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NEW TOPOLOGICAL INDICES FOR FINITE AND INFINITE SYSTEMS

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Summary: Three kinds of newly defined topological indices are presented and their mathematical characteristics are shown. They are compared with other topological indices and a correlation with the boiling points of saturated hydrocarbons is shown. Their formulas in finite systems and their values in infinitely large systems are presented.

1. Introduction

Topological indices [1] are values which are used to characterize the topological structure of molecules graph-theoretically. These are applied for analyzing the relations between structure and activity [2]. The method to obtain topological indices are classified into two kinds; the first is to use topological distance and the second is to utilize connectivity.

Topological indices depending on connectivity are further classified as follows: the first depends on the structure of the graph [3], the second is Hosoya's Z-index [1] which depends on the adjacency-number and the third depends on the orders of vertices of the graphs [3][6]. We treat the last case here.

The Zagreb group studied two kinds of topological indices by using order d_i of vertex i [4].

$$M_1(G) = \sum_{i=1}^{N} {d_i}^2 \qquad (1,1)$$

$$M_2(G) = \sum_{(i,j)} d_i d_j \qquad (1,2)$$

The summation in eq.(1,2) is concerned with all edges in a graph. These topological indices were obtained when the total π energy of conjugated compounds was studied.

Randić proposed the connectivity X(G) of a graph [5].

$$X(G) = \sum_{(i,j)} (d_i d_j)^{-1/2} \qquad (1,3)$$

This index was introduced in order to explain the branching of acyclic hydrocarbons [3][5].

The present author has devised the Simple Topological Index S(G) which is defined as the product of orders of points and is used to analyze the branching of saturated hydrocarbons [6],

$$S(G) = \prod_{i=1}^{N} d_i \qquad (1,4)$$

Other newly defined topological indices using orders d_i are reported in section 2 and the relations are given as to the numbers of vertices, edges and newly defined topological indices, A(G), G(G), and H(G) in section 3-1. Comparison with some other topological indices which were given by other authors are discussed in section 3-2. Application to thermodynamic data is also given in section 3-3. The formulas of the topological indices for fitite systems and the limiting values for the infinitely large systems are shown in section 3-4.

2. Definition

The quantity I(G) is defined first.

$$I(G) = \sum_{i=1}^{N} 1/d_i \qquad (2,1)$$

where d_i is the order of each vertex i of graph G and N is the number of vertices.

Then the quantity H(G) is called the Harmonic Topological Index ;

$$H(G) = N/I(G) \qquad (2,2)$$

The values of I(G) and H(G) of simple graphs are given in TABLE 1.

TABLE 1. The values of Harmonic Topological Index H(G).

N[a]	I(G)[b]	H(G)[c]
1	∞	0.00
2	2.00	1.00
3	2.50	1.20
4	3.00	1.33
2m3	3.33	1.20
5	3.50	1.42
2m4	3.83	1.30
22m3	4.25	1.17
6	4.00	1.50
2m5	4.33	1.38
3m5	4.33	1.38
22m4	4.75	1.26
23m4	4.66	1.28
7	4.50	1.55
2m6	4.83	1.44
3m6	4.83	1.44
3e5	4.83	1.44
23m5	5.16	1.35
24m5	5.16	1.35
22m5	5.25	1.33
33m5	5.25	1.33
223m4	5.58	1.25

a) Abbreviation of the compounds; For example 223m4 means 2,2,3-trimethylbutane. b) See text and eq.(2,1). c) See eq.(2,2).

3. Results and Discussion

3-1. Mathematical Relations.

$$A \geqq G \geqq H \qquad (3,1)$$

where $A = (d_1+d_2+ \cdots\cdots +d_N)/N \qquad (3,2)$

$$G = (d_1 d_2 \cdots\cdots d_N)^{1/N} \qquad (3,3)$$

$$H = N/(1/d_1+1/d_2+ \cdots\cdots +1/d_N) = N/I \qquad (2,2)$$

The quantities A and G are called the Arithmetic Topological Index and the Geometric Topological Index respectively.

