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M. Raji and G. Jayalalitha

IFS and Metric Space in Structure of Benzene

M. Raji[b)], and G. Jayalalitha [a)]

Department of Mathematics, School of Basic Sciences, Vels Institute of Science Technology and Advanced Studies, Chennai 600117, India

[a)]Corresponding author: g.jayalalithamaths.sbs@velsuniv.ac.in
[b)]rajialagumurugan@gmail.com

Abstract. *This paper explains about the molecular graph of Benzene. The distance between any pair of points in a graph is the number of lines in a shortest path. Measure of the distance is given by metric space. This metric space gives total measure of Linear Benzenoid Compounds which can be proved by theorems and it leads to complete metric space. This is covered by fractals.*

Key words: *Molecular Graph, Metric Space, Fractals.*

INTRODUCTION

Graph theory is a model to demonstrate many relations in real life applications [1]. A molecular graph can be a mathematical structure which provides a picturing of a molecule, taking under consideration the interior connectivity of atoms within the molecule through bonds. Consider Molecular Graph whose atoms and bonds are specified by vertices and edges respectively. The molecular graph of linear benzenoid compounds is a set of hexagons arranged on a horizontal line where each pair of adjacent hexagons shares a vertical edge [3, 4 and 5]. In Graph Theory, Points and lines are considered as vertices and edges respectively. A graph is connected if there is a path between any two points. A walk can be a sequence of vertices and edges of a graph. A walk is said to be a closed walk if the starting and ending vertices are identical [2].

A metric space is a pair (M, ρ) where M is a non-empty set and ρ: M x M → R is a real valued function called a metric on M, with the following properties (i) Positive Definite, (ii) Symmetric, (iii) Triangle inequality. Theorem states that A metric space M is compact if and only if any family of closed sets with finite intersection property has non-empty intersection. In a metric space M ,the following are equivalent : M is compact⇔Any infinite subset of M has a limit point⇔M is sequentially compact⇔M is totally bounded and complete and states that given a metric space M, with metric ρ, a mapping $T : M \to M$ is a contraction if $\rho(T(x), T(y)) \leq c\,\rho(x, y)$ for some $c < 1$ and for all $x, y \in X$. If equality holds everywhere, then we call S a contracting similarity [9].

In 1975, the mathematician Benoit Mandelbrot minted the word fractal**.** This word was drawn from the Latin word fractus which means broken or fractured. Fractal Geometry gives a general structure for the study of nature shapes. Many fractals have a fine structure which is made up of small pieces that resemble the whole part. If the replication is comparably an equivalent at every scale, then it is called a self-similar pattern. Self-similarities are not only properties of the fractals which will be used to define them. The important mechanism of fractal geometry is dimension in its many forms. Iterated function systems show a method of finding dimensions. The attractors of an iterated function system may represent Organic Compounds. Fractal concepts are used on various branches of science as Biology, Chemistry, Physics and Computer graphics [6, 7and 8].

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METHODS AND DISCUSSION

In this paper, Consider the graph G_M are finite, connected, and simple. We denote by V the vertex set of G_M and by E the edge set of G_M. The well Known one is such that this distance ρ can form a metric on V (G_M). FIGURE 1, FIGURE 2 and FIGURE 3 can be represented by the molecular graph of Benzene, Naphthalene and Anthracene respectively [10, 11].

