Tables of Non-Adjacent Numbers, Characteristic Polynomials and Topological Indices. I. Tree Graphs

Kimiko Mizutani (水 谷 公 子), **Keiko Kawasaki** (河 崎 啓 子) and **Haruo Hosoya** (細 矢 治 夫)

Department of Chemistry, Ochanomizu University,
Bunkyo-ku, Tokyo

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A topological index Z_G has been defined 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[1];

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

the integer m being the maximum number for k. It has been shown that Z_G is reflected from the topological nature of G, *i.e.*, branching mode and ring closure, and that topologically similar graphs with or without a ring are related to each other through their Z_G values.

The $p(G, k)$ numbers can be enumerated from a given graph G just by counting and the Z_G value for a complicated graph can be obtained with a composition principle by decomposing G into smaller sub-graphs. For a tree graph (a graph without a ring) having N points the $p(G, k)$ numbers can also be obtained from the characteristic polynomial $P_G(X)$ of G as

$$P_G(X) = \det|X\boldsymbol{E} + \boldsymbol{A}|$$

$$= \sum_{k=0}^{m} (-1)^k p(G, k) X^{N-2k} , \tag{2}$$

if one is given an adjacency matrix $\boldsymbol{A}$. An adjacency matrix $\boldsymbol{A}$ for G with N points is defined as a square matrix of the order N with the following elements

$$(\boldsymbol{A})_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

and is shown to be mathematically equivalent to G.

However, for a non-tree graph eq. (2) is not valid because of " contaminating terms " arising from a ring-counting in decomposing the det $|XE+A|$ into a polynomial of X. This problem is closely related to an *unsolved* problem in the graph theory that no analytical expression has been given for counting the number of polygons with $n \geqq 5$.[2)]

Although it has been pointed out by Harary that one-to-one correspondence between tree graphs and characteristic polynomials is not always observed for larger N, no example has been given in literatures. This problem is important if one considers a coding system (or a naming system with a set of numbers) for graphs or structural isomers of chemical compounds, say saturated hydrocarbons.

In relation to these two problems no analysis has been given whether a distance matrix $\boldsymbol{D}$ is useful for solving them or not. A distance matrix $\boldsymbol{D}$ for G with N points is defined as a square matrix of the order N with elements

$$(\boldsymbol{D})_{ij} = \left\{ \begin{array}{l} \text{the number of lines for the shortest} \\ \text{path from the point } i \text{ to } j \end{array} \right. \tag{4}$$

In order to study these problems we have calculated the $p(\mathrm{G}, k)$'s, Z_{G}, $P_{\mathrm{G}}(X)$ and $\boldsymbol{D}$ for lower members of all the possible isomeric graphs with zero and a few rings. The results have been punched on cards for sorting.

In this paper we only consider tree graphs. The $p(\mathrm{G}, k)$'s and Z_{G} for all the possible tree graphs with $N \leqq 10$ are tabulated in Table I.[4)] Each entry is classified as A or B depending that it corresponds to the carbon atom skeleton of a saturated hydrocarbon or not. The typical of the graphs in the group B is a *star* which consists of a central point and $N-1$ bonds radiating from it.

It is evident that among all the isomeric tree graphs (A+B) with the same number of points N a linear (or a normal) graph ($\bar{N}$) and a star graph (N^*) have, respectively, the largest and the smallest Z_{G} numbers, namely,

$$Z_{\bar{N}} = \left\{ \left(\frac{1+\sqrt{5}}{2} \right)^{N+1} - \left(\frac{1-\sqrt{5}}{2} \right)^{N+1} \right\} \Big/ \sqrt{5}$$

(Binét's formula for the Fibonacci numbers) (5)

$$Z_{N^*} = N$$

In general the graphs in the group B have smaller Z_{G} numbers than the group A, since Z_{G} decreases with branching. Although the classification between the groups A and B was made from the chemical point of view, it is interesting to note the following observation. The five A isomers of the graphs with $N=6$ are assigned consecutive five integers from 9 to 13, while the star graph (B1) which is the only entry of the graph B has an isolation Z_{G} number 6. This is also the case with the graphs with $N=7$: the Z_G's of the group B are 7 and 11, while the nine graphs of the group A have consecutive nine integers from 13 to 21.

