Simple Topological Index
—— A Newly Devised Index Characterizing The Topological Nature of Structural Isomers of Saturated Hydrocarbons ——

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Abstract

A simple topological index which is defined as the product of orders at vertexes of a graph is presented and compared with other indexes including Hosoya's index. Its characteristic is studied and an application is considered for the thermodynamic data, including boiling points. Simple composition principles are also given.

1. Introduction

Several years ago H. Hosoya set forth Topological Index[1,2,3,4] and tabulated its values[5,6] which were calculated by an electronic computer.

He defined the Topological Index for a graph G as the sum of the non-adjacent numbers p (G, k)'s, where p (G, k) is the number of ways in which such k bonds are chosen from G that no two of them are connected ;

$$Z_G = \sum_{k=0}^{m} p(G, k) \qquad (1)$$

the integer m being the maximum number for k. He could show that Z_G is reflected from the topological nature of G, i. e., branching mode and ring closure.

Now we propose an incomplete but simpler topological index which we can calculate easily without an electronic computer and discuss some natures of the index.

2. Results and Discussion

2.1. Definition and characteristics

A simple topological index (STI) is proposed for a connected graph G representing the carbon skeleton of a saturated hydrocarbon.

We define the simple topological index P_G for a graph G as the product of the order d (G, k)'s, where d (G, k) is the number of edges which radiate from the k-th vertex ;

$$P_G = \prod_{k=1}^{N} d(G, k) \qquad (2)$$

the integer N being the number of vertexes of the graph G.

The d (G, k) numbers can be enumerated from a given graph G just by counting. The P_G values for a complicated graph can be obtained with a kind of composition principle by decomposing G into smaller subgraphs as shown later.

In this paper we only consider tree graphs. The d (G, k)'s and P_G for all the possible

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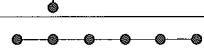
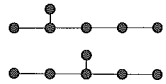
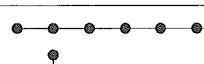
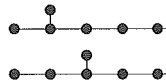
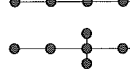
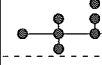
tree graph with $N \leqq 7$ are tabulated in Table I. The numbering of graphs are the same ones given in the paper of Hosoya.[5]

Each entry is classified as A or B depending on whether it corresponds to the carbon atom skeleton of a saturated hydrocarbon or not. The typical graphs in group B is a star graph which consists of a central point (vertex) and N-1 bonds (edges) radiating from it.

Table I. Simple Topological index P_G

N	No.	Graphs G	Factors n_1	n_2	n_3	n_4	n_5	n_6	P	Z
1	1		0	−1	0	0			$(\frac{1}{2})$	1
2	1		2	0	0	0			1	2
3	1		2	1	0	0			2	3
4	1		2	2	0	0			4	5
	2		3	0	2	0			3	4
5	1		2	3	0	0			8	8
	2		3	1	1	0			6	7
	3		4	0	0	1			4	5
6	1		2	4	0	0			16	13
	2		3	2	1	0			12	11
	3		3	2	1	0			12	12
	4		4	1	0	1			8	9
	5		4	0	2	0			9	10
	B 1		5	0	0	0	1		5	6
7	1		2	5	0	0			32	21
	2		3	3	1	0			24	18
	3		3	3	1	0			24	19
	4		3	3	1	0			24	20
	5		4	2	0	1			16	14
	6		4	1	2	0			18	17
	7		4	1	2	0			18	15
	8		4	2	0	1			16	16
	9		5	0	1	1			12	13
	B 1		5	1	0	0	1	0	7	11
	B 2		6	0	0	0	0	1	6	7

The P_G values for $N=8$ and ring compounds will be given elsewhere.[9]

It is evident that among all the isomeric tree graphs with the same number of vertexes N a linear graph ($\bar{N}$) and a star graph (N*) have, respectively, the largest and the smallest P_G numbers, i. e.,

$$P_{\bar{N}}=2^{N-2} \qquad (N\geq 2) \tag{3}$$

$$P_{N}{}^{*}=N-1 \qquad (N\geq 2) \tag{4}$$

This inclination is the same as Hosoya's Z.

The Simple Topological Index P_G is not defined for $N=1$. If we venture to define it we can give 1/2 to P_G according to (3).