The next relation is taken from the graph theory;

$$\sum_{i=1}^{N} d_i = 2e , \qquad (3,4)$$

where e is the number of edges in graph G. Therefore, from eqs. (3,2) and (3,4).

$$A = 2e/N \qquad (3,5)$$

Equation (3,5) means that for all isomers, (i.e., where each isomer has the same value of N) the Arithmetic Topological Index A(G) is the same for all isomers.

Simple Topological Index S(G) is defined [6] as in eq. (1,4), therfore,

$$G = S^{1/N} \qquad (3,6)$$

If eqs.(2,2), (3,5) and (3,6) are substituted into eq.(3,1), the following eq. is obtained.

$$2e/N \geq S^{1/N} \geq H = N/I \qquad (3,7)$$

The above equation shows the relationship among the number of vertices N, the number of edges e, Simple Topological Index S (or Geometric Topological Index $S^{1/N}$), Harmonic Topological Index H, and I.

3-2. Comparison with Other Indices.

The six kinds of values M_1, M_2, Z, S, H and G for heptane isomers are compared in TABLE 2. M_1, M_2, S, H and G have almost the same ability of classifying graphs with the same number of vertices, namely, isomers. The Hosoya's Z-index is the most effective index among the six indices.

TABLE 2. Comparison among the six indices.

Substances	M_1	M_2	Z	S	H	G
7	22	20	21	32	1.55	1.64
2m6	24	22	18	24	1.44	1.57
3m6	24	23	19	24	1.44	1.57
3e5	24	24	20	24	1.44	1.57
23m5	26	26	17	18	1.35	1.51
24m5	26	24	15	18	1.35	1.51
33m5	28	28	16	16	1.33	1.48
22m5	28	26	14	16	1.33	1.48
223m4	30	30	13	12	1.25	1.42

A=2e/N=2 6/7=1.71 for all heptane isomers.

For N=6 there is one pair of graphs with the same value of H but with different structures. Let us call them isovalue graphs. Namely in the case of N=6, 2m5 and 3m5 have the same H value of 1.38. Similar cases can be seen in TABLE 2.

Although isovalues are not useful for classifying graphs, the present topological indices H and G can be caluculated quite easily.

3-3 Application to Thermodynamic Properties.

The relationship between the Harmonic Topological Index H(G) and the boiling points t_b of acylic hydrocarbons is given in TABLE 3, where N and n are the number of carbon atoms and the number of isomers respectively, and A, B, C, and D are the constants in the following formulas

$$t_b = A + BH \qquad (3.8)$$

$$t_b = C + DZ \qquad (3,9)$$

Although the Harmonic Topological Index has many isovalues it has good correlation with the boiling point t_b.

TABLE 3. Relation between the Harmonic Topological index H and boiling point t_b of saturated hydrocarbons.

N	n	A	B	r	C	D	r'
5	3	-113.96	106.76	0.98	-34.87	8.90	0.99
6	5	-31.70	67.43	0.92	12.38	4.32	0.97
7	9	-2.45	65.09	0.87	48.22	2.32	0.88

Note: r and r' are correlation coefficients.

3-4. The Formula in Finite Systems and the Values for Infinitely large Systems of the Present Topological Indices.

3-4-1. The Formulas for Finite Systems.

The formulas of A, G, and H in various graphs are given as functions of the number of vertices N:

1) Star graphs (Fig.1).

$$A = 2(1-1/N)$$

$$G = (N-1)^{1/N}$$

$$H = (1-1/N)/(1-2/N+2/N^2)$$

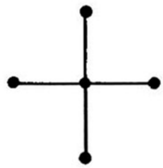

Fig. 1 Star graph with N=5.

2) Comb graphs (Fig.2).

$$A = 2(1-1/N)$$

$$G = 3^{(1-2/N)/2}$$

$$H = 3/(2+2/N)$$

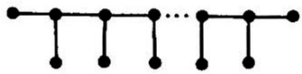

Fig. 2 Comb graph.

3) Cycle graphs (Fig.3).

