REVIEW OF RESEARCH
IMPACT FACTOR : 5.7631(UIF) ISSN: 2249-894X
VOLUME - 1 | ISSUE - 1 | MARCH - 2019

APPLICATION OF GRAPH TREE IN ORGANIC ALIPHATIC COMPOUND ALKANE

Dr.Berdewad O.K. and Tiwade S.S
Dept. of Mathematics, DigambarraoBindu College, Bhokar
Dept. of Chemistry, DigambarraoBindu College, Bhokar

ABSTRACT :

Graphs without cycles (called acyclic graphs) are probably the most essential graphs of with regards to computer science. The several kind of data structure regarded as tree in computer sciences have fundamental graphs that are the tree in graph theory. Trees are vital graphs. Simply because of the fact that lot of the application of graph theory contain trees. In this paper we have discussed how trees are used in various field and application to ethane compound. Also proved the some result on tree.

KEYWORDS : *Graph Theory, Tree, Chemistry, Alkane, Ethane*

INTRODUCTION

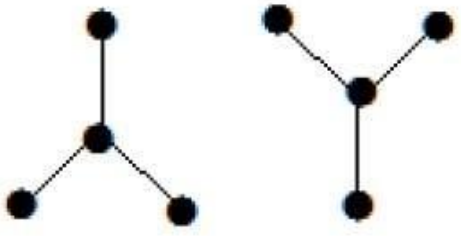
Trees are used in chemistry to model molecules, in sports to show tournament schedules, and in social science to model hierarchies, thus, the tree [3]. In 1857, Cayley discovered the important class of graphs called trees by considering the changes of variables in the differential calculus. This study had a lot of implications in theoretical chemistry [4]. The complicated techniques mainly concerned the enumeration of graphs having precise properties. Enumerative graph theory then rose from the results of Cayley and the essential results published by Pólya between 1935 and 1937 and the generalization of these by De Bruijn in 1959[4]. Cayley linked his effects on trees with the current research of chemical composition [4]. The fusion of the ideas coming from mathematics with those coming from chemistry is at the origin of graph theory[4].

Application of Graph Theory in various fields:

Graph theory concepts are mostly used to study and models are used in different applications in various areas. They include construction of bonds in the field of chemistry, study of atoms and study of molecules.trees and graphs in many application of computer science for example operating system manages hard file by using tree data structure to search it in big O(lgn). Compiler use trees to evaluate expressions of language. Trees are used in many applications: analysis of algorithms, compilation of algebraic expressions, theoretical models of computation, etc.[5]Tree is used in dictionary to fined specific word in millions of words. Graph is also used in many application of computer science. Graph theory also used in the sociology, example to explore the mechanisms in diffusion and actors prestige can be measured. Graph theory is used in biology and the efforts of the conversation where a vertex denotes the regions in that certain species exist and then the edges denotes movement or migration path between the regions. This information is very significant when seeing the breeding patterns or finding the spread of parasites, disease and to study about the migration impact which affect other species also.

Definition: In graph theory,a tree is a special kind of graph follow a particular set of rules [7].

A tree is an undirected graph in which any two vertices are connected by *exactly one* path [6].A *tree* is a connected forest with no loop. A collection of forest is a tree.For example, Figure shows below an example of a tree.



Theorem [8]: IfG *is a tree if and only if there is unique path between any two vertices in* G *and* G *has without loops*

Proof: Let G is tree. Since G is connected without loop, there is unique path between any two vertices in G. Let there be two distinct paths between two vertices u and v of G. Thus, theunion of these two paths contain a cycle which is contradicts the fact that, G is tree [9]. Hence there is unique path between any two vertices of a tree.

Conversely, Let G is a graph with n vertices and m edges. Let there is unique path between any two vertices in G [8]. So G is connected then there are no loops in G. If G contains cycles then there are distinct paths between u and v, which is contradiction [9].Thus G is connected with no cycle. Hence Gis a tree.

Theorem: Eliminating any edge disconnects the graph.