Thus, besides the upper and lower limits of the Z_G numbers (eq. (5)) of the isomeric graphs (A+B), it is interesting to know the lower limit of Z_G for the group A. The graphs having the smallest Z_G numbers in the group A with $N \leqq 15$ are given in Table II together with their Z_G's.

Finally let us take a closer look at the set of $p(G, k)$ numbers of the characteristic polynomials. From Table I it is observed that for the graphs with $N \leqq 8$ there is one-to-one correspondence between G and $P_G(X)$, while for $N \geqq 9$ there are several couples of graphs with an identical characteristic polynomial or an identical set of $p(G, k)$ numbers but with different structures. Let us call them isopolynomial graphs. They are tabulated in Table III.

In Appendix a flow chart for obtaining the $p(G, k)$ numbers for a given graph G with or without rings is shown.

References

1) H. Hosoya: Bull. Chem. Soc. Japan, to be published.
2) Although Harary gives in Ref. 3) an analytical expression for counting the number of pentagons, it was found mistaken.
3) F. Harary: Graph Theory (Addison-Wesley Publ. Co., Reading, Mass. 1969).
4) All the tree graphs with $N \leqq 10$ are given by Harary[3).

Table I-1

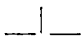
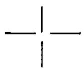
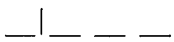
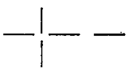
N	No	Graph(G)	p(G,k) k = 0	1	2	3	Z
1	1	.	1				1
2	1	—	1	1			2
3	1	— —	1	2			3
4	1	— — —	1	3	1		5
	2		1	3			4
5	1	— — — —	1	4	3		8
	2		1	4	2		7
	3		1	4			5
6	A1	— — — — —	1	5	6	1	13
	2		1	5	5		11
	3		1	5	5	1	12
	4		1	5	3		9
	5		1	5	4		10
6	B1		1	5			6

Table I-2 N = 7

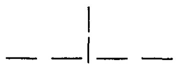
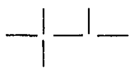
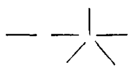
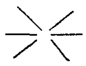
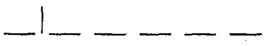
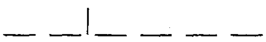
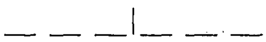
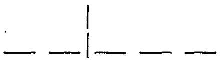
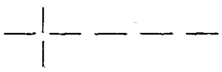
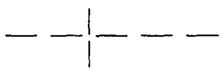
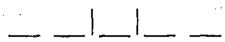
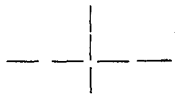
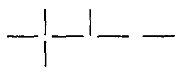
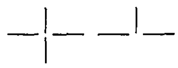
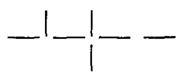
No	Graph(G)	p(G,k) k = 0	1	2	3	Z
A1		1	6	10	4	21
2		1	6	9	2	18
3		1	6	9	3	19
4		1	6	9	4	20
5		1	6	7		14
6		1	6	8	2	17
7		1	6	8		15
8		1	6	7	2	16
9		1	6	6		13
B1		1	6	4		11
2		1	6			7

Table I-3 N = 8

No	Graph(G)	p(G;k)					Z
		k = 0	1	2	3	4	
A1		1	7	15	10	1	34
2		1	7	14	7		29
3		1	7	14	8	1	31
4		1	7	14	8		30
5		1	7	14	9	1	32
6		1	7	12	3		23
7		1	7	13	6		27
8		1	7	13	5		26
9		1	7	13	4		25
10		1	7	12	5		25
11		1	7	13	7	1	29
12		1	7	13	7		28
13		1	7	12	7	1	28
14		1	7	11	3		22
15		1	7	11			19
16		1	7	11	4		23

