Applications of Graph Theory and Trees in the Cayley Theorem for Calculating the Number of Isomers in Compounds Alkanes

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ABSTRACT

Cayley's theorem, in principle, can be used in determining the isomers of alkanes lot, which was originally limited to the calculation of the number of isomers of manual calculation, the method of "drawing and counting." Graph structure of the alkane is a tree (the tree).
By proving that the alkane is a tree graph of a satisfying E (G) = V (G) with a value of V (G) = 3n + 2 and E (G) = 3n +1, -1. Alkane with the chemical formula CnH2n +2 where each node has degree one or four points, so that the calculations used 4-Cayley.
Based on the theorem of Cayley was able to show that many alkane isomers can be determined through the summation of many Bicentered Centered Tree and Tree. Centered Tree is a tree with one center that has a formula C2h (z) = ΣC2h, nz^n and Bicentered Tree is a tree with exactly two centers (centers are always close together) which has the formula B2h +1 (z) = ΣB 2h+1, nz^n

***Keywords : Cayley's theorem*, Isomers in Compound Alkanes, tree.**

1. PREFACE

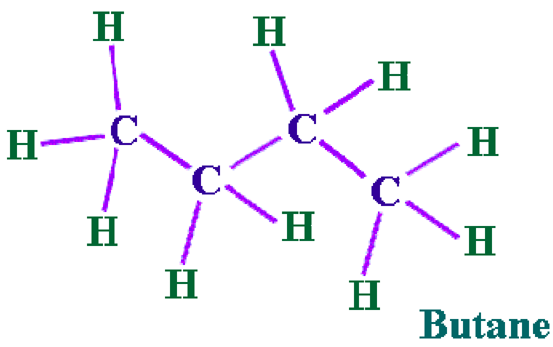
Graph theory was first introduced in 1736 by a famous Swiss mathematician named Euler. Graph theory first emerged to solve the puzzle Konigsberg bridge problem is very difficult to be solved at the time. Konigsberg Prussia is a town in eastern Germany. Approximately one hundred years after the birth of writing Euler, no significant developments relating to graph theory. 1847, GR Kirchhoff (1824-1887) succeeded in developing the theory of tree (Tree Theory) is used in solving electrical network problems. Ten years later, Arthur Cayley (1821-1895) also uses the concept of a tree to describe the problem of hydrocarbon chemistry [3] (Heri Sutarno, 2005: 65). Along with time and technological advances that increasingly sophisticated, graph theory has penetrated the disciplined application of science and help make it easier for people to solve problems. Emphasizing the use of graphs to model problems.

This theory is also very useful to develop a structured model in various situations. In the implementation of this theory is often found in the field of electro, organic chemistry, computer science, and so forth. Even the current graph theory used in the field of mass-ecology, geography, anthropology, genetics, physics, electronics, information processing, architectural design, and. In chemistry, graph theory can be applied in quantum electronic structures, molecular mechanics, simulated condensation phase, the design of the structure of molecules, polymers, topography, potential energy, and biological macromolecules (including proteins). Lately, graphics applications, especially related to the molecular structure of isomers, ie molecules that contain carbon [7] (Reisha Humaria, 2007: 1). As with any organic compounds, coordination compounds, known also isomers.

According to Kristian H. Sugiyarto (2006: 2.13) [4] isomers are compounds that have the same molecular formula but have different structures. Furthermore, in accordance with Reisha Humaria (2007: 1) [6] the chemical isomer is a very important concept in modern chemistry. At the beginning of isomers are known in chemistry, the number of isomers of a compound is determine and calculated by drawing (Drawing and Count Methods). This method is carried out on compounds that have a simple structure. However, in general, we need a method to calculate a more complex compound isomers. The development of science in chemistry, scientists led research in calculating the number of isomers. For example, in 1874 the number of isomers of a chemical compound with many Cayley graph concept.

The research was continued by George Polya by using combinatorial to determine the number of isomers of a chemical compound. Polya theory is very relevant for this type of combinatorial calculations. Determination of isomers in chemistry was not done arbitrarily. There are special rules in determining, for example in the naming of compounds in each structure is formed. Despite having the same molecular formula but different structural isomers that have different properties. In graph theory calculation of the number of isomers can be done easily by ignoring chemical properties. Because the isomers graph calculations with chemical properties do not affect the results. Graphs with tree theory can be used easily to solve problems in chemistry, especially in determining the isomers of alkanes lot.

