

TOPOLOGICAL INDEX AND FIBONACCI NUMBERS WITH RELATION TO CHEMISTRY

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INTRODUCTION

This paper deals with the discussion on the graphical aspects of the Fibonacci numbers through the topological index [1] which has been defined by the present author for non-directed graphs.¹

A graph G consists of points (vertices or atoms) and lines (edges or bounds) [2, 3]. We are concerned with such connected non-directed graphs that have no loop (a line joining to itself) and no multiple lines (double or triple bonds). An adjacency matrix A for graph G with N points is a square matrix for the order N with elements

$$(1) \quad a_{ij} = \begin{cases} 1 & \text{if the points } i \text{ and } j \text{ are neighbors,} \\ 0 & \text{otherwise.} \end{cases}$$

The matrix character is independent of the way of the numbering of the points. A characteristic polynomial or a secular polynomial $P(X)$ is defined as²

$$(2) \quad P(X) = \det |A + XE| = \sum_{i=0}^N b_i X^{N-i},$$

where E is a unit matrix of the order N and X is a scalar variable.

Consider a series of path progressions $\{S_N\}$, for which $P(X)$ can be expressed as (see [4])

$$(3) \quad P(X) = \sum_{k=0}^m (-1)^k \binom{N-k}{k} X^{N-2k},$$

where N is the number of points and m is $[N/2]$. Examples are shown in Table 1 on the following page.

¹Originally this idea came out quite independently from other works especially published in mathematical journals. However, thanks to the communications from the colleagues in this field, several important papers were found to be relevant to this problem. In this paper the relevant papers will be cited as many as possible.

²Alternative definition

$$(2') \quad P(X) = (-1)^N \det |A - XE|$$

can be chosen, which, however, makes no difference in the following discussion.

Table 1

N	G(S _N)	$\binom{N-k}{k} = p(G, k)$					$\sum_{k=0}^m p(G, k) = Z = f_N$
		k = 0	1	2	3	4	
1	●	1					1
2	—	1	1				2
3	— —	1	2				3
4	— — —	1	3	1			5
5	— — — —	1	4	3			8
6	— — — — —	1	5	6	1		13
7	— — — — — —	1	6	10	4		21
8	— — — — — — —	1	7	15	10	1	34

On the other hand, from the combinatorial theory we know the following relation under the name of Lucas (see [5, 6]).

$$(4) \quad f_N = \sum_{k=0}^m \binom{N-k}{k},$$

where f_N is the N^{th} Fibonacci number, which is defined as

$$(5) \quad \begin{aligned} f_0 &= f_1 = 1, * \\ f_N &= f_{N-1} + f_{N-2} \quad (N = 2, 3, \dots) . \end{aligned}$$

The sums of the absolute values of the coefficients of the characteristic polynomial for the graph $\{S_N\}$ form the Fibonacci series. This is not new. Turn Table 1 counter-clockwise by 45 degrees, and we get the Pascal's triangle or the pyramid of binomial coefficients, from which the Fibonacci numbers can be obtained by adding the coefficients diagonally (just the reverse of the above procedure!). (See [7].)

Let us consider the physical meaning of the combination $\binom{N-k}{k}$. Consider a group of $N - k$ points which are linearly arranged as in Fig. 1a. Choose an arbitrary set of k points (black circles), place k additional points (crosses) one-by-one below them, and join all the N points together by drawing consecutive $N - 1$ lines as in Fig. 1b to get a path progression with N points, or $N - 1$ lines. This means that the value $\binom{N-k}{k}$ is the number of ways in which k disconnected lines (vertical lines in Fig. 1b) are chosen from graph S_N .

*Alternative definition can be used as $f_1 = f_2 = 1$.