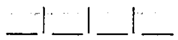
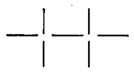
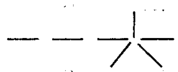
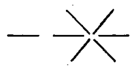
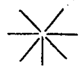
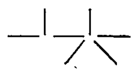
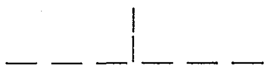
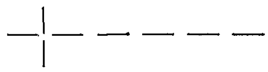
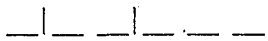
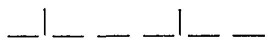
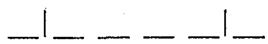
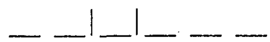
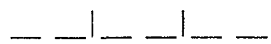
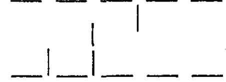
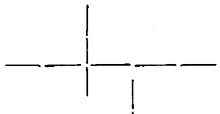
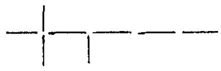
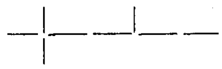
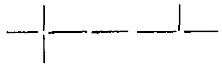
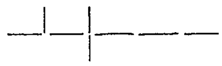
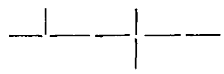
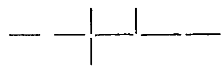
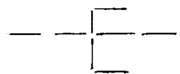
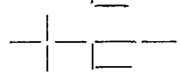
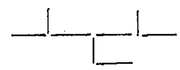
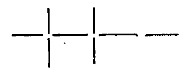
No	Graph(G)		p(G,k)				Z
		k = 0	1	2	3	4	
17		1	7	12	4		24
18		1	7	9			17
B1		1	7	9			17
2		1	7	9	3		20
3		1	7	5			13
4		1	7				8
5		1	7	8			16

Table I-4 N = 9

No	Graph(G)	p(G,k) k = 0	1	2	3	4	Z
A1		1	8	21	20	5	55
2		1	8	20	16	2	47
3		1	8	20	17	4	50
4		1	8	20	17	3	49
5		1	8	20	18	5	52
6		1	8	20	18	4	51
7		1	8	18	10		37
8		1	8	19	14	2	44
9		1	8	19	13		41
10		1	8	19	13	2	43
11		1	8	19	12		40
12		1	8	18	12	2	41
13		1	8	19	15	3	46
14		1	8	19	14	3	45
15		1	8	18	12		39
16		1	8	19	15	2	45

No	Graph(G)	p(G,k) k = 0	1	2	3	4	Z
17		1	8	19	14	2	44
18		1	8	18	14	3	44
19		1	8	19	16	4	48
20		1	8	17	9		35
21		1	8	17	7		33
22		1	8	17	6		32
23		1	8	17	10		36
24		1	8	18	12	2	41
25		1	8	18	10		37
26		1	8	17	8		34
27		1	8	17	11	2	39
28		1	8	18	16	5	48
29		1	8	17	10		36
30		1	8	17	12	2	40
31		1	8	18	12		39
32		1	8	15	6		30