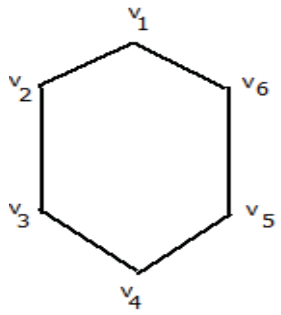

FIGURE 1. Molecular graph of Benzene

The following computations give the distance between each and every vertices of Benzene (FIGURE 1)
$\rho(v_1,v_1) = 0;\rho(v_1,v_2) = 1;\ \rho(v_1,v_3)= 2\ ;\ \rho(v_1,v_4)= 3\ ;\rho(v_1,v_5)= 2\ ;\rho(v_1,v_6) =1;\rho(v_2,v_1) =1;\rho(v_2,v_2) = 0;$
$\rho(v_2,v_3) = 1;\rho(v_2,v_4)= 2;\ \rho(v_2,v_5) = 3;\ \rho(v_2,v_6) =2\ ;\rho(v_3,v_1) = 2;\rho(v_3,v_2) = 1;\rho(v_3,v_3) =0;\rho(v_3,v_4)= 1;$
$\rho(v_3,v_5) = 2;\rho(v_3,v_6) = 3;\ \rho(v_4,v_1) = 3;\ \rho(v_4,v_2) = 2;\rho(v_4,v_3) = 1;\rho(v_4,v_4) = 0;\rho(v_4,v_5) =1;\rho(v_4,v_6)= 2;$
$\rho(v_5,v_1) = 2;\rho(v_5,v_2) = 3;\ \rho(v_5,v_3) = 2;\ \rho(v_5,v_4) = 1;\rho(v_5,v_5) = 0;\rho(v_5,v_6) = 1.$

In the Molecular graph of Benzene , all its vertices belong to the Vertex set of the molecular graph of Benzene satisfying the properties here V = { v_1,v_2,v_3,v_4,v_5,v_6}.A walk starts from v_1 to v_2 through their edges ,then $v_2 \rightarrow v_3 \rightarrow v_4 \rightarrow v_5 \rightarrow v_6 \rightarrow v_1$ through their edges. Here a walk starts from v_1 and ends with v_1. Hence the Molecular graph of Benzene contains a closed walk. The Molecular graph of Benzene is a metric under distance function ρ (u, v).

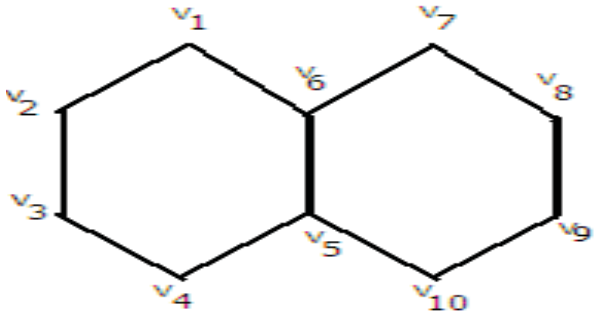

FIGURE 2. Molecular graph of Naphthalene

The following computations give the distance between each and every vertices of Naphthalene (FIGURE 2)
$\rho(v_1,v_1) = 0;\rho(v_1,v_2) =1;\rho(v_1,v_3)= 2;\rho(v_1,v_4)= 3\ ;\rho(v_1,v_5) =2\ ;\rho(v_1,v_6)=1;\rho(v_1,v_7) =2\ ;\ \rho(v_1,v_8) = 3;\ \rho(v_1,v_9) = 4;$
$\rho(v_1,v_{10})= 3;\rho(v_2,v_1) =1;\rho(v_2,v_2)= 0\ ;\rho(v_2,v_3) =1;\rho(v_2,v_4)= 2;\rho(v_2,v_5)=3;\rho(v_2,v_6) =2;\ \rho(v_2,v_7) = 3;\rho(v_2,v_8) = 4;$
$\rho(v_2,v_9) = 5;\rho(v_2,v_{10}) = 4;\rho(v_3,v_1)=2;\rho(v_3,v_2) = 1;\rho(v_3,v_3) = 0;\rho(v_3,v_4) =1;\rho(v_3,v_5) =2;\rho(v_3,v_6) = 3;\rho(v_3,v_7) = 4;$
$\rho(v_3,v_8) = 5;\rho(v_3,v_9) = 4;\rho(v_3,v_{10})= 3;\rho(v_4,v_1) =3;\rho(v_4,v_2)= 2;\rho(v_4,v_3) = 1;\rho(v_4,v_4) = 0;\rho(v_4,v_5) =1;\rho(v_4,v_6) = 2;$
$\rho(v_4,v_7) = 3;\rho(v_4,v_8) = 4;\rho(v_4,v_9)=3;\rho(v_4,v_{10})=2;\rho(v_5,v_1) = 2;\rho(v_5,v_2) = 3;\rho(v_5,v_3) =2;\rho(v_5,v_4) =1\ ;\ \rho(v_5,v_5) = 0;$
$\rho(v_5,v_6) = 1;\rho(v_5,v_7) = 2;\rho(v_5,v_8) =3;\rho(v_5,v_9) =2;\rho(v_5,v_{10})=1;\rho(v_6,v_1) =1;\rho(v_6,v_2) =2;\rho(v_6,v_3) = 3;\ \rho(v_6,v_4) = 2;$
$\rho(v_6,v_5) = 1;\rho(v_6,v_6)= 0;\rho(v_6,v_7)=1;\rho(v_6,v_8) =2;\rho(v_6,v_9) =3;\rho(v_6,v_{10}) =2;\rho(v_7,v_1) = 2;\rho(v_7,v_2) =3\ ;\ \rho(v_7,v_3)= 4;$
$\rho(v_7,v_4) = 3;\rho(v_7,v_5) = 2;\rho(v_7,v_6) =1;\rho(v_7,v_7) =0;\rho(v_7,v_8) =1;\rho(v_7,v_9) = 2;\rho(v_7,v_{10}) = 3;\rho(v_8,v_1) =3;\rho(v_8,v_2) = 4;$