Generally P_G is written as

$$P_G=1^{n_1}2^{n_2}3^{n_3}4^{n_4}\cdots\cdots d_m^{n_m} \tag{5}$$

and we have

$$n_1+n_2+n_3+\cdots\cdots+n_m=N \tag{6}$$

where n_1, n_2, --- are the non-negative integers. The n_i shows there are n_i of the orders d_i' s in a graph G. The d_m is the maximum order of graph. Especially in the linear saturated hydrocarbons we have

$$P_G=1^{n_1}2^{n_2}3^{n_3}4^{n_4} \tag{7}$$

$$n_1+n_2+n_3+n_4=N \tag{8}$$

It is well known that the sum of the orders of edges equals to twice of the number of edges, i. e.,

$$n_1d_1+n_2d_2+\cdots\cdots+n_md_m=2E(N-1) \tag{9}$$

where E is the number of edges. From eqs. (6) and (9), we have

$$2(n_1+n_2+\cdots\cdots+n_m-1)=n_1d_1+n_2d_2+\cdots\cdots+n_md_m \tag{10}$$

Eq. (10) shows the relation between n_i' s and d_i' s.

The graphs having the smallest P_G numbers in the group A are given in Table II with their factors, P_G's and Z_G's.

Table II shows the same result as Hosoya's except for the graph Nos. 9.32 and 9.45 (see Ref. 5).

For $N\geq 6$ there are several couples of graphs with the same set of factors but with different structures. Let us call them isofactorgraphs. For example in the case of $N=6$, there is one kind of isofactor $P\ (6, 2)=P\ (6, 3)=1^3\times 2^2\times 3$, where the first number in the parentheses is N and the second one is the numbering of graphs. For the graph with $N=7$, there are three kinds of isofactors ; $P\ (7, 2)=P\ (7, 3)=P\ (7, 4)=24$, $P\ (7, 5)=P\ (7, 8)=16$, $P\ (7, 6)=P\ (7,7)=18$.

The existence of isofactors is not desirable for the classifying graphs. However the simplicity in calculating the Simple Topological Index makes up for the fault. Although the classification A and B is artificial from a mathematical view point, it is interesting for us to compare group A and B on chemical aspects. In general the graphs in the group B

Table II. The smallest P_G values.

N	No.	Factors				P	Z
		n_1	n_2	n_3	n_4		
4	2	3	0	1	0	3	4
5	3	4	0	0	1	4	5
6	4	4	1	0	1	8	9
7	9	5	0	1	1	12	13
8	18	6	0	0	2	16	17
9	32	6	1	0	2	32	30
	34	6	1	0	2	32	24
10	45	7	0	1	2	48	43
	46	7	0	1	2	48	40

Table III. The comparison among four kinds of indexes.

Graph	M_1	M_2	Z	P
A 1	22	20	21	32
2	24	22	18	24
3	24	23	19	24
4	24	24	20	24
5	28	26	14	16
6	26	26	17	18
7	26	24	15	18
8	28	28	16	16
9	30	30	13	12
B 1	34	32	11	7
2	42	36	7	6

have smaller P_G values than the group A, since P_G decreases with branching as Z_G does. The A group of the graphs with $N=6$ and 7 have almost continuous integers exeept for the one for linear graphs which has isolating upper P_G number. On the other hand the P_G's of the group B have isolating lower P_G values compared with the ones of the group A's.

2.2. Comparison with other indexes

Several other topological indexes are reported elsewhere.[7]

Especially we noticed after creating our index P_G that two of them of Zagreb group[8] have relation with ours ;

$$M_1(G)=\sum_{j=1}^{N} d_j^2 \tag{11}$$

$$M_2(G)=\sum_{\text{edges}} d_i d_j \tag{12}$$

The first seems over all vertexes of G and the second over all edges in G.

We compare the four kinds of values M_1, M_2, Z and P with $N=7$ in the Table III. M_1, M_2 and P have almost the same ability of classifying graphs with the same number of vertexes, namely chemically speaking isomers with the same number of carbons. But P_G is the most easy index to be calculated because that is obtained by just multiplying. The Topological Index of Hosoya is of course the most effective index among the four kinds of indexes.

However we need a table to know their values. On the other hand we do not need any table to know the P_G values. We can know it just by knowing the orders of graph G and by multiplying them.

2.3. Application for thermodynamic data

Now we study the relationship between the Simple Topological Index P_G and the boiling points t_b of linear saturated hydrocarbons in Table IV. N and n are the number

Table IV a. The relation between the Simple Topological Index and Boiling Points.

N	n	A	B	r
4	2	−33.19	11.23	1.00
5	3	−15.38	6.64	0.97
6	5	36.17	2.11	0.93
7	9	68.15	0.96	0.95
8	18	99.44	0.39	0.75

Table IV b. The relation between the Topological Index and Boiling Points.