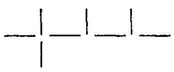
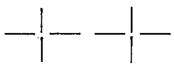
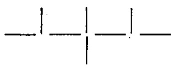
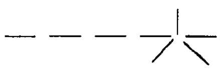
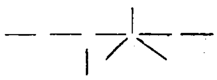
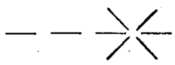
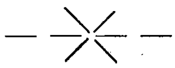
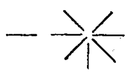
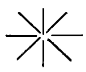
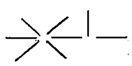
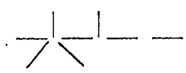
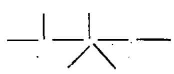
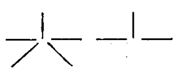
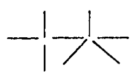
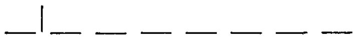
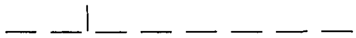
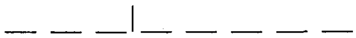
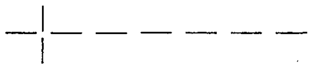
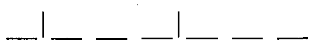
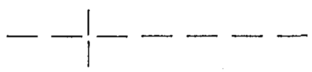
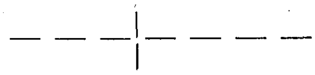
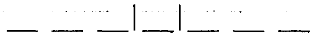
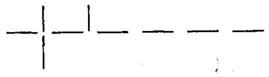
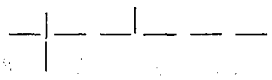
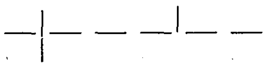
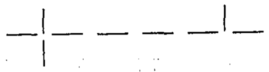
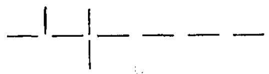
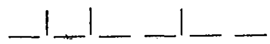
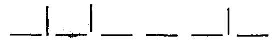
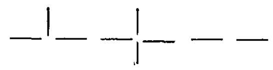
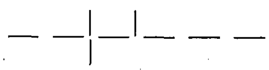
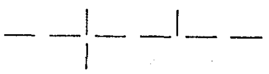
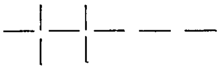
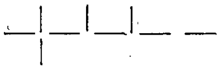
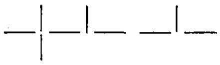
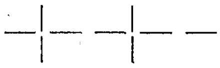
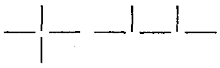
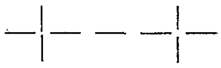
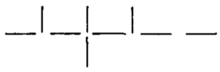
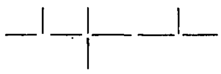
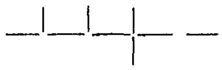
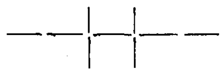
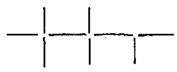
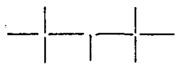
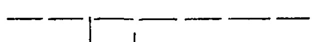
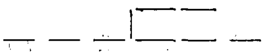
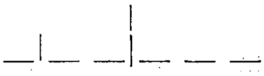
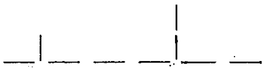
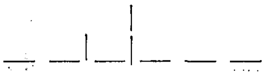
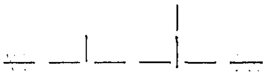
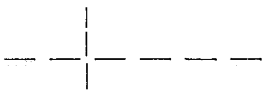
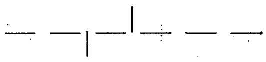
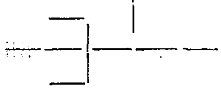
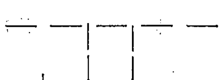
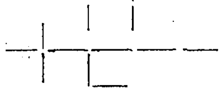
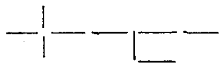
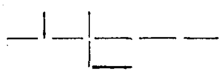
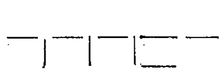
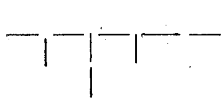
No	Graph(G)	p(G,k) k = 0	1	2	3	4	Z
33		1	8	16	6		31
34		1	8	15			24
35		1	8	16	8		33
B1		1	8	15	4		28
2		1	8	15	7		31
3		1	8	15	10	2	36
4		1	8	11			20
5		1	8	11	4		24
6		1	8	6			15
7		1	8				9
8		1	8	10			19
9		1	8	14	4		27
10		1	8	14	6		29
11		1	8	14			23
12		1	8	12			21

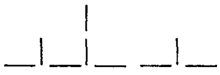
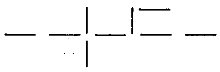
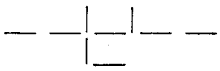
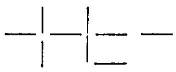
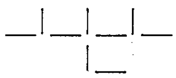
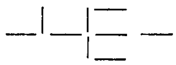
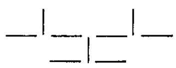
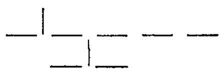
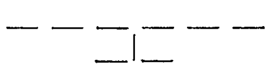
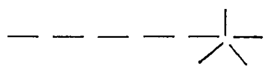
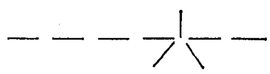
Table I-5 N = 10