$A = G = H = 2.$

Namely the values do not depend on N.

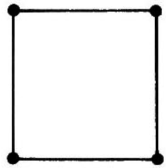

Fig. 3 Cycle graph with N=4.

4) Path graphs (Fig.4).

$A = 2(1-1/N)$

$G = 2^{1-2/N}$

$H = 1/(1/N + 1/2)$

Fig. 4 Path graph.

5) Ladder graphs (Fig.5).
(Linear polyomino graphs)

$A = 3-4/N$

$G = 2^{4/N}\ 3^{1-4/N}$

$H = 3/(1+2/N)$

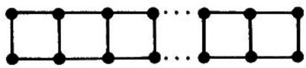

Fig. 5 Ladder graph.

6) Tower graphs (Fig.6).
(n $\times$ 4 torus)

$A = 4-8/N$

$G = 3^{8/N}\ 4^{1-8/N}$

$H = 12/(3+8/N)$

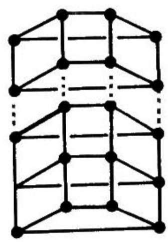

Fig. 6 Tower graph.

7) Window graphs (Fig.7).

$A = 3$

$G = 2^{12/N} 3^{1-8/N}$

$H = 3/(1+1/N)$

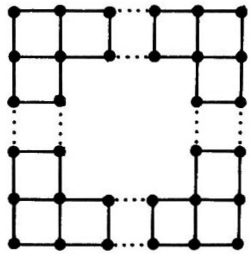

Fig. 7 Window graph.

8) Centipede graphs (Fig.8).

$A = 2(1-1/N)$

$G = 4^{(N-2)/3N}$

$H = 4/(3+2/N)$

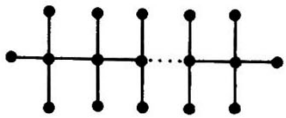

Fig. 8 Centipede graph.

9) Complete graphs (Fig.9).

$A = G = H = N-1$

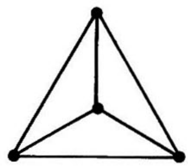

Fig. 9 Complete graph wtih N=4.

10) $l \times m \times n$ Lattice graphs.

The size of the lattice is $l \times m \times n$, namely $N=lmn$. If D_i is assumed to be the number of vertices which have order i, then

$D_3 = 8$

$D_4 = 4\ (l+m+n-6)$

$D_5 = 2[(l-2)(m-2)+(m-2)(n-2)+(n-2)(l-2)]$

$D_6 = lmn-2(lm+mn+nl)+4(l+m+n)-8$

using the above D_i's, A, G, and H are expressed as follows;

$$A = 3D_3/N + 4D_4/N + 5D_5/N + 6D_6/N$$

$$G = 3^{D_3/N} \cdot 4^{D_4/N} \cdot 5^{D_5/N} \cdot 6^{D_6/N}$$

$$H = 1/(D_3/3N + D_4/4N + D_5/5N + D_6/6N)$$

3-4-2. The Values for Infinitely Large Systems.

The following three kinds of values are defined as N becomes infinite:

$$\alpha = \lim_{N\to\infty} A$$

$$\gamma = \lim_{N\to\infty} G$$

$$\chi = \lim_{N\to\infty} H$$

The values α, γ and χ are given in TABLE 4.
The values A, G, and H remain finite in almost all cases as N goes up infinity. The finiteness is a remarkable feature of the indices α, γ and χ.

The physical data of substances of infinite scale will be discussed by using the present topological indices α, γ and χ.

TABLE 4. The limiting values α, γ and χ for the present topological indices of various series of graphs

Graphs	α	γ	χ
Star Graph	2	1	1
Comb Graph	2	$\sqrt{3}$	3/2
Cycle Graph	2	2	2
Path Graph	2	2	2
Ladder Graph	3	3	3
Tower Graph	4	4	4
Window Graph	3	3	3
Centipide Graph	2	$\sqrt[3]{4}$	4/3
Complete Graph	∞	∞	∞
Lattice Graph	6	6	6

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