

Research Article

The General $(\alpha, 3)$ -Path Connectivity Indices of Polycyclic Aromatic Hydrocarbons

Haiying Wang  and Chuantao Li

School of Science, China University of Geosciences (Beijing), Beijing, 100083, China

Correspondence should be addressed to Haiying Wang; whycht@126.com

Received 15 June 2018; Accepted 26 August 2018; Published 5 September 2018

Academic Editor: Luisa Di Paola

Copyright © 2018 Haiying Wang and Chuantao Li. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

The general (α, t) -path connectivity index of a molecular graph originates from many practical problems such as three-dimensional quantitative structure-activity (3D QSAR) and molecular chirality. It is defined as ${}^tR_\alpha(G) = \sum_{P^t=v_{i_1}v_{i_2}\cdots v_{i_{t+1}} \in G} [d(v_{i_1})d(v_{i_2})\cdots d(v_{i_{t+1}})]^\alpha$, where the summation is taken over all possible paths of length t of G and we do not distinguish between the paths $v_{i_1}v_{i_2}\cdots v_{i_{t+1}}$ and $v_{i_{t+1}}\cdots v_{i_2}v_{i_1}$. In this paper, we focus on the structures of Polycyclic Aromatic Hydrocarbons (PAH_n), which play a role in organic materials and medical sciences. We try to compute the exact general $(\alpha, 3)$ -path connectivity indices of this family of hydrocarbon structures. Furthermore, we exactly derive the monotonicity and the extremal values of ${}^3R_\alpha(PAH_n)$ for any real number α . These valuable results could produce strong guiding significance to these applied sciences.

1. Introduction

1.1. Application Background. In many fields like physics, chemistry, and electric network, the boiling point, the melting point, the chemical bonds, and the bond energy are all important quantifiable parameters in their fields.

To understand physicochemical properties of chemical compounds or network structures, we abstractly define different concepts, collectively named *topological descriptors* or *topological indices* after mathematical modelings. We called them different names such as Randić index and Zagreb index. Different index represents its corresponding chemical structures in graph-theoretical terms via arbitrary molecular graph. A large number of articles about related all *topological indices* are proposed and based on edges or vertices in molecular graph [1–3].

In the last decades, as a powerful approach, these two-dimensional topological indices have been used to discover many new drugs such as Anticonvulsants, Anineoplastics, Antimalarials or Antiallergics, and Silico generation ([4–8]). Therefore, the practice has proven that the topological indices and quantitative structure-activity relationships (QSAR) have

moved from an attractive possibility to representing a foundation stone in the process of drug discovery and other research areas ([9–12]).

Most importantly, with the further study of chemical indices and drug design and discovery, three-dimensional molecular features (topographic indices) and molecular chirality are also presented. It is more and more urgent to study the three-dimensional quantitative structure-activity (3D QSAR) such as molecular chirality. Actually, so far there have been few results expect that one related definition which is generally mentioned in [7].

1.2. Notations. Throughout this paper, we always let $G = (V(G), E(G))$ be a simple molecular graph with the vertex set $V(G)$ and the edge set $E(G)$. Denote the numbers of vertices and edges by $|V(G)|$ and $|E(G)|$ respectively. In physicochemical graph theory, the vertices and the edges correspond to the atoms and the bonds, respectively. Two vertices u and v are *adjacent* if there exists an edge $e = uv$ between them in G . The number of its adjacent vertices is called *degree* of u , denoted by $d_G(u)$ or $d(u)$. The set of all of neighbors of u is denoted by $N_G(u)$ or $N(u)$. Specially, a vertex

in G is called *pendant* if its degree is one. All other notations and terminologies are referred to [13].

With the intention of extending the applicability of the general Randić index, L.B.Kier, L.H.Hall, E. Estrada, and coworkers considered *the general (α, t) -path connectivity index* of G as

$${}^t R_\alpha(G) = \sum_{P^t = v_{i_1} v_{i_2} \cdots v_{i_{t+1}} \subseteq G} [d(v_{i_1}) d(v_{i_2}) \cdots d(v_{i_{t+1}})]^\alpha, \quad (1)$$

where the summation is taken over all possible paths of length t of G and we do not distinguish between two paths $v_{i_1} v_{i_2} \cdots v_{i_{t+1}}$ and $v_{i_{t+1}} \cdots v_{i_2} v_{i_1}$ ([4, 5]).