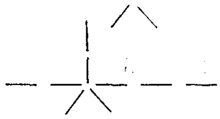
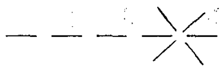
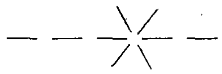
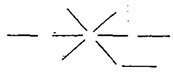
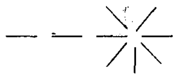
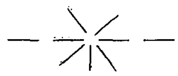
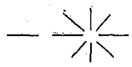
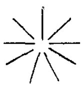
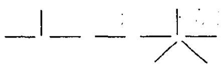
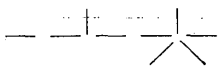
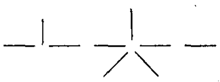
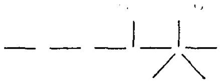
No	Graph(G)	k = 0	1	2	3	4	5	Z
		p(G,k)						
A1		1	9	28	35	15	1	89
2		1	9	27	30	9		76
3		1	9	27	31	12	1	81
4		1	9	27	31	11		79
5		1	9	27	31	11	1	80
6		1	9	25	22	3		60
7		1	9	26	27	8		71
8		1	9	26	26	5		67
9		1	9	26	26	6		68
10		1	9	26	26	7		69
11		1	9	26	25	4		65
12		1	9	25	24	7		66
13		1	9	26	28	10	1	75
14		1	9	26	27	8		71
15		1	9	26	27	10	1	74
16		1	9	25	24	5		64

No	Graph(G)	p(G,k) k = 0	1	2	3	4	5	Z
17		1	9	26	28	9		73
18		1	9	24	20	3		57
19		1	9	24	18			52
20		1	9	24	18	3		55
21		1	9	24	17			51
22		1	9	24	21	4		59
23		1	9	25	24	6		65
24		1	9	25	23	6		64
25		1	9	25	22	4		61
26		1	9	24	19			53
27		1	9	25	23	5		63
28		1	9	25	21			56
29		1	9	24	19	4		57
30		1	9	24	22	6		62
31		1	9	24	20	5		59
32		1	9	24	22	5		61

No	Graph(G)	p(G,k) k = 0	1	2	3	4	5	Z
33		1	9	25	25	9	1	70
34		1	9	22	15			47
35		1	9	23	17	3		53
36		1	9	23	15			48
37		1	9	22	11			43
38		1	9	23	14			47
39		1	9	22	9			41
40		1	9	23	19	4		56
41		1	9	23	16			49
42		1	9	23	18	4		55
43		1	9	24	20	4		58
44		1	9	22	17	4		53
45		1	9	21	12			43
46		1	9	21	9			40
47		1	9	27	32	14	1	84
48		1	9	27	32	13	1	83

No	Graph(G)	p(G,k) k = 0	1	2	3	4	5	Z
49		1	9	27	32	12		81
50		1	9	26	28	9		73
51		1	9	26	27	7		70
52		1	9	26	27	9		72
53		1	9	26	29	11	1	77
54		1	9	26	28	11	1	76
55		1	9	25	26	10	1	72
56		1	9	26	29	11		76
57		1	9	25	26	8		69
58		1	9	25	28	12	1	76
59		1	9	26	30	13	1	80
60		1	9	24	21	3		58
61		1	9	24	19	3		56
62		1	9	24	23	6		63
63		1	9	25	25	8		68
64		1	9	25	25	7		67

No	Graph(G)	p(G,k) k = 0	1	2	3	4	5	Z
65		1	9	25	23	4		62
66		1	9	24	21	5		60
67		1	9	24	23	7		64
68		1	9	24	24	9	1	68
69		1	9	22	17	3		52
70		1	9	23	20	4		57
71		1	9	24	25	9		68
72		1	9	23	17			50
73		1	9	24	20			54
74		1	9	25	24	4		63
75		1	9	26	28	8		72
B1		1	9	22	13			45
2		1	9	22	16	3		51