Since settlement in the graph is very simple and uncomplicated as if determined through chemical, with record properties that affect the calculation ignored. To overcome these problems, alkanes should be modeled. Graf with a variety of theories is very suitable for modeling of chemical compounds. In the modeling using graphs, which binds the elements represented as nodes and chemical bonds that occurs is denoted by the rib. Graph to form compounds that have the sense that a compound found in nature said to be stable if it has a shape like that modeled in graphical form. For example, modeling is a compound Butane (C4H10).



Picture 1. Image Modeling with Graph in Compound Butane

2. METHOD

The method of writing paper used are book study method, hypothesis and analysis of the case. After the writer read various articles on Cayley, the author tried to synthesize a way to get the amount of chemical compounds. In determining the formula in getting the number of chemical compounds, the author uses references from the internet. By using the formula, Cayley's theorem applies to count the number of isomers of compounds Alkanes.

3. BASIC THEORY

3.1 Definition of Graph

The definition of a graph is the set of vertices connected by edges. Mathematically, a graph G is defined as the set of pairs (V, E), which in this case:

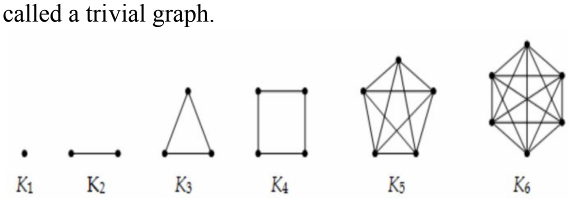
V = non-empty set of nodes (vertices or nodes) = {v1, v2, ..., vn}

and

edge set E = (edges) connecting a pair of nodes = {, e1 e2, ..., en}

or can be written brief with the notation G = (V, E).

[7] States the above definition that V can not be empty, while E can be empty. So, it is possible to graph does not have a single side, but concluded there must be, at least one. Graf who has only one node without a side of fruit called a trivial graph.



Picture 2. Several modeling graph

3.2 KIND OF GRAPH

Based on the presence or absence of a bracelet or double-side on the graph, then the graph are classified into two types:

1. Simple graphs
   Graph that does not contain a bracelet and double-side is called a simple graph.
2. Unsimple-graf/multigraf
   Unsimple Graph or coil segment containing the called non-simple graphs (graphs or unsimple multigraf).

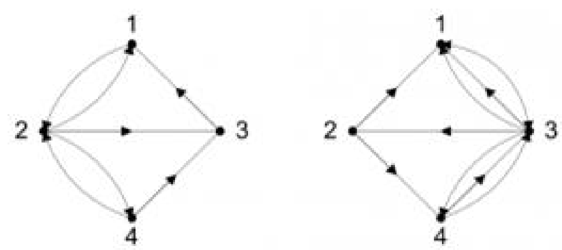
Based on the number of nodes in the graph, then in general graphs can be classified into two types:

1. Graphics up to (limited graphics).
   Limited graph is a graph of the number of vertices, n, finite.
2. Graph of infinite (unlimited graph).
   Graph the number of vertices, n, there is no limited number called an infinite graph.

Based on the orientation direction, the graph is generally divided into 2 types:

1. Non-directed graph (directed graph).
   Graph that has no known side orientation of non-directed graph.
2. Digraph (directed graph)
   Graph in which each side is given the orientation of the direction referred to as a digraph.

Two graphs in the figure 3 are a directed graph



Picture 3. Directed Graph

3.3 Definition of Tree

The tree is a special chart. The definition of a tree is as follows: "The tree of non-directed graph contains no circuits connecting" Some trees can be made into the forest.

Forest is:

- a collection of trees from each other, or
- no graph connect that does not contain circuits. Each component in the graph connect it is a tree.

Theorem of Tree

Let G = (V, E) is takberarah simple graph and the number of vertices n. So, all statements below are equivalent:

1. G is a tree.
2. Each pair of vertices in G can connect with a single trajectory.
3. G connected and has m = n - 1 pc side.
4. G contains no circuit and have m = n - 1 pc side.
5. G contains no circuits and the addition of one hand on the graph will make only one circuit.
6. G connected and all sides are the bridge. Above theorem can be regarded as another definition of the tree. [5]

3.4 Graph Cayley

In mathematics, also known as the Cayley graph Cayley color graph. This concept was introduced by Arthur Cayley, which is the basis for understanding the theory of Cayley. [7] (Weisstein, 2008: 1). The set of generators of the group is the set of elements of the group itself, which allows the repetition of the generator and the generator can produce a combination of elements of the group.