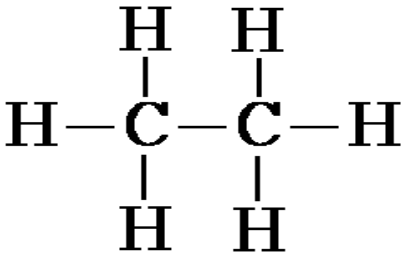
Proof: Suppose that we remove edge u—v. Since a tree contained a unique path between u and v, that path must have been u—v. Therefore, when that edge is removed, no path remains, and so the graph is disconnected.

Theorem: Every tree with at least two vertices has at least two leaves.

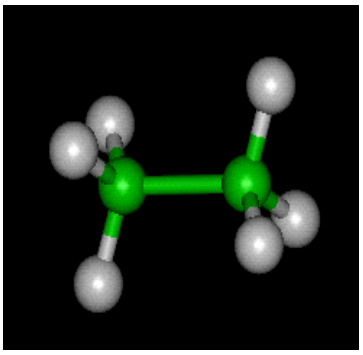
Proof: Let $v_1, v_2, ..., v_m$ be the sequence of vertices on a longest path in G[1]. Then m ≥2, since a tree with two vertices must contain at least one edge. There cannot be an edge $v_1 — v_i$ for 2 <i ≤ m; otherwise, vertices $v_1, v_2, ..., v_i$ would from a cycle. Furthermore, there cannot be an edge $u — v_1$ where u is not on the path; otherwise, we could make the path longer. Therefore, the only edge incident to v_1 is $v_1 — v_2$, which means that v_1 is a leaf. By a symmetric argument, v_m is a second leaf.[2]

Application of graph theory to aliphatic compound:

Graph theory is used in mathematically simulates molecules and put on understanding of the physical properties of aliphatic compound. A few physical compounds properties namely boiling point are related to the shape of a given compound. This is particularly true for compounds called as alkanes.Alkanes are an organic compound made up of only of carbon and hydrogen atoms [10].For instance, of an alkane is ethane as shown in figure 1



Ethane is a colorless, odorless, and flammable gas with a chemical formula of **C2H6**.Each carbon atom has four chemical bonds each with one chemical bond. Consequently, hydrogen atom can be removed without losing information onmolecules. Ethane thus produced is represented by the carbon tree shown in figure 2



Carbon tree can be represented as map by replacing carbon atom with vertices. Chemical bonds are represented as edges of the graph.

Conclusion:

The several kind of data structure regarded as tree in computer sciences have fundamental graphs that are the tree in graph theory.This study had a lot of implications in theoretical chemistry [4].In this paper we have study the graph tree and their application in ethane compound.

References :

1. "Graphs." ocw.mit.edu. Massachusetts Institute of Technology Course Notes, Week 5 6.042J/18.062J, Fall '05: Mathematics for Computer Science, 10 Mar. 2005. Web. 19 Feb. 2019. <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-042jmathematics-for-computer-science-fall-2005/readings/ln5.pdf>.
2. scielo.br.N.p.,n.d.Web.19Feb.2019.<http://www.scielo.br/scielo.php?script=sci_arttext&pid=S0100-60452016000400279.
3. "Graph Theory for the Middle School.." *dc.etsu.edu*. East Tennessee State University Digital Commons @ East Tennessee State University, 8 Oct. 2006. Web. 19 Feb. 2019. <https://dc.etsu.edu/cgi/viewcontent.cgi?article=3590&context=etd>.
4. https://en.wikibooks.org/wiki/Transportation Geography and Network Science/Graph theory
5. https://web.itu.edu.tr/gencata/courses/GT/GTlecture2.pdf
6. https://en.wikipedia.org/wiki/Tree_%28graph_theory%29
7. http://academics.triton.edu/faculty/ebell/6%20-%20Graph%20Theory%20and%20Trees.pdf
8. https://www.whitman.edu/mathematics/cgt_online/book/section05.05.html
9. 9.http://compalg.inf.elte.hu/~tony/Oktatas/TDK/FINAL/Chap%204.PDF.
10. https://www.chem.fsu.edu/chemlab/chm1046course/hydrocarbons.html