According to the definition above, it is clear that the general (α, t) -path connectivity index of a graph is a real number and an important invariant under graph automorphism. It is closely related to the structures of a molecular graph. For any molecular material, only by mastering its structure can we calculate its exact value of the general (α, t) -path connectivity index.

In this paper, we focus on the structures of Polycyclic Aromatic Hydrocarbons, for short PAH_n , which play a role in organic materials and medical science. Then we try to compute the general $(\alpha, 3)$ -path connectivity indices of this family of hydrocarbon structures. Furthermore, we exactly derive the monotonicity and the extremal values of ${}^3 R_\alpha(PAH_n)$ for any real number α . The valuable results could produce strong guiding significance to these applied sciences.

For convenience, it is necessary to simplify some basic concepts and notations in PAH_n . An i -vertex denotes a vertex with degree i , and a (j, k) -edge stands for an edge connecting a j -vertex with a k -vertex. Let m_{jk} denote the number of (j, k) -edge.

Let $v_{i_0} v_{i_1} \cdots v_{i_t}$ be a path P^t of length t in PAH_n , that is, $P^t = v_{i_0} v_{i_1} \cdots v_{i_t}$. And $(d(v_{i_0}), d(v_{i_1}), \dots, d(v_{i_t}))$ is called its degree sequence. Then it is obvious that there are all three types $(1, 3, 3, 1)$, $(1, 3, 3, 3)$, and $(3, 3, 3, 3)$ of degree sequences of 3-paths in PAH_n . Let m_{1331} , m_{1333} , and m_{3333} denote the numbers of the 3-paths of the degree sequence types $(1, 3, 3, 1)$ and $(1, 3, 3, 3)$ and $(3, 3, 3, 3)$ in PAH_n , respectively.

2. Polycyclic Aromatic Hydrocarbons (PAH_n)

Large Polycyclic Aromatic Hydrocarbons are ubiquitous combustion products and belong to more important hydrocarbon molecules. They have been implicated as carcinogens and play a role in organic materials and medical science [14].

As we known, Polycyclic Aromatic Hydrocarbons have great significance as molecular analogues of graphite as candidates for interstellar species and as building blocks of functional materials for device applications. In addition, synthetic routes to Polycyclic Aromatic Hydrocarbons are available. Therefore, much detailed knowledge of all molecular features would be necessary for the tuning of molecular properties towards specific applications.

Polycyclic Aromatic Hydrocarbons can be regarded as graphene sheets composed of free radicals of saturated suspended bonds and vice versa; graphene sheets can be interpreted as an infinite number of PAH molecules. The

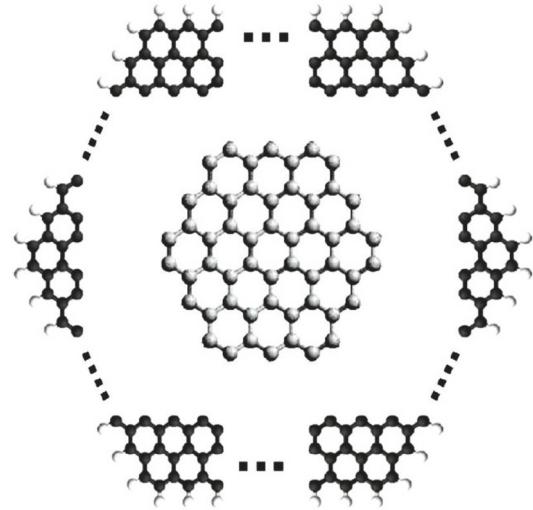


FIGURE 1: The general representation of Polycyclic Aromatic Hydrocarbon.