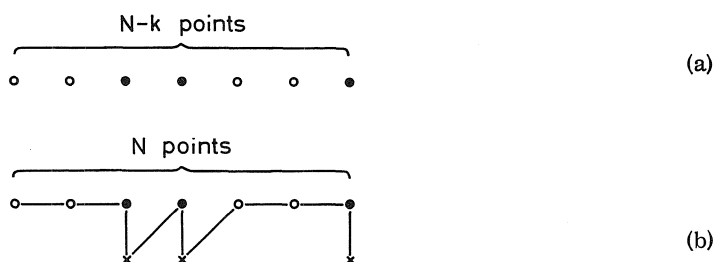


Fig. 1 Physical Meaning of $\binom{N-k}{k}$

TOPOLOGICAL INDEX [1]

Encouraged by the simple relation above, let us develop a more general theory. Define a non-adjacent number $p(G, k)$ for graph G as the number of ways in which k disconnected lines are chosen from G . A Z -counting polynomial $Q(Y)$ and a topological index Z are defined respectively as

$$(6) \quad Q(Y) = \sum_{k=0}^m p(G, k) Y^k$$

and

$$(7) \quad Z = \sum_{k=0}^m p(G, k) = Q(1) \quad . \quad (\text{See [1].})$$

Note that for the series of path progressions $\{S_N\}$ in Table 1, the $p(G, k)$ number is nothing else but $\binom{N-k}{k}$, namely, the absolute value of the coefficients of the X^{N-2k} term in the characteristic polynomial $P(X)$. Thus we get

$$(8) \quad Z_{S_N} = f_N$$

or for brevity




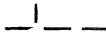
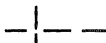
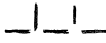
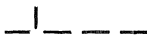
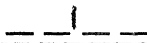
$$(8') \quad S_N = f_N \quad .$$

Further, for any tree graph with or without branches but with no cycles, the following relation can be proved by term-to-term inspection of the expansion of $\det |A + XE|$ into $P(X)$:

$$(9) \quad P(X) = \sum_{k=0}^m (-1)^k p(G, k) X^{N-2k} \quad (G \in \text{Tree}) \quad .$$

Examples are shown in Table 2. More comprehensive tables of $p(G, k)$ and Z numbers have been published for smaller tree [8] and non-tree [9] graphs. For non-tree graphs, Eq. (9) no longer holds but $P(X)$ can be expressed as the sums of the contributions like the right-

Table 2

G	p(G,k)				Z
	k = 0	1	2	3	
	1	3			4
	1	4			5
	1	5			6
	1	4	2		7
	1	5	3		9
	1	5	4		10
	1	5	5		11
	1	5	5	1	12

hand side of Eq. (9) of subgraphs of G . (See [10, 11].) As well as the characteristic polynomial [12, 13] the topological index does not uniquely determine the topology of a graph. However, it is generally observed that the Z value gets smaller with branching and larger with cyclization. Thus for a group of graphs with the same number of points, Z roughly represents the topological nature of the graph. For evaluating the Z values of larger and complicated graphs, the following composition principles are useful. They can be proved by the aid of $Q(Y)$. (See [1, 10].)

COMPOSITION PRINCIPLES (CP)

Composition Principle 1 (CP1). (See [1].) Consider a graph G in Fig. 2a and choose from it a line ℓ , (1) Delete line ℓ and we get subgraphs L and M . (2) Delete all the lines in L and M that were incident to ℓ and we get subgraphs A, B, \dots, F . Then the topological index Z for G can be obtained as

$$(10) \quad G = L \times M + A \times B \times C \times D \times E \times F.$$

For applying this principle there is no restriction in the number of subgraphs incident to the chosen line ℓ , since the Z values of a point graph (S_1) and a vacant graph (S_0) are both unity,