$\rho(v_8,v_3) = 5;\rho\ (v_8,v_4)= 4;\rho\ (v_8,v_5)=3;\rho(v_8,v_6)=2;\rho(v_8,v_7) = 1;\rho\ (v_8,v_8) =0;\rho(v_8,v_9) = 1;\rho(v_8,v_{10}) = 2\ ;\ \rho\ (v_9,v_1) = 4;$
$\rho(v_9,v_2) = 5;\rho\ (v_9,v_3) = 4;\rho\ (v_9,v_4)=3;\rho\ (v_9,v_5)=2;\rho\ (v_9,v_6) =3;\rho(v_9,v_7)= 2;\rho\ (v_9,v_8) =1;\rho\ (v_9,v_9)= 0\ ;\ \rho\ (v_9,v_{10}) = 1;$
$\rho(v_{10},v_1)= 3;\rho(v_{10},v_2) =4;\rho(v_{10},v_3)=3;\rho(v_{10},v_4) = 2;\rho(v_{10},v_5) =1;\rho(v_{10},v_6)=2;\rho(v_{10},v_7)=3;\rho(v_{10},v_8) =2;\rho\ (v_{10},v_9) = 1;$
$\rho(v_{10},v_{10}) = 0.$
Hence the Molecular graph of Naphthalene is a metric under distance function ρ(u,v) and is a closed walk.