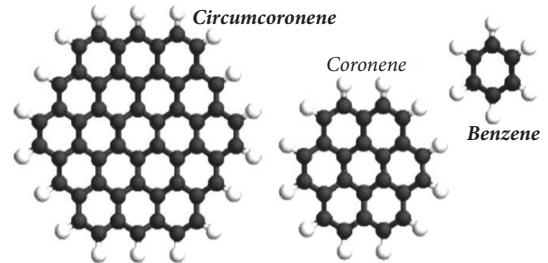


FIGURE 2: The first three graphs of Polycyclic Aromatic Hydrocarbon.

successful application of Polycyclic Aromatic Hydrocarbons in modeling of graphite surface has been reported and references have been provided. The family of Polycyclic Aromatic Hydrocarbons have similar properties with Benzenoid system (Circumcoronene Homologous Series of Benzenoid) ([9–12]). Thus, molecular structures of Polycyclic Aromatic Hydrocarbons play a key role in particular.

For any positive integer n , let PAH_n be the general representation of this Polycyclic Aromatic Hydrocarbon shown in Figure 1. To understand more structures of PAH_n , the first three members of this hydrocarbon family are given in Figure 2, where PAH_1 is called Benzene with 6 carbon atoms (C) and 6 hydrogen (H) atoms, PAH_2 the Coronene with 24 carbon atoms and 12 hydrogen atoms, PAH_3 Circumcoronene with 54 carbon atoms, and 18 hydrogen atoms.

From Figure 1, there are $6n^2$ carbon atoms and $6n$ hydrogen atoms in PAH_n , denoted $N(H) = 6n$ and $N(C) = 6n^2$, respectively. Thus, this molecular graph has $6n^2 + 6n$ atoms (or vertices); satisfying the degrees of each hydrogen atom is 1 and each carbon atom is 3. That is, $|V(PAH_n)| = 6n^2 + 6n$ and $|E(PAH_n)| = (3 \times 6n^2 + 1 \times 6n)/2 = 9n^2 + 3n$.

In Figure 1, each hydrogen atom has just one edge/bond between only one carbon atom and any carbon atom just has three bonds with carbon atoms or hydrogen atom. The

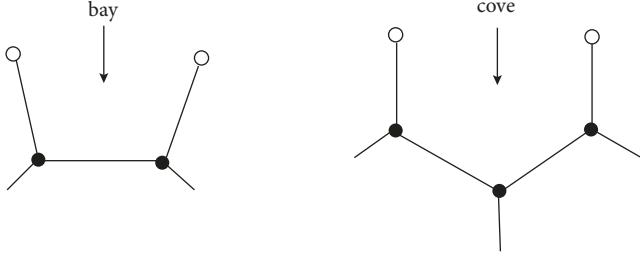


FIGURE 3: Structure of a bay and a cove.

edge/bond set of Polycyclic Aromatic Hydrocarbon can be divided into two partitions, $(1, 3)$ -edge set and $(3, 3)$ -edge set. Thus

$$m_{13} = N(H) = 6n, \quad (2)$$

and

$$m_{33} = |E(PAH_n)| - N(H) = 9n^2 - 3n. \quad (3)$$

If one goes along the perimeter of Polycyclic Aromatic Hydrocarbon System, then there are only two types of structures, which are named *bays* and *coves*, respectively. A *bay* is a structural feature formed by a 1-vertex (hydrogen atom), followed by two consecutive 3-vertices (carbon atoms) and then followed by a 1-vertex (hydrogen atom). A *cove* is a structural feature formed by a 1-vertex (hydrogen atom), followed by three consecutive 3-vertices (carbon atoms) and then followed by a 1-vertex (hydrogen atom). See Figure 3.

A 1-vertex (hydrogen atom) is *proper* if it just belong to coves, not on any bay. Denote the numbers of its bays, coves and proper 1-vertices by $N(\text{bays})$, $N(\text{coves})$, and $N(\text{proper 1-vertices})$, respectively. According to the structures of PAH_n with $n \geq 2$, we have

$$N(\text{bays}) = 6 \quad (4)$$

$$N(\text{coves}) = 6(n-1) \quad (4)$$

and

$$\begin{aligned} N(\text{proper 1-vertices}) &= N(H) - 2N(\text{bays}) \\ &= (6n) - 2 \cdot 6 = 6(n-2). \end{aligned} \quad (5)$$

3. Main Results on the Value ${}^3R_\alpha(PAH_n)$

Let PAH_n be the general representation of Polycyclic Aromatic Hydrocarbons molecules for any positive integer n (see Figure 1). Let $P^3 = v_{i_0}v_{i_1}v_{i_2}v_{i_3}$ be any 3-path in which e_1, e_2 , and e_3 are the edges of this 3-path and $v_{i_0}v_{i_1} = e_1$, $v_{i_1}v_{i_2} = e_2$, and $v_{i_2}v_{i_3} = e_3$. And we call e_2 the midedge of this 3-path.

