



ORDERING OF MOLECULES ACCORDING TO THE CONNECTIVITY

SUDHIR KUMAR MISHRA* and A. N. SINGH^a

University Dept. of Chemistry, Rajendra College Campus Chapra (J.P.U. CHAPRA) (Bihar) INDIA

^aDeptt. of Physics, J. P. University, CHAPRA (Bihar) INDIA

(Received : 14.03.2012; Revised : 29.03.2012; Accepted : 31.03.2012)

ABSTRACT

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 .

Key words: Connectivity index, Isomer ordering.

INTRODUCTION

The definition of the connectivity index $C(\lambda) = C(\lambda; G) = G(G)$ can be found in the preceding paper¹ where the ordering of alkanes with regarding $C(\lambda)$ is discussed. It was shown¹ 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 as shown in Fig. 1, where R and S denote arbitrary fragments. Clearly, G_1 and G_2 represent a pair of constitutional isomers. It is necessary that R consists of more than a single vertex (otherwise G_1 and G_2 would coincide implying $C(\lambda; G_1) = C(\lambda; G_2)$ for all λ , therefore, it is assumed that the degree δ_x 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, 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 to the molecular graphs G_1 and G_2 one obtains:

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

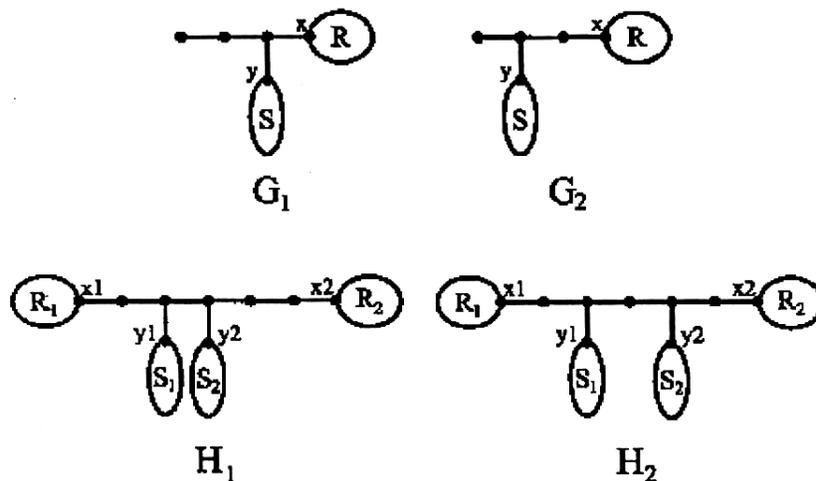


Fig. 1: The structure of the molecular graphs considered in Theorems 1 and 2 and the labeling of their fragments and vertices

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

From which

$$C(\lambda, G_1) - C(\lambda, G_2) = 2^\lambda + (3 \delta_x)^\lambda - 3^\lambda - (2 \delta_x)^\lambda = (3^\lambda - 2^\lambda) (\delta_x^\lambda - 1) \quad \dots(1)$$

As $\delta_x > 1$, the expression on the right-hand side of Eq. (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:

$$C(\lambda, H_1) = (\delta_{x_1} \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot 2)^\lambda + (2 \cdot \delta_{x_2})^\lambda + (3 \cdot \delta_{y_1})^\lambda + (3 \cdot \delta_{y_2})^\lambda + C(R_1) + C(R_2) + C(S_1) + C(S_2)$$

$$C(\lambda, H_2) = (\delta_{x_1} \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot 3)^\lambda + (3 \cdot 2)^\lambda + (2 \cdot \delta_{x_2})^\lambda + (3 \cdot \delta_{y_1})^\lambda + (3 \cdot \delta_{y_2})^\lambda + C(R_1) + C(R_2) + C(S_1) + C(S_2)$$

for which

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

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

The other words: Theorem 2 claims that by moving any two substituent 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 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 $\tau_8 = \{18\}$.

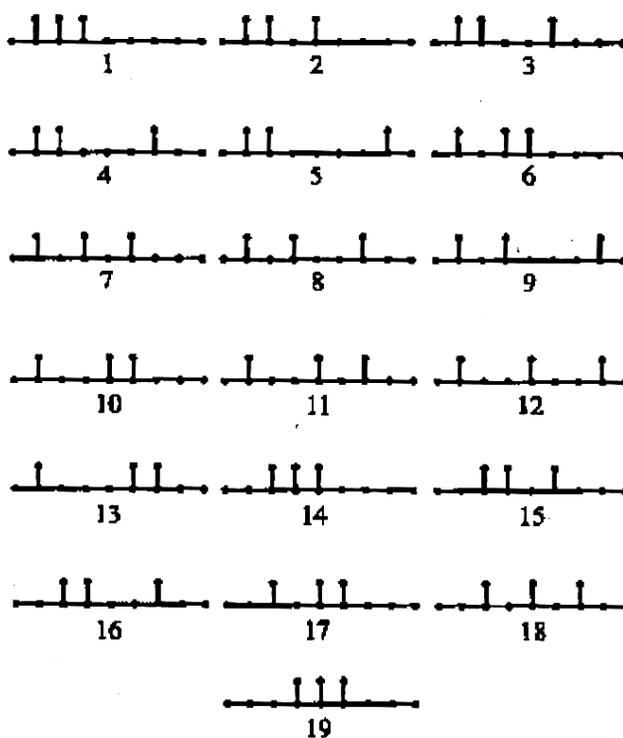


Fig. 2: Molecular graphs of the 19 isomeric trimethylnonanes

Let T_i be any element of the τ_i $i = 1, 2, \dots, 8$. 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:

$$C(\lambda, T_1) < C(\lambda, T_7) \text{ for } \lambda < 1 \text{ and } C(\lambda, T_1) > C(\lambda, T_7) \text{ for } \lambda > 1;$$

$$C(\lambda, T_1) < C(\lambda, T_8) \text{ for } \lambda < -0.2838 \text{ and } \lambda > 0 \text{ and } C(\lambda, T_1) > C(\lambda, T_8) \text{ for } -0.2838 < \lambda < 1;$$

$$C(\lambda, T_2) < C(\lambda, T_8) \text{ for } \lambda < 1 \text{ and } C(\lambda, T_2) > C(\lambda, T_8) \text{ for } \lambda > 1;$$

$$C(\lambda, T_3) < C(\lambda, T_4) \text{ for } \lambda < 1 \text{ and } C(\lambda, T_3) > C(\lambda, T_4) \text{ for } \lambda > 1;$$

$$C(\lambda, T_3) < C(\lambda, T_8) \text{ for } \lambda < 2.3686 \text{ and } C(\lambda, T_3) > C(\lambda, T_8) \text{ for } \lambda > 2.3686.$$

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

REFERENCES

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