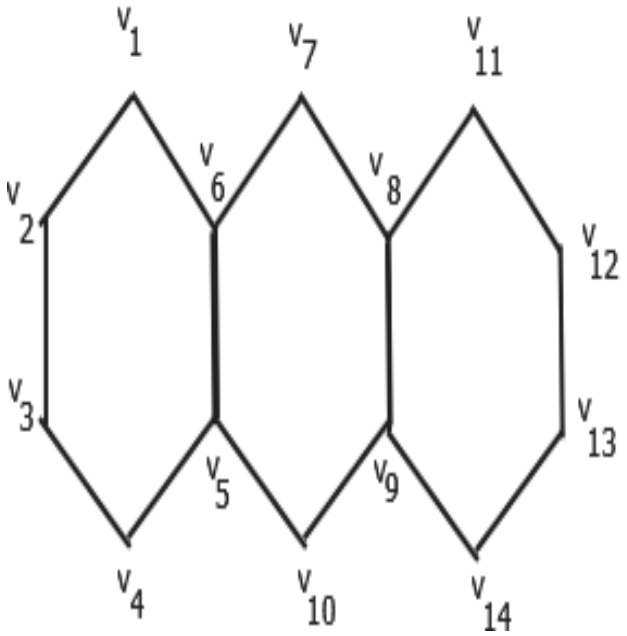

FIGURE 3. Molecular graph of Anthracene

The following computations give the distance between each and every vertices of Anthracene (FIGURE 3)
$\rho(v_1,v_1) = 0;\rho(v_1,v_2) =1;\rho(v_1,v_3)= 2;\rho(v_1,v_4)= 3;\rho\ (v_1,v_5) =2\ ;\rho\ (v_1,v_6)=1;\rho\ (v_1,v_7) =2\ ;\ \rho\ (v_1,v_8) = 3;\ \rho(v_1,v_9) = 4;$
$\rho(v_1,v_{10})=3;\rho(v_1,v_{11})=4;\rho(v_1,v_{12})=5;\rho(v_1,v_{13})=6;\rho(v_1,v_{14})=5;\rho(v_2,v_1)=1;\rho(v_2,v_2)=0;\rho(v_2,v_3)=1;\rho(v_2,v_4)=2;\ \rho(v_2,v_5)=3;$
$\rho(v_2,v_6)=2;\rho(v_2,v_7)=3;\ \rho(v_2,v_8)=4;\ \rho(v_2,v_9)=5;\rho(v_2,v_{10})=4;\rho(v_2,v_{11})=5;\rho(v_2,v_{12})=6;\rho(v_2,v_{13})=7;\rho(v_2,v_{14})=6;\rho(v_3,v_1)=2;$
$\rho(v_3,v_2)=1;\rho(v_3,v_3)=0;\ \rho(v_3,v_4)=1;\ \rho(v_3,v_5)=2;\ \rho(v_3,v_6)=3;\ \rho(v_3,v_7)=4;\ \rho(v_3,v_8)=5;\ \rho(v_3,v_9)=4;\rho(v_3,v_{10})=3;\rho(v_3,v_{11})=6;$
$\rho(v_3,v_{12})=7;\rho(v_3,v_{13})=6;\rho(v_3,v_{14})=5;\rho(v_4,v_1)=3;\rho(v_4,v_2)=2;\rho(v_4,v_3)=1;\ \rho(v_4,v_4)=0;\ \rho(v_4,v_5)=1;\ \rho(v_4,v_6)=2;\ \rho(v_4,v_7)= 3;$
$\rho(v_4,v_8)=4;\rho(v_4,v_9)=3;\rho(v_4,v_{10})=2;\rho(v_4,v_{11})=5;\rho(v_4,v_{12})=6;\rho(v_4,v_{13})=5;\rho(v_4,v_{14})=4;\rho(v_5,v_1)=2;\rho(v_5,v_2)=3;\rho\ (v_5,v_3)=2;$
$\rho(v_5,v_4)=1;\rho(v_5,v_5)=0;\rho(v_5,v_6)=1;\rho(v_5,v_7)=2;\rho(v_5,v_8)=3;\rho(v_5,v_9)=2;\rho(v_5,v_{10})=1;\rho(v_5,v_{11})=4;\rho\ (v_5,v_{12})=5;\rho(v_5,v_{13})= 4;$
$\rho(v_5,v_{14})=3;\rho(v_6,v_1)=1;\rho(v_6,v_2)\ =2;\rho(v_6,v_3)=3;\rho(v_6,v_4)\ =2;\rho(v_6,v_5)=1;\rho(v_6,v_6)= 0;\rho\ (v_6,v_7)=1;\rho(v_6,v_8)\ =2;\rho(v_6,v_9)\ =3;$
$\rho(v_6,v_{10})=2;\rho(v_6,v_{11})=3;\rho(v_6,v_{12})=4;\rho(v_6,v_{13})=5;\rho(v_6,v_{14})=4;\rho(v_7,v_1)=2;\rho(v_7,v_2)=3;\rho(v_7,v_3)=4;\rho(v_7,v_4)=3;\rho(v_7,v_5)= 2;$
$\rho(v_7,v_6)=1;\rho(v_7,v_7)=0;\rho(v_7,v_8)=1;\rho(v_7,v_9)=2;\rho(v_7,v_{10})=3;\rho(v_7,v_{11})=2;\rho(v_7,v_{12})=3;\rho(v_7,v_{13})=4;\rho(v_7,v_{14})=3;\rho(v_8,v_1)\ \ =3;$
$\rho(v_8,v_2)=4;\rho(v_8,v_3)=5;\rho(v_8,v_4)=4;\rho(v_8,v_5)=3;\rho(v_8,v_6)=2;\rho(v_8,v_7)\ =1;\rho\ (v_8,v_8)\ =0;\rho(v_8,v_9)\ =1;\rho(v_8,v_{10})=2;\rho(v_8,v_{11})\ =\ 1;$