In this section, we compute the general $(\alpha, 3)$ -path connectivity indices of a family of Polycyclic Aromatic Hydrocarbons. The indices should reflect directly the material natural properties.

Theorem 1. For any real number α and positive integer $n \geq 1$, the general $(\alpha, 3)$ -path connectivity indices of PAH_n are equal to

$$\begin{aligned} {}^3R_\alpha(PAH_n) &= 2 \cdot 3^{2\alpha+1} \cdot [2 \cdot 3^{2\alpha+1} \cdot n^2 + 2 \cdot 3^\alpha \\ &\quad \cdot (2 - 3^{\alpha+1}) \cdot n + (1 - 2 \cdot 3^\alpha + 3^{2\alpha})]. \end{aligned} \quad (6)$$

Proof. In Polycyclic Aromatic Hydrocarbon PAH_n with $n \geq 1$, there are all three types of 3-paths in which degree sequences are $(1, 3, 3, 1)$ $(1, 3, 3, 3)$ and $(3, 3, 3, 3)$, respectively. Assume that $P^3 = v_{i_0}v_{i_1}v_{i_2}v_{i_3}$ is an arbitrary 3-path in which degree sequence is $(d(v_{i_0}), d(v_{i_1}), d(v_{i_2}), d(v_{i_3}))$. Denote $v_{i_0}v_{i_1} = e_1$, $v_{i_1}v_{i_2} = e_2$ and $v_{i_2}v_{i_3} = e_3$, where e_2 is its midedge. It is clear that e_2 is not $(1, 3)$ -edge.

(1) $n = 1$. By the structures of Benzene (see Figure 2), it is easy to obtain

$$\begin{aligned} m_{1331} &= 6; \\ m_{1333} &= 2 \cdot N(H) = 12; \\ m_{3333} &= 6. \end{aligned} \quad (7)$$

Thus

$$\begin{aligned} {}^3R_\alpha(PAH_1) &= \sum_{P^3=v_{i_1}v_{i_2}v_{i_3}v_{i_4} \subseteq PAH_1} [d(v_{i_1})d(v_{i_2})d(v_{i_3})d(v_{i_4})]^\alpha \\ &= m_{1331} \cdot (1 \times 3 \times 3 \times 1)^\alpha + m_{1333} \cdot (1 \times 3 \times 3 \times 3)^\alpha \\ &\quad + m_{3333} \cdot (3 \times 3 \times 3 \times 3)^\alpha \\ &= 6 \cdot (3)^{2\alpha} + 12 \cdot (3)^{3\alpha} + 6 \cdot (3)^{4\alpha} \\ &= 2 \cdot 3^{2\alpha+1} \cdot [1 + 2 \cdot 3^\alpha + 3^{2\alpha}]. \end{aligned} \quad (8)$$

(2) $n \geq 2$. First, we compute the total number of distinct 3-paths in PAH_n . For any e_2 , which is $(3, 3)$ -edge and not $(1, 3)$ -edge, there exist four distinct 3-paths in which midedges are the same e_2 but other parts are different $(3, 3)$ -edges. Only when e_2 traverses all $(3, 3)$ -edge one time in PAH_n , will it produce all distinct 3-paths in PAH_n since any 3-paths with distinct midedges will be different. Then

$$\begin{aligned} N(P^3) &= 4m_{33} = 4 \cdot [|E(PAH_n)| - N(H)] \\ &= 4 \cdot [(9n^2 + 3n) - 6 \cdot n] = 12n(3n-1). \end{aligned} \quad (9)$$

Second, we consider m_{1331} . According to the structure of Polycyclic Aromatic Hydrocarbon PAH_n , only bays can produce 3-paths of the type $(1, 3, 3, 1)$. And one produces one 3-path of this type. Thus,

$$m_{1331} = N(\text{bays}) = 6. \quad (10)$$

Consider m_{1333} . It is clear that each 1-vertex (hydrogen atom) can produce different 3-paths of the type $(1, 3, 3, 3)$.