$$(11) \quad S_0 = S_1 = 1.$$

Application of CP1 to the terminal line of graph S_N gives the recursion formula

$$(12) \quad S_N = S_{N-1} + S_{N-2}.$$

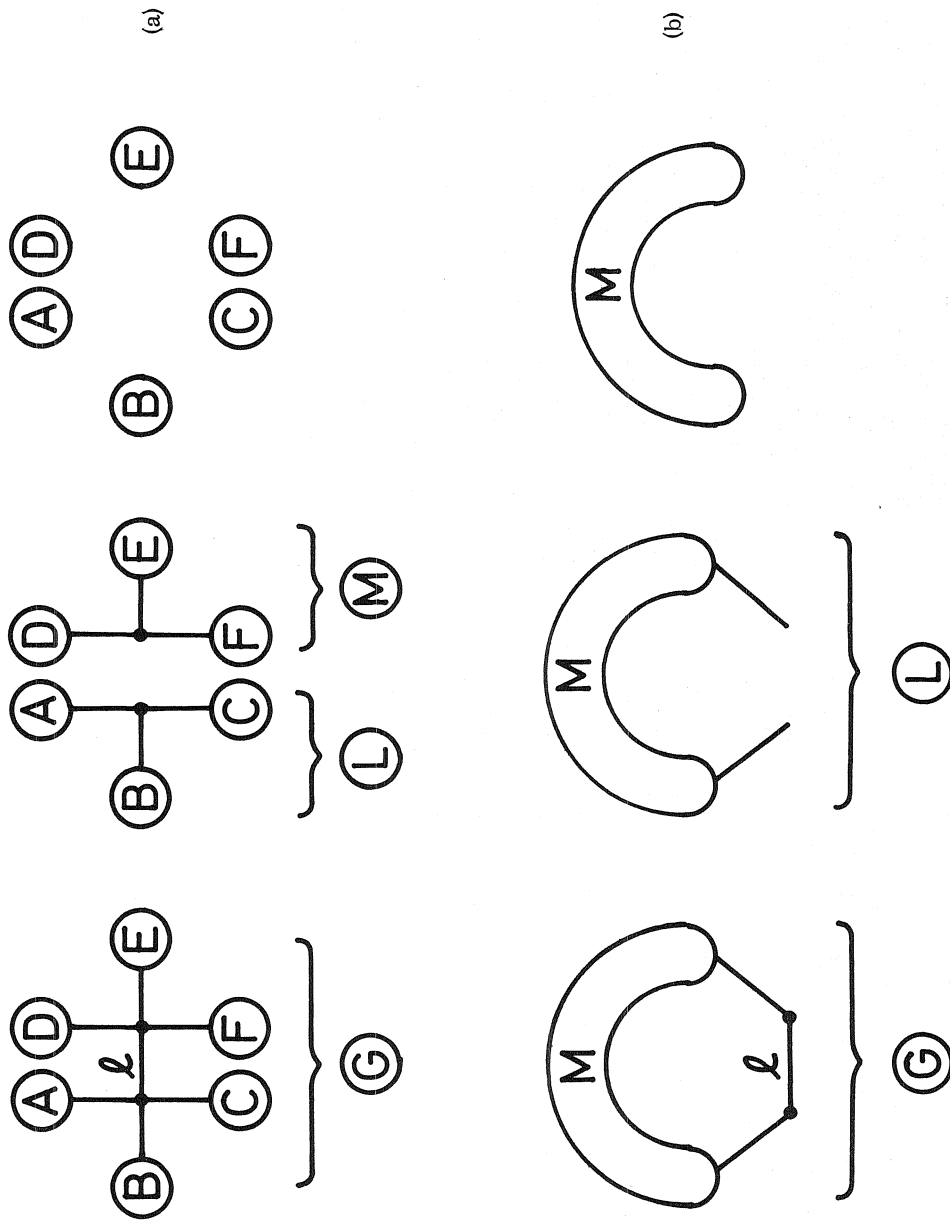


Fig. 2 Composition Principle 1

Comparison of Eqs. (11) and (12) with Eq. (5) yields Eq. (8).

For graph S_N with even $N (= 2n)$ we get the relation

$$(13) \quad S_{2n} = S_n^2 + S_{n-1}^2$$

by choosing the central line as ℓ . This is the graphical equivalent of the relation for the Fibonacci numbers [5-7]

$$(14) \quad f_{2n} = f_n^2 + f_{n-1}^2 .$$

Similarly, we get

$$(15) \quad S_{2n+1} = S_n(S_{n+1} + S_{n-1})$$

or

$$(16) \quad f_{2n+1} = f_n(f_{n+1} + f_{n-1}) .$$

Corollary to CP1. If the line to be deleted is a member of a cycle, the deletion gives only one subgraph L as in Fig. 2b. In this case, we have

$$(17) \quad G = L + M .$$

By use of this corollary the Z values for the series of N -membered cycles (N -gon, abbreviated as C_N) are obtained as in Table 3. It is apparent from Eq. (17) that

$$(18) \quad C_N = S_N + S_{N-2}$$

and the series of these Z values form what are known as the Lucas sequences $\{g_N\}$; namely, (see [5])

$$(19) \quad \begin{aligned} C_N &= g_N \\ g_1 &= 1, \quad g_2 = 3 \\ g_N &= g_{N-1} + g_{N-2} . \end{aligned}$$









