match no. 25 pp. 131-140 1990

# A PROPERTY OF THE SIMPLE TOPOLOGICAL INDEX

Ivan Gutman

*Faculty of Science, University of Kragujevac, P.O.Box 60*

*YU-34000 Kragujevac, Yugoslavia*

(Received September 1989)

Abstract. The simple topological index of a hydrocarbon is the product of vertex degrees of the respective molecular graph. It is shown that two isomers have equal simple topological indices if and only if their molecular graphs have identical vertex degree sequences.

## Introduction

Let G be a graph and $v_1, v_2, \ldots, v_n$ its vertices. The *degree* $d_i = d_i(G)$ of the vertex $v_i$ is the number of vertices adjacent to $v_i$. The vertices of G can always be labelled so that $d_1 \le d_2 \le \ldots \le d_n$. Then the ordered n-tuple $(d_1, d_2, \ldots, d_n)$ is called the *vertex degree sequence* of the graph G and is denoted by $\mathbf{d}(G)$. Two graphs G and H with equal numbers of vertices are said to have *identical* vertex degree sequences if $d_i(G) = d_i(H)$ for all $i = 1, 2, \ldots, n$. Then we write $\mathbf{d}(G) = \mathbf{d}(H)$.

Graphs representing saturated hydrocarbons (either complete molecular graphs or skeleton graphs) [1] have vertex degrees less than or equal to four. This is, of course, due to the tetravalency of the carbon atom. Further, molecular graphs are necessarily connected and, consequently, they do not possess vertices of degree zero (i.e. isolated vertices). Therefore for molecular graphs $d_1 \geq 1$ and $d_n \leq 4$.

Several topological indices defined via the vertiex degrees of the molecular graph have been proposed in the chemical literature. A recent systematic examination of these indices has been undertaken in the paper [2], where also references to the previous works in this area can be found. Three topological indices which are fully determined by means of **d**(G) are M(G), I(G) and S(G), first introduced in refs. [3], [2] and [4], respectively. They are defined as follows:

$$M(G) = \sum_{i=1}^{n} d_i^2 \tag{1}$$

$$I(G) = \sum_{i=1}^{n} 1/d_i \tag{2}$$

$$S(G) = \prod_{i=1}^{n} d_i \tag{3}$$

The quantity S defined via Eq. (3) is called [2,4] the *simple topological index*.

We note in passing that according to Euler's theorem

$$\sum_{i=1}^{n} d_i = 2m \tag{4}$$

where m denotes the number of edges of the corresponding graph.

From Eqs. (1)-(3) it is evident that if two graphs have identical vertex degree sequences, then their M, I and S indices coincide. It is somewhat less straightforward to see whether the reverse of these statements are also obeyed, namely whether non-identical vertex degree sequences imply different M, I and S values.

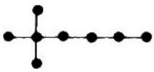
As a matter of fact, it is quite easy to design pairs of molecular graphs with non-identical vertex degree sequences, having equal M, I or S indices. Below are depicted the simplest such examples. Observe that $M(G_1) = M(G_2)$, $I(G_3) = I(G_4)$, $S(G_5) = S(G_6)$.

$G_1$ $G_2$ $G_3$ $G_4$

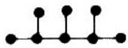
$G_5$ $G_6$

The natural objection to the above examples is that they correspond to pairs of non-isomeric hydrocarbons. On the other hand the topological indices M, I and S, as well as the great majority of other graph invariants considered in the chemical literature, are usually applied for the study of molecular properties of groups of isomers. Therefore one may ask the question whether there are pairs of molecular graphs with equal numbers of vertices and edges (which correspond to isomers), but with non-identical vertex degree sequences, whose topological indices M, I or S coincide.

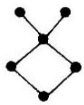
In the case of the quantities M and I the answer to the above question is confirmative. This is illustrated by the following examples. By easy calculation one can verify that $M(G_7) = M(G_8)$, $M(G_9) = M(G_{10})$ and $I(G_{11}) = I(G_{12})$, $I(G_{13}) = I(G_{14})$.