(i) For any improper 1-vertex H which belongs to some bay, it can produce three 3-paths of the type $(1, 3, 3, 3)$. Since

each bay has two different 1-vertices (hydrogen atoms), each bay goes with all six 3-paths of the type $(1, 3, 3, 3)$. Thus, all improper vertices (hydrogen atoms) produce a total of thirty-six 3-paths of the type $(1, 3, 3, 3)$.

(ii) For any proper 1-vertex (hydrogen atom), it may produce four 3-paths of the type $(1, 3, 3, 3)$. Then all proper 1-vertices (hydrogen atoms) go with all

$$N(\text{proper 1-vertices}) \cdot 4 \quad (11)$$

3-paths of the type $(1, 3, 3, 3)$.

Combining (i) and (ii), we have

$$\begin{aligned} m_{1333} &= 36 + N(\text{proper 1-vertices}) \cdot 4 \\ &= 36 + 6(n-2) \cdot 4 = 24n - 12. \end{aligned} \quad (12)$$

$$\begin{aligned} {}^3R_\alpha(PAH_n) &= \sum_{P^3=v_{i_1}v_{i_2}v_{i_3}v_{i_4} \subseteq PAH_n} [d(v_{i_1})d(v_{i_2})d(v_{i_3})d(v_{i_4})]^\alpha = m_{1331} \cdot (1 \times 3 \times 3 \times 1)^\alpha + m_{1333} \cdot (1 \times 3 \times 3 \times 3)^\alpha \\ &+ m_{3333} \cdot (3 \times 3 \times 3 \times 3)^\alpha = 6 \cdot (3)^{2\alpha} + (24n-12) \cdot (3)^{3\alpha} + (36n^2 - 36n + 6) \cdot (3)^{4\alpha} = 3^{2\alpha} \cdot [4 \cdot 3^{2\alpha+2} \cdot n^2 + 4 \cdot 3^{\alpha+1} \\ &\cdot (2 - 3^{\alpha+1}) \cdot n + (6 - 4 \cdot 3^{\alpha+1} + 2 \cdot 3^{2\alpha+1})] = 2 \cdot 3^{2\alpha+1} \cdot [2 \cdot 3^{2\alpha+1} \cdot n^2 + 2 \cdot 3^\alpha \cdot (2 - 3^{\alpha+1}) \cdot n + (1 - 2 \cdot 3^\alpha + 3^{2\alpha})]. \end{aligned} \quad (15)$$

□

4. The Monotonicity and the Extremal Values of ${}^3R_\alpha(PAH_n)$

Let PAH_n be the general representation of the Polycyclic Aromatic Hydrocarbons molecules for any positive integer n . In this section, we approach the monotonicity and the extremal values of ${}^3R_\alpha(PAH_n)$ for any real number α and $n \geq 3$.

Let

$$\begin{aligned} {}^3R_\alpha(PAH_n) &= 2 \cdot 3^{2\alpha+1} \cdot [2 \cdot 3^{2\alpha+1} \cdot n^2 + 2 \cdot 3^\alpha \\ &\cdot (2 - 3^{\alpha+1}) \cdot n + (1 - 2 \cdot 3^\alpha + 3^{2\alpha})]. \end{aligned} \quad (16)$$

Denote

$$\begin{aligned} f(n) &= 2 \cdot 3^{2\alpha+1} \cdot n^2 + 2 \cdot 3^\alpha \cdot (2 - 3^{\alpha+1}) \cdot n \\ &+ (1 - 2 \cdot 3^\alpha + 3^{2\alpha}). \end{aligned} \quad (17)$$

For any real number α , we have $2 \cdot 3^{2\alpha+1} > 0$. Then ${}^3R_\alpha(PAH_n)$ has the same monotonicity with the function $f(n)$.