N	n	A'	B'	r'
4	2	−56.65	11.23	1.00
5	3	−34.87	8.90	0.99
6	5	12.38	4.32	0.97
7	9	48.22	2.32	0.96
8	18	81.69	1.22	0.88

of carbons and the number of isomers respectively. A, B, A' and B' are constants in the following formula ;

$$t_b\ (°C)=A+B\ P \tag{13}$$

$$t_b\ (°C)=A'+B'\ Z \tag{14}$$

r and r' are the correlation coefficients. Although the Simple Topological Index has many isofactors they have good correlations with boiling points t_b. Hosoya's index has of course better correlation with them but there is not so great difference between the degrees of correlations of the two indexes.

2.4. A simple composition principle

Finally we thought about a kind of composition principle. Consider a graph G in Fig. I_a, I_b or I_c and choose from it a line l. (1) Delete line l and we get subgraphs L′ and M′. · (2) Add a line to each position of L′ or M′ where the deleted line l existed, we get graphs L and M.

Then the Simple Topological Index P_G for G can be obtained as

$$P_G=P_L P_M \tag{15}$$

P_G values of a point graph is 1/2 by definition as mentioned above. Application of the principle to the terminal line of the linear (or normal) graphs $\bar{N}$ gives the following equation ;

$$P_{\bar{N}}=P_2 P_{\bar{N}} \tag{16}$$

For Graph $\bar{N}$ with even N $(=2k)$ we get the relation

$$P_{2k}=P_{k+1}{}^2 \tag{17}$$

by choosing the central line as l. We gain the following equation similarly

$$P_{2k+1}=P_{k+1}\ P_{k+2} \tag{18}$$

If the line to be deleted is a member of a cycle, the deletion gives only one subgraph L′. The adding lines gives a graph L (Fig. II). In this case we have a simple relation ;

$$P_G=P_L \tag{19}$$

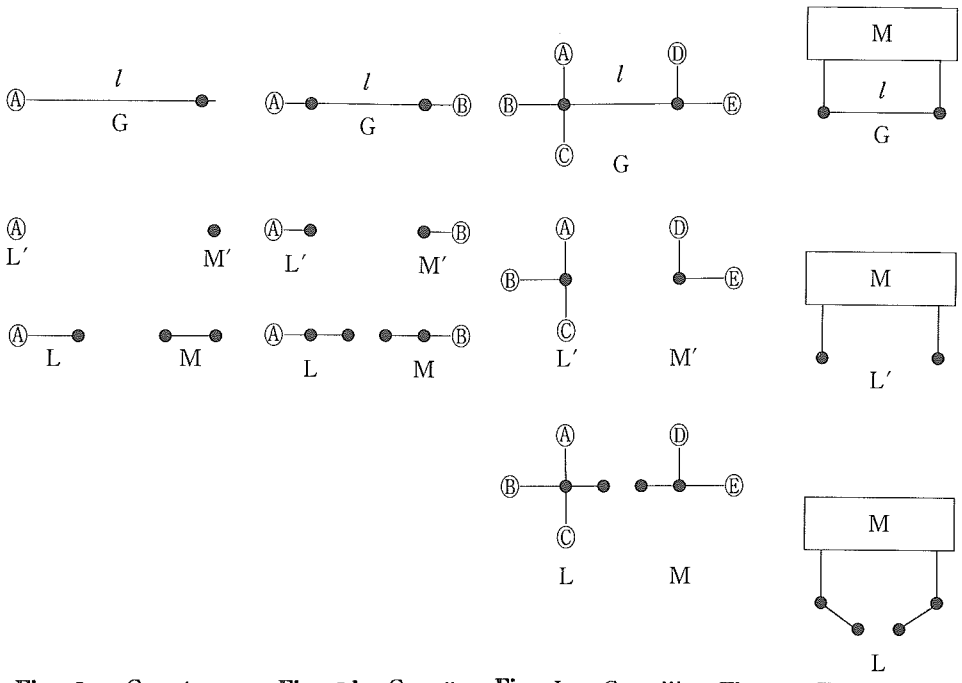


Fig. I a Case i **Fig. I b** Case ii **Fig. I c** Case iii **Fig. II** The case of a cycle.

Calculation of the Simple Topological Indexes for the tree graph with N's larger than 7 and for the mono- and bicyclic groups will be published in a coming paper[9].

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