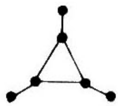
$G_7$



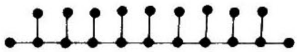
$G_8$



$G_9$

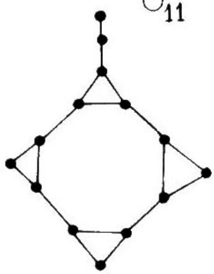


$G_{10}$

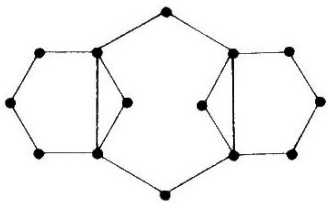


$G_{11}$

$G_{12}$



$G_{13}$



$G_{14}$

A method for the construction of examples of this kind is outlined in the Appendix.

## The Main Results

The main results of this work are the following two statements.

Let G and H denote two connected graphs with equal numbers of vertices (n) and edges (m). The maximum vertex degrees of G and H are then $d_n(G)$ and $d_n(H)$, respectively.

Theorem 1. If $d_n(G) \leq 5$ and $d_n(H) \leq 5$, then $S(G) = S(H)$ holds if and only if $\mathbf{d}(G) = \mathbf{d}(H)$.

Bearing in mind that molecular graphs have maximum vertex degrees not greater than four, we arrive at the following immediate consequence of Theorem 1.

Corollary 1.1. Isomeric saturated hydrocarbons have equal simple topological indices if and only if the respective molecular graphs have identical vertex degree sequences.

Corollary 1.1 means that *the simple topological index has the highest possible isomer-discriminating power* among topological indices based (solely) on the vertex degree sequence of the molecular graph. In this sense the simple topological index is superior to other previously proposed indices of the same kind [2], in particular to the quantities M and I. Thus Corollary 1.1 can be understood as a justification for the usage in chemical studies of the recently introduced quantity S [2,4]. It also provides an argument against inventing furhter vertex-degree-sequence-based topological indices.

Proof of Theorem 1. Denote by $n_i$ the number of vertices of G whose vertex degrees are equal to i. It is clear that the numbers $n_1, n_2, n_3, \ldots$ determine **d**(G) and vice versa.

Suppose that $d_n(G) \le 5$. Then

$$n_1 + n_2 + n_3 + n_4 + n_5 = n \qquad (5\ a)$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 + 5n_5 = 2m \qquad (5\ b)$$

$$2^{n_2}\, 3^{n_3}\, 4^{n_4}\, 5^{n_5} = S \qquad (6)$$

Recall that (5 b) is just another way of writing formula (4).

Since S is a positive integer it has a unique decomposition into prime factors, viz.

$$S = 2^a\, 3^b\, 5^c \qquad (7)$$

Comparing (6) and (7) one deduces

$$n_2 + 2n_4 = a \qquad (5\ c)$$

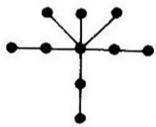
$$n_3 = b \qquad (5\ d)$$

$$n_5 = c \qquad (5\ e)$$

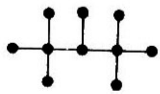
The relations (5 a)-(5 e) provide a system of five linear equations in five unknowns ($n_1$ to $n_5$). This system has a unique solution, implying that it is impossible to find another graph H with n vertices and m edges, such that **d**(H) ≠ **d**(G) and S(H) = S(G).

This proves the "only if" part of Theorem 1. Its "if" part should be obvious from Eq. (3). ■

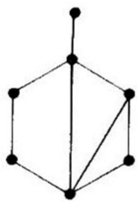
The below examples $G_{15}$ and $G_{16}$ as well as $G_{17}$ and $G_{18}$ show that the value 5 for the maximum vertex degree in Theorem 1 is the best possible.



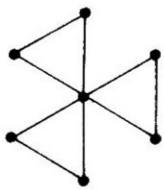
$G_{15}$



$G_{16}$



$G_{17}$



$G_{18}$

Note that $d_{10}(G_{15}) = 6$, $d_{10}(G_{16}) = 4$ as well as $d_7(G_{17}) = 4$, $d_7(G_{18}) = 6$.

The construction of the graphs $G_{15}$, $G_{16}$, $G_{17}$ and $G_{18}$ is based on the following reasoning.