Consider the quadratic function $f(n)$ on a variable n with $a = 2 \cdot 3^{2\alpha+1}$ and $b = 2 \cdot 3^\alpha \cdot (2 - 3^{\alpha+1})$. Since $a = 2 \cdot 3^{2\alpha+1} > 0$ for any $\alpha \in (-\infty, +\infty)$, the quadratic function $f(n)$ is increasing in the interval $[n_0, +\infty)$, where $n_0 = \max\{1, \lceil -b/2a \rceil\}$. For any $\alpha \in (-\infty, +\infty)$, $-b/2a = 1/2 - 1/3^{\alpha+1} < 1/2 < 1$. So the general $(\alpha, 3)$ -path connectivity indices of Polycyclic Aromatic Hydrocarbons PAH_n are increasing in the interval $[1, +\infty)$.

Consider m_{3333} . Since there are all three types of 3-paths in which degree sequences are $(1, 3, 3, 1)$, $(1, 3, 3, 3)$ and $(3, 3, 3, 3)$ in PAH_n , we have

$$m_{1331} + m_{1333} + m_{3333} = N(P^3), \quad (13)$$

which induces

$$\begin{aligned} m_{3333} &= N(P^3) - m_{1331} - m_{1333} \\ &= 12n(3n-1) - 6 - (24n-12) \\ &= 36n^2 - 36n + 6. \end{aligned} \quad (14)$$

By usage of the definition, we can compute the general $(\alpha, 3)$ -path connectivity index of Polycyclic Aromatic Hydrocarbon PAH_n as follows:

Theorem 2. For any $\alpha \in (-\infty, +\infty)$, the general $(\alpha, 3)$ -path connectivity indices of Polycyclic Aromatic Hydrocarbons PAH_n are increasing in the interval $[1, +\infty)$. Therefore, the minimal value happens when $n = 1$.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

This research is supported by the Natural Science Foundation of China (no. 11701530) and the Fundamental Research Funds for the Central Universities (nos. 2652015193 and 2652017146).

References

- [1] M. Randić, "On characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.
- [2] M. Lu, L. Zhang, and F. Tian, "On the Randic index of cacti," *MATCH -Communications in Mathematical and in Computer Chemistry*, vol. 56, no. 3, pp. 551–556, 2006.
- [3] S. Wang and B. Wei, "Sharp Bounds of Multiplicative Zagreb Indices of k-Trees," *Discrete Applied Mathematics*, vol. 180, pp. 168–175, 2015.

- [4] L. B. Kier and L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, NY, USA, 1976.
- [5] L. B. Kier, W. J. Murray, M. Randic, and L. H. Hall, "Molecular Connectivity V: Connectivity Series Concept Applied to Density," *Journal of Pharmaceutical Sciences*, vol. 65, no. 8, pp. 1226–1230, 1976.
- [6] L. B. Kier and L. H. Hall Wiley, New York, NY, USA, 1986.
- [7] E. Estrada, G. Patlewicz, and E. Uriarte, "From molecular graphs to drugs. A review on the use of topological indices in drug design and discovery," *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, vol. 42, no. 6, pp. 1315–1329, 2003.
- [8] R. Zanni, M. Galvez-Llompart, R. García-Domenech, and J. Galvez, "Latest advances in molecular topology applications for drug discovery," *Expert Opinion on Drug Discovery*, vol. 10, no. 9, pp. 945–957, 2015.
- [9] I. Gutman, *Advances in the Theory of Benzenoid Hydrocarbons 2, Topics in Current Chemistry*, vol. 162, Springer, Berlin, Germany, 1992.
- [10] I. Gutman, "Extremal hexagonal chains," *Journal of Mathematical Chemistry*, vol. 12, no. 1-4, pp. 197–210, 1993.
- [11] I. Gutman and S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer, Berlin, Germany, 1989.
- [12] I. Gutman and S. J. Cyvin, *Advances in the Theory of Benzenoid Hydrocarbons, Topics in Current Chemistry*, vol. 153, Springer, Berlin, Germany, 1990.
- [13] J. A. Bondy and U. S. R. Murty, *Graph Theory with Applications*, MacMillan, New York, NY, USA, 1976.
- [14] U. E. Wiersum and L. W. Jenneskens, "Gas Phase Reactions in Organic Synthesis," Y. E. Valle, Ed., pp. 143–194, Gordon and Breach Science Publishers, Amsterdam, The Netherlands, 1997.