No	Graph(G)	p(G;k) k = 0	1	2	3	4	5	Z
3		1	9	22	16			48
4		1	9	22	19	5		56
5		1	9	22	22	9	1	64
6		1	9	18	5			33
7		1	9	18	9			37
8		1	9	18	13	3		44
9		1	9	13				23
10		1	9	13	5			28
11		1	9	7				17
12		1	9					10
13		1	9	21	8			39
14		1	9	21	9			40
15		1	9	21	11			42
16		1	9	21	12			43

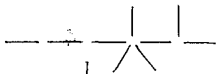
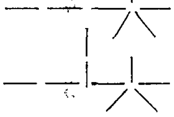
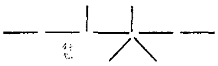
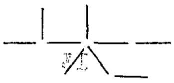
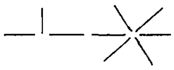
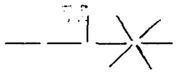
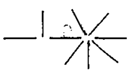
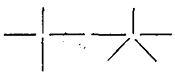
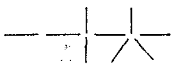
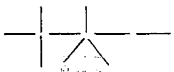
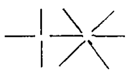
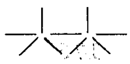
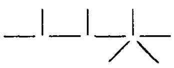
No	Graph(G)	p(G,k) k = 0	1	2	3	4	5	Z
17		1	9	21	14			45
18		1	9	21	13			44
19		1	9	21	15	3		49
20		1	9	21	17	4		52
21		1	9	17				27
22		1	9	17	5			32
23		1	9	17	8			35
24		1	9	12				22
25		1	9	19				29
26		1	9	19	8			37
27		1	9	19	9			38
28		1	9	15				25
29		1	9	16				26
30		1	9	20	8			38
31		1	9	20	12			42

Table II

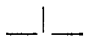
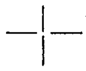
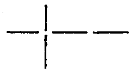
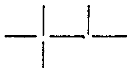
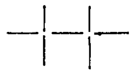
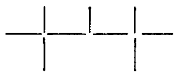
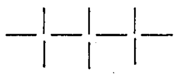
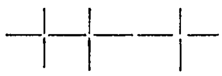
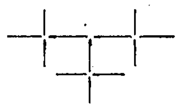
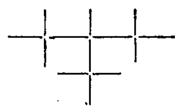
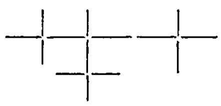
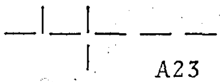
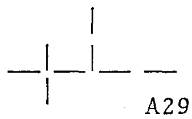
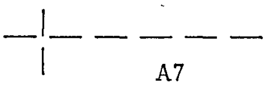
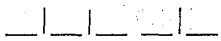
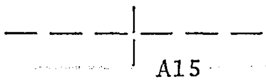
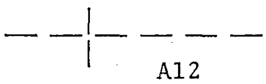
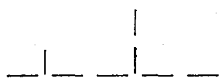
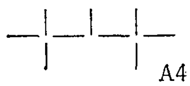
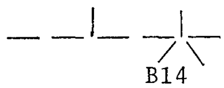
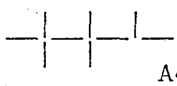
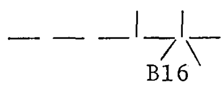
N	Graph(G)	Z_G
4		4
5		5
6		9
7		13
8		17
9		24
10		40
11		56
12		81
13		112
14		176
15		264

Table III

N	Graph(G)		Z_G
9	 A23	 A29	36
	 A7	 A25	37
	 A15	 A31	39
	 A12	 A24	41
	 A8	 A17	44
10	 A46	 B14	40
	 A45	 B16	43
	 A7	 A14	71
	 A17	 A50	73

APPENDIX

CALCULATION OF P(G,k)