Then Eq. (18) is equivalent to the relation

$$(20) \quad g_N = f_N + f_{N-2} .$$

From the correspondence relation of Eq. (19), a monogon and a digon may be defined, respectively, as a point graph $C_1 (= S_1)$ and a graph C_2 with two points joined by two lines (see Table 3).*

*By extending this definition a topological index for a graph with multiple bonds can be defined.

Table 3

N	$G(C_N)$	k = 0	p(G, k)				Z
			1	2	3	4	
1		1					1
2		1	2				3
3		1	3				4
4		1	4	2			7
5		1	5	5			11
6		1	6	9	2		18
7		1	7	14	7		29
8		1	8	20	16	2	47

Composition Principle 2 (CP2). (See [8].) Consider a graph G in Fig. 3 and choose from it a point p . The number of the lines incident to point p should be at least two but not necessarily be six as in this example. (1) Divide them into two groups. In this case, we chose the division as (a, b, c) and (d, e, f) . (2) Delete a group of lines a, b and c in G , and we get subgraphs A, B, C and M . (3) Delete another group of lines d, e and f in G , and we get subgraphs D, E, F and L . (4) Delete both of the groups of lines a, b, \dots, f in G , and we get subgraphs A, B, \dots, F . With these subgraphs we have

$$(21) \quad G = A \times B \times C \times M + D \times E \times F \times L - A \times B \times C \times D \times E \times F.$$

Composition Principle 3 (CP3). Further consider a graph G in Fig. 4a in which two subgraphs A and B are joined by path progression S_3 , i. e., three consecutive lines. (1) Delete a line from S_3 and rejoin the two resultant subgraphs to get L . (2) Delete one more line from S_2 in L and rejoin the subgraphs to get M . The Z value for G is given by (see Fig. 4)

$$(22) \quad G = L + M.$$

This is also applied to the case in which A and B are joined with two paths to form a cycle to give the relation (19) (Fig. 4b).