Example 2.13

Suppose that Z 6 is the addition operation modulo 6 is a group, 6 Z = {0, 1, 2, 3, 4, 5}. Generator set is {1}, {2, 5}, {2, 3, 4}. Is derived as follows:

For {1}
1.0 = 0
1.1 = 1
1.2 = 2
1.3 = 3
1.4 = 4
1.5 = 5

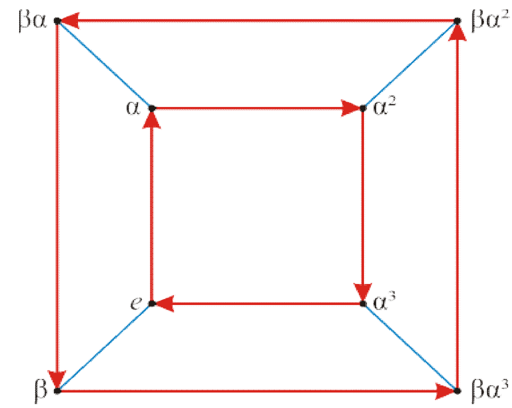
For {2, 5}
2.0+ 5.0 = 0
2.1+ 5.1 = 1
2.2+ 5.2 = 2
2.3+ 5.3 = 3
2.4+ 5.4 = 4
2.5+ 5.5 = 5

For {2, 3, 4}
1.0 + 3.1 + 4.2 = 5
2.1 + 3.1 + 4.2 = 1
2.3 + 3.1 + 4.3 = 3
2.1 + 3.2 + 4.2 = 4
2.5 + 3.4 + 4.2 = 0
2.1 + 3.4 + 4.3 = 2
[2]

Suppose that G is a group and S is the set of generators. Cayley graph G = G (G, S) is a colored directed graph (colored Directed Graph), which was established as follows:

a. Each element g G is expressed as the nodes: the set of vertices V (G) of G given by G.
b. Each element S s expressed as a color for each.
c. G € g, s € S, the nodes in accordance with the elements g and gs are combined by a directed edge-colored, ie cs. Therefore, the edge set E (G) consists of pairs (g, gs), with s € S as a provider of color.

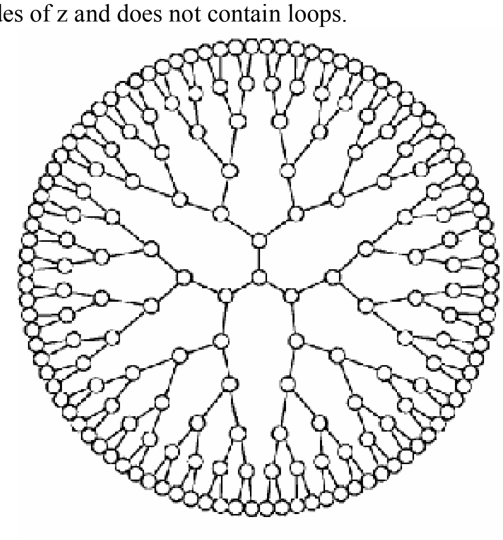
Cayley graphs on dihedral group D4 of two elements, such as α and β will be described by Figure 4. Red arrows in Figure 4 is a left multiplication by α elements. While the element β is the opposite of itself, the blue line represents the left multiplication by elements of β are not trends. Therefore this graph is formed, which has eight nodes, eight arrows, and four ribs. Cayley table in D4 group can be determined through a group of α, β | α^4 β^2 = e =, αβ = $\beta\alpha^3$.



Picture 4. Cayley graphs on dihedral groups

3.5 Cayley's Tree

Cayley or called by Bethe Lattice, introduced by Hans Bethe in 1935. Cayley with coordination number z is the branching graph of every vertex to connect with other nodes of z and does not contain loops.

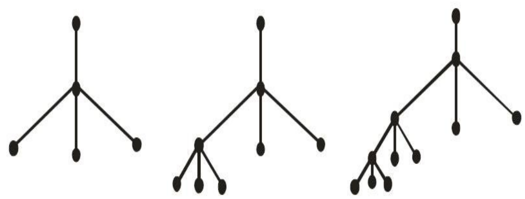


Picture 5. ***Cayley***

4 DISCUSSION AND ANALYSIS

4.1 Determination the Number of k-Cayley

In this section we will discuss the determination of the k-Cayley widely used in the calculation of many isomers of alkanes. Where in the calculation will use the concept Becentered Centered Tree and Tree. Given that the acyclic alkanes are tree-like structure, then the calculation of alkane isomers by using the basic concept of Cayley. Alkane with the chemical formula Cn H2n + 2 where each node has degree one or four, then in this discussion uses the concept of 4-Cayley. **Figure 6** below shows the 4-Cayley



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(a) (b) (c)

Figure 6

(a) Alkanes with n=1 in form *Cayley*

(b) Alkanes with n=2 in form *Cayley*

(c) Alkanes with n=3 in form *Cayley*

Figure 6 can be described as an evolving structure of the central node with all nodes arranged around the node at the previous level as an example in **Figure 7**.