Suppose that $d_n(G) = 6$. Then instead of Eqs. (5 a), (5 b) and (6) we have

$$n_1 + n_2 + n_3 + n_4 + n_5 + n_6 = n \tag{8 a}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 + 5n_5 + 6n_6 = 2m \tag{8 b}$$

$$2^{n_2} 3^{n_3} 4^{n_4} 5^{n_5} 6^{n_6} = S \tag{9}$$

Bearing in mind Eq. (7) we now conclude that

$$n_2 + 2n_4 + n_6 = a \tag{8 c}$$

$$n_3 + n_6 = b \tag{8 d}$$

$$n_5 = c \tag{8 e}$$

Relations (8 a)-(8 e) represent a system of five linear equations in six unknowns ($n_1$ to $n_6$). This system must have one solution in which $n_1$ to $n_6$ are non-negative integers (corresponding to the graph G), but may have other such solutions as well.

Eqs. (8 a)-(8 e) imply

$$n_4 + 2n_6 = 2m - n - (a + 2b + 4c) \tag{10}$$

From (10) is seen that if the choice $n_4 = 2p$, $n_6 = q$ satisfies (8a)-(8e), then also the choice $n_4 = 2q$, $n_6 = p$ will satisfy the same system. The simplest pairs of non-negative integers satisfying the system (8) would thus be $n_4 = 0$, $n_6 = 1$ and $n_4 = 2$, $n_6 = 0$.

Making a further simplification, namely assuming that $n_5 = 0$, we easily find pairs of graphs G, H having equal S values but different vertex degree sequences.

## Appendix: Constructing Molecular Graphs with Equal M and I

Consider a molecular graph G with n vertices and m edges, whose maximum vertex degree is four. Then, using the same notation as in the proof of Theorem 1, we have

$$n_1 + n_2 + n_3 + n_4 = n \tag{11}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m \tag{12}$$

$$n_1 + 4n_2 + 9n_3 + 16n_4 = M \tag{13}$$

$$n_1 + n_2/2 + n_3/3 + n_4/4 = I \tag{14}$$

From Eqs. (11)-(13) we obtain

$$2n_3 + 6n_4 = M + 2n - 6m \tag{15}$$

which means that if $n_3 = 3p$, $n_4 = q$ satisfies Eqs. (11)-(13), then also $n_3 = 3q$, $n_4 = p$ is a solution of the same system. Choosing $p = 0$ and $q = 1$ we immediately arrive at the pairs of graphs $G_7$, $G_8$ and $G_9$, $G_{10}$.

In a completely analogous manner Eqs. (11), (12) and (14) render

$$4n_3 + 9n_4 = 12I + 12m - 18n \tag{16}$$

Bearing in mind that 12I is necessarily an integer we see that the system of equations (11), (12), (14) has two sets of integer solutions given by $n_3 = 9p$, $n_4 = 4q$ and $n_3 = 9q$, $n_4 = 4p$. The choice $p = 1$, $q = 0$ results then in the examples $G_{11}$, $G_{12}$ and $G_{13}$, $G_{14}$.

It is clear from the above analysis that if the maximum vertex degree of the molecular graph G is equal to three, then both M and I are uniquely determined by **d**(G). In this case **d**(G) ≠ **d**(H) would imply M(G) ≠ M(H) as well as I(G) ≠ I(H).

If Eqs. (13) and (14) are to be obeyed simultaneously, then the system (11)-(14) has a unique solution. This makes possible the formulation of the following result.

Theorem 2. Isomeric hydrocarbons have equal topological indices M and in the same time equal topological indices I if and only if the respective molecular graphs have identical vertex degree sequences.

*Acknowledgement*. This paper was produced during the author's visits to Hokkaido University (Sapporo), Shizuoka University (Shizuoka), Kyoto University (Kyoto), Hiroshima University (Hiroshima) and Ochanomizu University (Tokyo). The financial support of the Japan Society for the Promotion of Science is gratefully acknowledged.

References

[1] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin 1986, pp. 19-20.
[2] H. Narumi, *Match* **22**, 195 (1987).
[3] I. Gutman, B. Ruščić, N. Trinajstić and C. F. Wilcox, *J. Chem. Phys.* **62**, 3399 (1975).
[4] H. Narumi and M. Katayama, *Mem. Fac. Eng. Hokkaido Univ.* **16**, 209 (1984).