RECURSIVE SEQUENCES

A recursive sequence $\{a_N\}$ is defined as

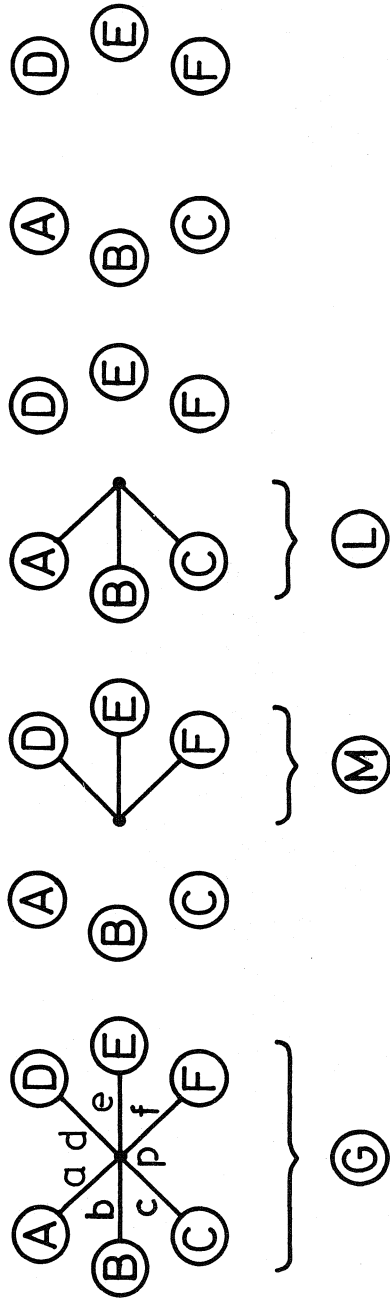


Fig. 3 Composition Principle 2

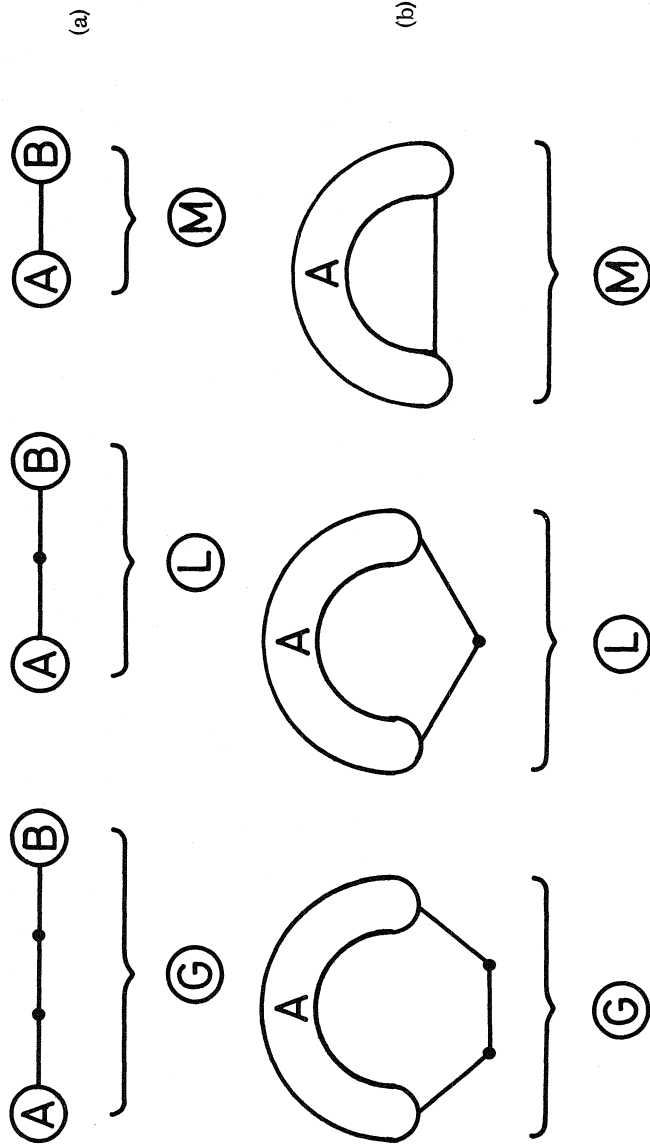


Fig. 4 Composition Principle 3

$$(23) \quad a_N = \sum_{i=1}^k C_i a_{N-i} .$$

Both of the Fibonacci and Lucas sequences are the special cases with $C_1 = C_2 = 1$, $C_i = 0$ ($i > 2$) but with different initial conditions. One can find a number of graphical series whose topological indices form recursive sequences as in Fig. 5. They can be proved by the composition principles. More interesting graphical sequences might be discovered through the topological index.

The most important point in this discussion is that a number of relations in the recursive sequences can be inspected and proved by applying the composition principles to the graphical equivalent of the sequences.

APPLICATION TO CHEMISTRY

Let us confine ourselves to a class of chemical compounds, saturated hydrocarbons, whose topological structure is expressed as a structural formula. An example is shown in Fig. 6 for 2-methylbutane (a). Since carbon (C) and hydrogen (H) atoms, respectively, have tetra- and mono-valencies, for describing the whole structure only the carbon atom skeleton (b) is sufficient, which is equivalent to graph (c). The series of graphs in Table 1 are read in chemical language as methane, ethane, propane, butane, etc. They form a family of normal paraffins. Thus the topological indices of normal paraffins are shown to form the Fibonacci sequences. Table 3 indicates that the topological indices of cycloparaffins (cyclopropane . . .) form the Lucas sequences.

As was discussed earlier the topological index does not uniquely determine the topology of the molecular structure. For example, normal butane (the 4th entry in Table 1) and neopentane (the 2nd entry in Table 2) both have $Z = 5$. However, it was shown that the topological index can be used as a rough sorting device for coding the complicated structures of chemical compounds [14].