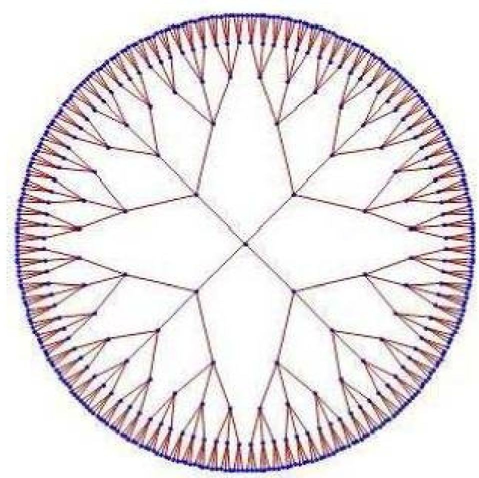


Figure 7. 4-Cayley

Figure 7 is Calley Tree by tree roots has z = 4, then the node at level k can be calculated by $N^k = z(z - 1)^{k-1}$ for $k \geq 0$

k = 1
$N_1 = 4(4 - 1)^{1-1}$
$N_1 = 4.(3)^0$
$N_1 = 4$

k = 2
$N_2 = 4(4 - 1)^{2-1}$
$N_2 = 4.(3)^1$
$N_2 = 12$

k = 3
$N_3 = 4(4 - 1)^{3-1}$
$N_3 = 4.(3)^2$
$N_3 = 36$

k = 4
$N_4 = 4(4 - 1)^{4-1}$
$N_4 = 4.(3)^3$
$N_4 = 108$

and so on until n.

A graph with unique vertex v is defined as a typical distance of a vertex v to another node. graphic Center is a node that has a single trait. graph can have a different number nodes in place. For trees, there are only two possibilities, namely:

1. A tree with exactly one center (Centered Tree).
2. A tree with exactly two centers (Bicenterd Tree), in this case the center is always adjacent .

For more detailed information, then Centered Tree and Tree Bicenterd is shown in Table 1 as follows:

Table 1 Many Determined Through Isomorphic Graph and Count Method Draw Method Table

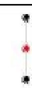
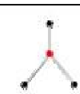
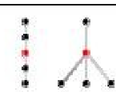
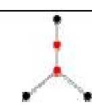
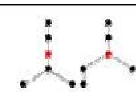
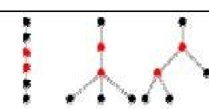
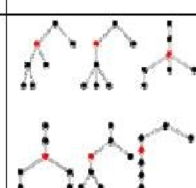
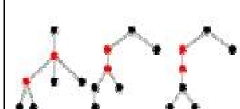
n	*Centered*	*Bicentered*	Total
1			1
2			1
3			1
4			2
5			3
6			5
7			9
...	...	...	...

Table 1. Centralized and bicentered calculation shows a way to Draw and Count method, but for subsequent calculations will use a more efficient way is with a formula that in the calculations aided by a Maple program. A tree with the longest path (diameter) 2m has a unique node called the center, at the midpoint of the long road 2m. In the tree with the longest path (diameter) 2m +1 there is a unique node pairs called bicenter, in the

middle of the track length 2m +1. Therefore, the calculation of isomers will be discussed based on the concept of central and bicenter.

4.1.1. *Centered Tree* C(z)

For k-Cayley, said h n T, is the number (k – 1) –ary are nodes and maximum tree height h. As a treaty, an empty tree has h = -1

For example, $T_h(z) = \sum T_{h,n} Z^n$, so

$T_{-1}(z) = 1$

$T_0(z) = 1 + z$

And for *h*>1

$T_{h+1}(z) = 1 + zS_{k-1}(T_h(z))$

4.1.2 *Bicentered Tree C(z)*

Suppose B2h+1,n is the number n k-tree bicenter Cayleys is the number of vertices and 2d +1 is the diameter of the tree.