$\rho(v_8,v_{12})=2;\rho(v_8,v_{13})=3;\rho(v_8,v_{14})=2;\rho(v_9,v_1)=4;\ \rho(v_9,v_2)=5;\ \rho(v_9,v_3)=4;\ \rho(v_9,v_4)=3;\ \rho(v_9,v_5)=2;\rho(v_9,v_6)=3;\ \rho(v_9,v_7)=2;$
$\rho(v_9,v_8)=1;\rho(v_9,v_9)=0;\ \ \rho(v_9,v_{10})=1;\ \ \rho(v_9,v_{11})=2;\ \ \rho(v_9,_{12})=3;\ \ \rho(v_9,v_{13})=2;\ \ \rho(v_9,v_{14})=1;\ \ \rho(v_{10},v_1)=3;\ \ \rho(v_{10},v_2)=4;$
$\rho(v_{10},v_3)=3;\ \rho(v_{10},v_4)=2;\ \rho(v_{10},v_5)=1;\ \rho(v_{10},v_6)=2;\ \rho(v_{10},v_7)=3;\ \rho(v_{10},v_8)=2;\ \rho(v_{10},v_9)=1;\ \rho(v_{10},v_{10})=0;\ \rho(v_{10},v_{11})=3;$
$\rho(v_{10},v_{12})=4;\ \rho(v_{10},v_{13})=3;\ \rho(v_{10},v_{14})=2;\ \rho(v_{11},v_1)=4;\ \rho(v_{11},v_2)=5;\ \rho(v_{11},v_3)=6;\ \rho(v_{11},v_4)=5;\ \rho(v_{11},v_5)=4;\ \rho(v_{11},v_6)=3;$
$\rho(v_{11},v_7)=2;\ \rho(v_{11},v_8)=3;\ \rho(v_{11},v_9)=2;\ \rho(v_{11},v_{10})=3;\ \rho(v_{11},v_{11})=0;\ \rho(v_{11},v_{12})=1;\ \rho(v_{11},v_{13})=2;\ \rho(v_{11},v_{14})=3;\ \rho(v_{12},v_1)=5;$
$\rho(v_{12},v_2)=6;\ \rho(v_{12},v_3)=7;\ \rho(v_{12},v_4)=6;\ \rho(v_{12},v_5)=5;\ \rho(v_{12},v_6)=4;\ \rho(v_{12},v_7)=3;\ \rho(v_{12},v_8)=2;\ \rho(v_{12},v_9)=3;\ \rho(v_{12},v_{10})=4;$
$\rho(v_{12},v_{11})=1;\ \rho(v_{12},v_{12})=0;\ \rho(v_{12},v_{13})=1;\ \rho(v_{12},v_{14})=2;\ \rho(v_{13},v_1)=6;\ \rho(v_{13},v_2)=7;\ \rho(v_{13},v_3)=6;\ \rho(v_{13},v_4)=5;\ \rho(v_{13},v_5)=4;$
$\rho(v_{13},v_6)=5;\ \rho(v_{13},v_7)=4;\ \rho(v_{13},v_8)=3;\ \rho(v_{13},v_9)=2;\ \rho(v_{13},v_{10})=3;\ \rho(v_{13},v_{11})=2;\ \rho(v_{13},v_{12})=1;\ \rho(v_{13},v_{13})=0;\ \rho(v_{13},v_{14})=1;$
$\rho(v_{14},v_1)=5;\ \rho(v_{14},v_2)=6;\ \rho(v_{14},v_3)=5;\ \rho(v_{14},v_4)=4;\rho(v_{14},v_5)=3;\ \rho(v_{14},v_6)=4;\ \rho(v_{14},v_7)=3;\ \rho(v_{14},v_8)\ =2;\rho\ (v_{14},v_9)\ =1;$
$\rho(v_{14},v_{10})\ =\ 2;\ \rho\ (v_{14},v_{11})\ =\ 3;\ \rho\ (v_{14},v_{12})=\ 2\ ;\ \rho\ (v_{14},v_{13})\ \ =\ 1\ ;\ \rho\ (v_{14},v_{14})=\ 0.$
Hence the Molecular graph of Anthracene is a metric under distance function ρ (u,v) and is a closed walk.