It was also shown that the topological index of a saturated hydrocarbon is correlated well with some of the thermodynamic quantities such as boiling point through its entropy, which is a measure of the degree of freedom in internal rotations of a flexible molecule [15].

Characteristic polynomials appear in the application of quantum mechanics to the study of the electronic structure of molecules. The simplest method is the Hückel molecular orbital method, in which the problem is reduced to obtaining the solution of a secular equation $P(X) = 0$ (see [10, 16, 17]).

SYNOPSIS

Define a topological index Z as the sum of the non-adjacent number, $p(G,k)$, which is the number of ways in which such k disconnected lines are chosen from graph G . The Z values for the path progressions $\{S_N\}$ form the Fibonacci sequences, while those for the

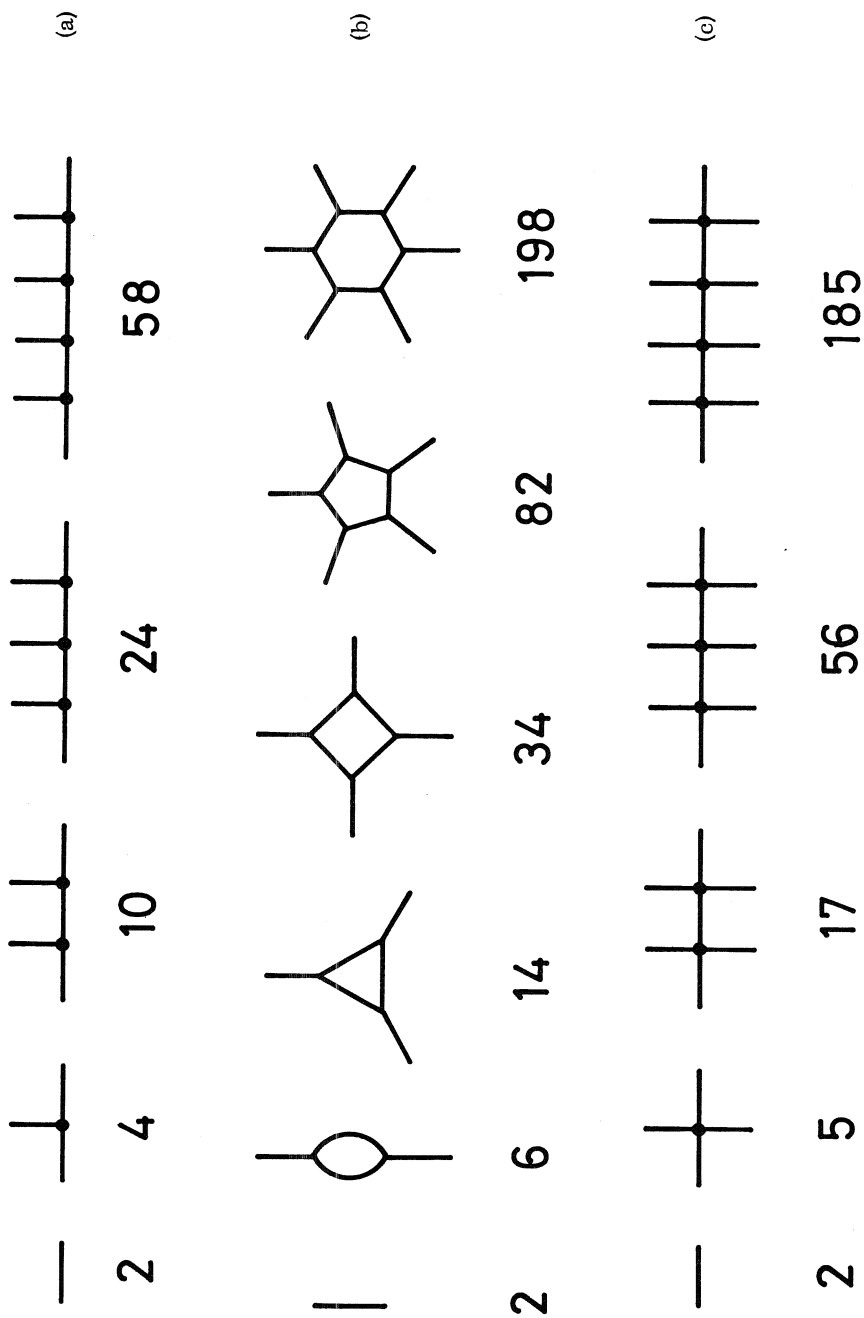


Fig. 5 Examples of Graphical Equivalent of Recursive Sequences
 $a_N = 2a_{N-1} + a_{N-2}$ for (a) and (b) and $a_N = 3a_{N-1} + a_{N-2}$ for (c).

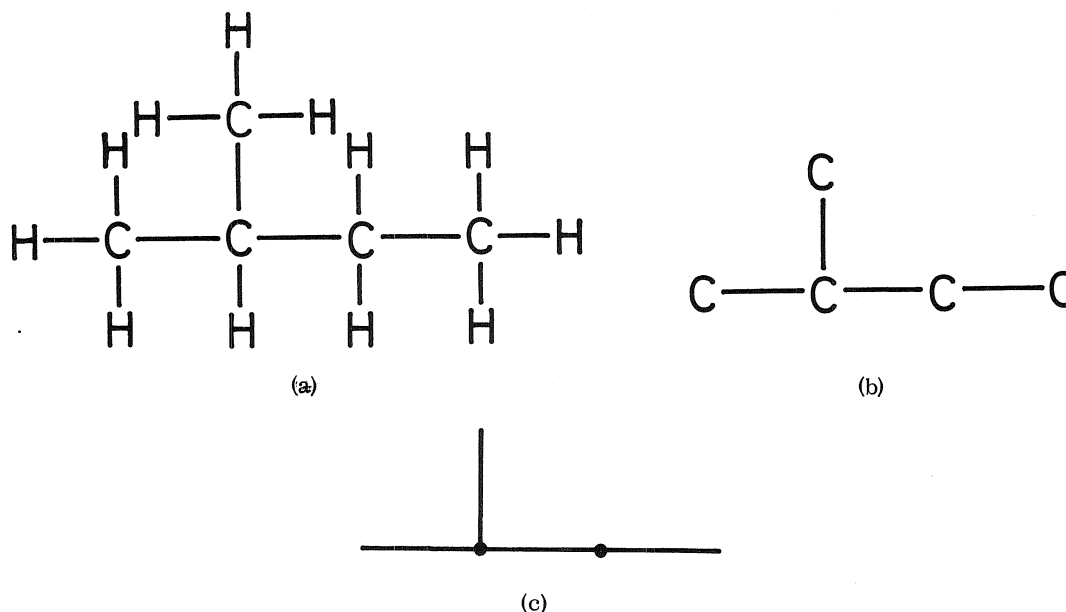


Fig. 6 Structure and Graph of 2-methylbutane

series of cycles $\{C_N\}$ the Lucas sequences. Many relations for them can be proved by the aid of the composition principles for Z . Application of Z to chemistry is discussed.

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BOOK REVIEW: I CHING GAMES

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I Ching Games of Duke Tan of Chou and C. C. T'ung, by H. Y. Li and Sibley S. Morrill, The Cadleon Press, P. O. Box 24, San Francisco, California 94101: 1971. 138 pages plus game pieces. \$5.95.

The I Ching Games, whose names translate as "The Wisdom Plan" and "The Beneficial to Wisdom Plan," are considered among the most important ever written, since they are thought to improve the player's ability to learn while advancing his psychological development. The first game is also called the Tangram, being a seven-piece dissection of a square into a smaller square, five isosceles right triangles, and a parallelogram, which can be re-assembled into an infinite variety of recognizable pictures. The 15-game is a dissection of a square to also include the circle, and the problems become jigsaw puzzles of a thousand delights.

The authors, as well as hoping to re-introduce the Tangram game and introduce the 15-game to the West for the first time, give a history of the games and describe their relationship to the I Ching, the ancient Chinese Book of Change, the oldest book now known.