Take $B_{2h+1,n}(z) = \sum B_{2h+1,n}z^n$

Bn is the number of k-Cayleys bicenter which has n vertices, and B (z) = ΣBnzn. Because bicenter tree rooted tree in accordance with the pair (k-1)-ary with a high right h obtained

$$B_{2h-1}(z) = S2(T_h(z)\ T_{h-1}(z))$$

Then a tree is obtained bicenter$B(z) = \sum B_{2h+1}(z)$

if it is obtained as described below

$$B(z) = B1(z) + B3(z) + B5(z) + B7(z) + B9(z) + ...$$

Table 2. Table many isomorphic graph defined through the concept of Cayley

n	*Centered*	*Bicentered*	Total
1	1	0	1
2	0	1	1
3	1	0	1
4	1	1	2
5	2	1	3
6	2	3	5
7	6	3	9
8	9	9	18
9	20	15	35
10	37	38	75
...	...	...	...

Number of **Table 2** states the graph isomorphic largely determined by the sum of Centered and Bicentered.

4.2 Graph Theory Application in Determining The Many Isomers of Alkanes

Isomers are compounds that have the same molecular formula but have different structures. In graph theory, in fact the same graph isomorphic isomer only in chemical properties is negligible. Because in graph theory further discuss only the structure, making it easier to count the many isomers of alkanes. Chemical compounds, especially alkanes are not easily described or modeled

It takes a special rule in the modeling of this chemical compound. Graf with a variety of theories is very suitable for modeling of chemical compounds. In chemistry, the chemical component to the formula CnH2n +2 called alkanes. CnH2n +2 n compounds containing carbon atoms and 2n +2 hydrogen atoms. In accordance with it's function in graph theory, a lot of vocabulary from the dictionary chemical that is converted to graphs with the goal of vocabulary in comprehension.

Table 3. Table of Chemical Terms

Chemical Term	The term in Graph
Structural formula	*Graph*
Atom	*Vertex*
Chemical Bond	*Edge*
Valency of atom	*Degree of vertex*
Acyclic structure	*Tree*
Isomers	*Isomorphic*

Cayley Theorem

C_nH_{2n+2} alkanes structure is a tree

Proof:

The number of vertice of C_nH_{2n+2} is

$n + (2n + 2) = 3n + 2$

Alkanes are molecules that each carbon atom has 4 bonds, while each hydrogen atom is only 1 fastener. Suppose that G is a graph as a model of Alkanes, then G has 3n +2 vertices. Further indicates that the number of sides in G is **3n +1**.

$V(G) = 3n+2$

$E(G) = ½ \sum d(V_i)$

$= ½ (d(C) + d(H))$

$= ½ (n.4 + (2n+2).1)$

$= (4n + 2n + 2)/2$

$= \mathbf{3n + 1}$

(proven)

Therefore, E (G) = V (G) -1, the structure of alkanes CnH2n +2 is a tree.

Form the structure of the chemical composition is a diagram that says the bond between atoms in the molecule. Molecular formula CnH2n +2 are not sufficient to identify the isomers, as long as there are isomers that have the same molecular formula but different structure. Therefore there needs to be depictions of the structure concerned.

The first three forms of alkanes can be presented in **Figure 6** as follows.

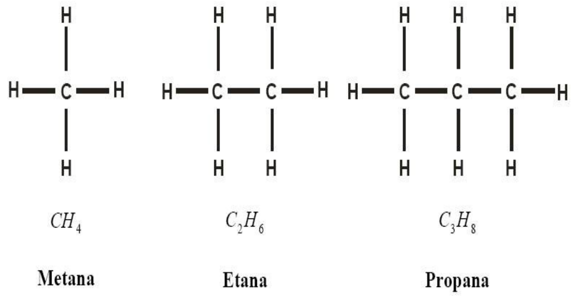


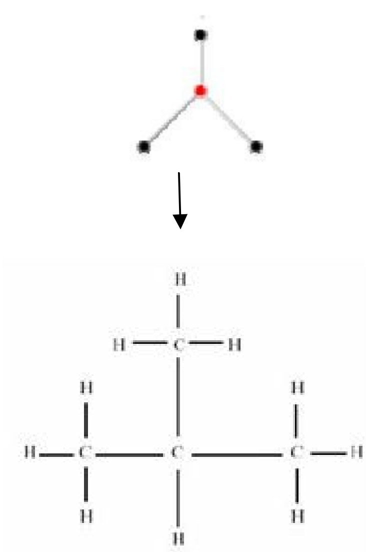
Figure 6. Three first form of Alkanes

The three types of alkanes above have only one isomer. For n> 4 can be obtained more than one isomer CnH2n +2. **Figure 7** are isomers of Butane and Pentane as determined using the Draw and Count method, which has two isomers of Butane and Pentane has three isomers. Calculation of isomers would be very easy to do when n is small, but very difficult to do when n is large, because it will take a long time, even the possibility of doing a big mistake. Therefore, the chapter is done through a mathematical calculation using the Cayley.