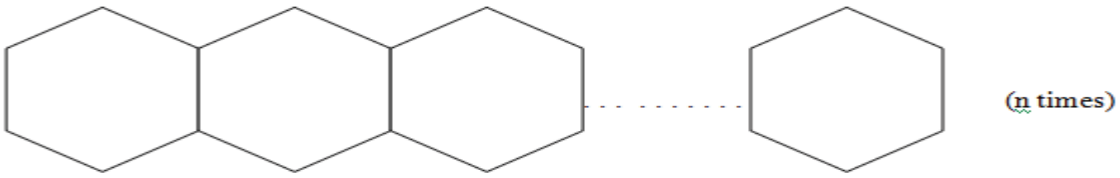

FIGURE 4. Molecular graph of Linear Benzenoid Compounds

There are $4h+2$ vertices in the molecular graph of Linear Benzenoid Compounds G_M.From FIGURE 4,we can say that for all vertices *u, v, w* belong to the Vertex set of the molecular graph of Linear Benzenoid Compounds satisfying the properties *(i)*$\rho(u, v) \geq 0$*;(ii)*$\rho(u, v)=\rho(v, u)$ *;(iii)*$\rho(u, w) \leq \rho(u, v) +\rho(v, w)$.Hence the Molecular graph of Linear Benzenoid Compounds G_M is a metric under distance function ρ(u ,v).The distance between points in G_M is less than some finite constant. By Metric criteria, it can be bounded. So G_M is bounded. In such a Molecular Graph, Interaction between cycles sharing some vertices and cycles linked by a path. This Molecular graph is a closed cycle. The molecular graph of Linear Benzenoid Compounds G_M is a closed walk. Hence the structure of Linear Benzenoid Compounds G_M is closed and bounded. Therefore, it is a compact. By equivalent properties, the molecular graph of Linear Benzenoid Compounds G_M is totally bounded and complete. So we may consider this as a Complete Metric Space [9].

Iterated Function Systems in Linear Benzenoid Compounds

Fractals preserve Self-similarity. These self-similarities are not only properties of the fractals which are used to define them. Iterated function systems can give this in a unified way. The axiom of an iterated function system (IFS) is that it finds a unique attractor, which is generally fractal [6, 12, and 13]. Here Molecular Graph of Linear Benzenoid Compounds G_M is represented by ɧ hexagons. Consider the molecular graph of Linear Benzenoid Compounds G_M as an iterated function system. Take a finite family of contractions $\{T_1, T_2, T_3, \ldots\ldots, T_n\}$ with n≥2 which is constructed by ɧ hexagons, is called an iterated function system. If $F= \bigcup_{i=1}^{n} T_i(F)$, then a non-empty compact subset F of G_M is an attractor. Consider G_M is any non empty subset (sub graph) of n-dimensional Euclidean space $\mathbb{R}^n$.

Theorem

Consider the iterated function system given by the contractions $\{T_1, T_2, T_3, \ldots, T_n\}$ on $G_M \subset \mathbb{R}^n$,so that $\left|T_i(v_i) - T_i(v_j)\right| \leq c_i \left|v_i - v_j\right|$ $(v_i, v_j) \in G_M$ with $c_i < 1$ for each i. Then there is a unique attractor F.

Proof. Define a transformation T on G_M by T (G) = $\bigcup_{i=1}^{n} T_i(G)$ for G ∈ T. That is, the graphs in T are transformed by T into other graphs of T. If $G_1, G_2 \in$ T ,then ρ(T(G_1), T(G_2)) = ρ ($\bigcup_{i=1}^{n} T_i(G_1)$, $\bigcup_{i=1}^{n} T_i(G_2)$) ≤ $\max_{1\leq i\leq m} \rho(T_i(G_1), T_i(G_2))$.If δ-neighbourhood $(T_i(G_1))_\delta$ contains $T_i(G_2)$ $\forall$ i,then $(\bigcup_{i=1}^{n} T_i(G_1))_\delta$ contains $\bigcup_{i=1}^{n} T_i(G_2)$ and conversely. By assumption, ρ (T (G_1), T (G_2)) ≤ $\max_{1\leq i\leq m} c_i$ ρ(G_1, G_2) . It may be concluded that d is a complete metric on T. Then T is a contraction on G_M which is complete. By Contraction mapping theorem [9], T has exactly one fixed point. So there is a unique set F ∈ T such that T (F) =F. Hence proved.

CONCLUSION

In this paper, it obtains that the molecular graph of Linear Benzenoid Compounds Satisfies Metric properties. Then it is a connected and closed. So its structure is a compact metric space as well as totally bounded and complete metric. It describes that an Iterated function systems gives an attractor. This paper initiates a relationship between

Graph Theory, Measures and Fractal Geometry that is discussed through distance function. It concludes that molecular graph of Linear Benzenoid Compounds is a fractal using contraction mapping which is proved.

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