $\lambda > 0$, then $3^\lambda > 2^\lambda$ and $\delta_x{}^\lambda > 1$, both factors $(3^\lambda - 2^\lambda)$ and $(\delta_x{}^\lambda - 1)$ are positive, and therefore their product is positive too. If $\lambda < 0$, then both $(3^\lambda - 2^\lambda)$ and $(\delta_x{}^\lambda - 1)$ are negative, and therefore their product is positive again.

Theorem 1 follows.

In other words: Theorem 1 claims that by moving any substituent towards the end (to the β-position) of a carbon-atom chain the connectivity index will necessarily decrease.

THE SECOND THEOREM

Consider the molecular graphs H_1 and H_2 of a pair of constitutional isomers, shown in Fig. 1, where R_1, R_2, S_1 and S_2 denote arbitrary fragments. This time the groups R_1, R_2, S_1, S_2 may be absent in which case the respective vertices x_1, x_2, y_1, y_2 have degree 1.

Theorem 2. For all non-zero values of λ, and for arbitrary R_1, R_2, S_1, S_2 (*cf.* Fig. 1), the connectivity index of H_1 is greater than the connectivity index of H_2.

Proof. Applying the definition of the connectivity index to the molecular graphs H_1 and H_2 one obtains:

$$C(\lambda, H_1) = (\delta_{x1} \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot 2)^\lambda + (2 \cdot \delta_{x2})^\lambda + \\ + (3 \cdot \delta_{y1})^\lambda + (3 \cdot \delta_{y2})^\lambda + C(R_1) + C(R_2) + C(S_1) + C(S_2)$$

$$C(\lambda, H_2) = (\delta_{x1} \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot \delta_{x2})^\lambda + (3 \cdot \delta_{y1})^\lambda + (3 \cdot \delta_{y2})^\lambda + C(R_1) + C(R_2) + C(S_1) + C(S_2)$$

from which

$$C(\lambda, H_1) - C(\lambda, H_2) = 9^\lambda + 4^\lambda - 2 \cdot 6^\lambda = (3^\lambda)^2 - 2(3^\lambda)(2^\lambda) + (2^\lambda)^2 = (3^\lambda - 2^\lambda)^2. \quad (2)$$

The expression of the right-hand side of (2) is evidently positive for all $\lambda \neq 0$. Theorem 2 follows.

In other words: Theorem 2 claims that by moving any two substituents from a vicinal into a non-vicinal mutual position the connectivity index will necessarily decrease.

AN APPLICATION

In order to illustrate the potentials of Theorems 1 and 2, the isomeric trimethylnonanes will be considered. There exist 19 distinct constitutional isomers of this kind, depicted and numbered in Fig. 2. These are grouped into 8 sets of *C*-equivalent[1] species, namely: $\tau_1 = \{1\}$, $\tau_2 = \{2, 3, 4, 6, 10, 13\}$, $\tau_3 = \{5\}$, $\tau_4 = \{7, 8, 11\}$, $\tau_5 = \{9, 12\}$, $\tau_6 = \{14, 19\}$, $\tau_7 = \{15, 16, 17\}$ and $\tau_8 = \{18\}$.

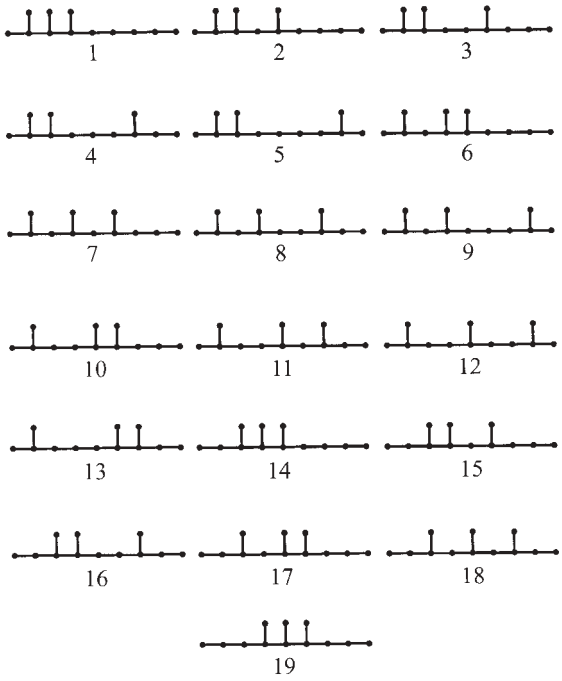

Fig. 2. Molecular graphs of the 19 isomeric trimethylnonanes.

Let T_i be any element of the set τ_i, $i = 1, 2, ..., 8$. Then by application of Theorem 1 one arrives at the following relations: $C(T_2) > C(T_3)$, $C(T_4) > C(T_5)$, $C(T_6) > C(T_1)$, $C(T_7) > C(T_2)$ and $C(T_8) > C(T_4)$. Application of Theorem 2 yields: $C(T_1) > C(T_2)$,

$C(T_2) > C(T_4)$, $C(T_3) > C(T_5)$, $C(T_6) > C(T_7)$ and $C(T_7) > C(T_8)$. In summary, the following orderings are established:

$$C(\lambda, T_6) > C(\lambda, T_1) > C(\lambda, T_2) > C(\lambda, T_3) > C(\lambda, T_5)$$
$$C(\lambda, T_6) > C(\lambda, T_7) > C(\lambda, T_8) > C(\lambda, T_4) > C(\lambda, T_5)$$
$$C(\lambda, T_7) > C(\lambda, T_2) > C(\lambda, T_4)$$

which hold irrespective of the value of the exponent $\lambda \neq 0$.

In fact, the only pairs of trimethylnonane isomers that cannot be ordered by means of Theorems 1 and 2 are T_1, T_7; T_1, T_8; T_2, T_8; T_3, T_4 and T_3, T_8. These, however, cannot be ordered at all (in the sense of Theorems 1 and 2), because their order depends on λ. Namely, by direct calculation one finds the following:

$C(\lambda, T_1) < C(\lambda, T_7)$ for $\lambda < 1$ and $C(\lambda, T_1) > C(\lambda, T_7)$ for $\lambda > 1$;
$C(\lambda, T_1) < C(\lambda, T_8)$ for $\lambda < -0.2838$ and $\lambda > 0$ and $C(\lambda, T_1) > C(\lambda, T_8)$ for $-0.2838 < \lambda < 0$;
$C(\lambda, T_2) < C(\lambda, T_8)$ for $\lambda < 1$ and $C(\lambda, T_2) > C(\lambda, T_8)$ for $\lambda > 1$;
$C(\lambda, T_3) < C(\lambda, T_4)$ for $\lambda < 1$ and $C(\lambda, T_3) > C(\lambda, T_4)$ for $\lambda > 1$;
$C(\lambda, T_3) < C(\lambda, T_8)$ for $\lambda < 2.3686$ and $C(\lambda, T_3) > C(\lambda, T_8)$ for $\lambda > 2.3686$.

Thus, in the case of trimethylnonanes Theorems 1 and 2 suffice to deduce all λ-independent orderings with respect to the connectivity index $C(\lambda)$.

И З В О Д

ДВЕ ТЕОРЕМЕ О ИНДЕКСИМА ПОВЕЗАНОСТИ

ИВАН ГУТМАН

Природно-математички факултет у Крагујевцу

Указано је на два општа случаја где је поредак молекула у односу на индекс повезаности $C(\lambda)$ исти за све вредности експонента λ.

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REFERENCES

1. I. Gutman, D. Vidović, A. Nedić, *J. Serb. Chem. Soc.* **67** (2002) 87.