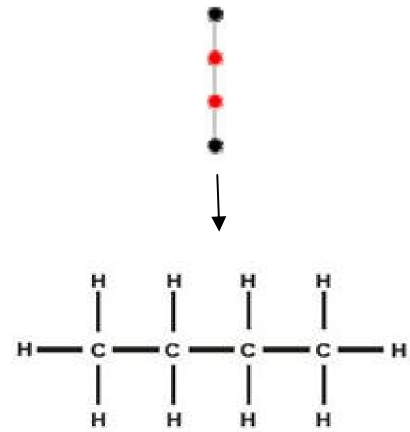
According to **Cayley's theorem** has been proved that alkanes are the trees when viewed in terms of mathematics. Therefore, for more details how the graphs are very important in theoretical chemistry, particularly in determining the number of isomers of alkanes, below will be presented in a graphical representation of the calculation of alkanes which of course uses the concept of Bicentered Centered Tree and Tree. Graph representation is presented in **Figure 7** that the compounds butane (C4H10) and compound Pentane (C5H12).

Representation of Graph in Butane (C_4H_{10})

Centered

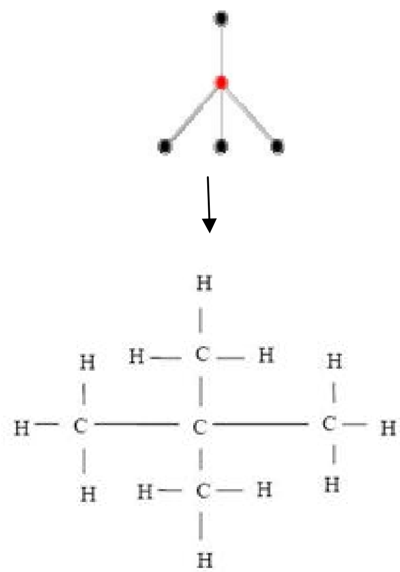


Bicentered

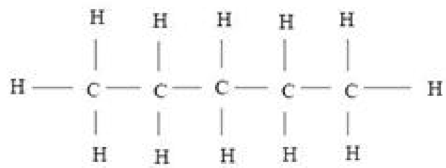


Representation of Graph in Pentane (C_5H_{12})

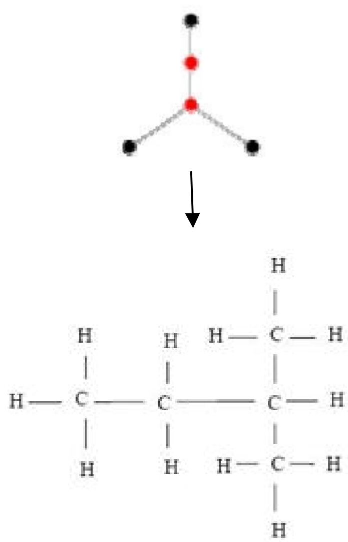
Centered



Centered



Bicentered



Picture 7. Butane and Pentane

Graphic representation of the compounds butane (C4H10) and compound Pentane (C5H12) through the concept and Bicentered Centered in **Figure 7** shows the relationship between graph theory and chemistry. Through the concept of Cayley graph theory to simplify many calculations alkane isomers. Therefore, many alkane isomers can be seen the results in **Table 2**, because in many alkane isomers determine exactly the same as in determining the graph isomorphic much can be formed from the molecular formula of alkanes is CnH2n +2.

5 CONCLUSION

The conclusion that can be drawn from the discussion in this paper is as follows:

1. The structure of chemical compounds, especially alkanes with the formula CnH2n +2 is the graph tree, because they meet E (G) = V(G) − 1. Does acyclic alkanes in which each vertex serajat one or four, so that in his discussion uses the concept of 4-Cayley.
2. The number of isomers of alkanes determined by the amount Bicentered Centered Tree and Tree. Are as follows:

n	*Centered*	*Bicentered*	Total
1	1	0	1
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4	1	1	2
5	2	1	3
6	2	3	5
7	6	3	9
8	9	9	18
9	20	15	35
10	37	38	75
...	...	...	...

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