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Constructions and Enumeration Methods for Cubic Graphs and Trees

Erica R. Gilliland
Butler University

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Read, approved, and signed by:

Thesis adviser(s): Prem Sharma — 4-22-'13
Date

Date

Reader(s): William Johnston — 4-22-2013
Date

Date

Certified by: Judith Harper Morrel — 9-16-13
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Constructions and Enumeration Methods for Cubic Graphs and Trees

Erica R. Gilliland

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Erica R. Gilliland

Under the supervision of Dr. Prem Sharma

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Contents

1 Introduction

The goal of this thesis is to study two related problems that, in the broadest terms, lie in a branch of mathematics called *graph theory*. The first problem examines some new techniques for constructing a Hamiltonian graph of least possible order and having a preassigned girth, and the second concerns the enumeration of a certain type of graphs called trees.

Graph theory is a highly developed subject with scores of textbooks and thousands of research articles devoted to it. The origins of graph theory predate Euclid's *Elements*, written c. 300 B.C. It was around 400 B.C. that Plato and his disciples proved that only five perfect polyhedra can exist in the 3-dimensional space we live in. Euclid's *Elements Book XIII*, devoted to the construction of these polyhedra, enumerates them thus: the tetrahedron (four triangular faces), the cube, the octahedron (eight triangular faces), the dodecahedron (12 pentagonal faces), and the icosahedron (20 triangular faces) [2]. According to the famed British philosopher and mathematician Bertrand Russell, *"Elements is certainly one of the greatest books ever written."* It is only fitting that an account of these so-called Platonic solids be a part of this hallowed book.

The five perfect polyhedra are much more than simply geometric specimens of perfection in nature. They contain the seminal idea behind what we today call the regular graphs. In fact, the tetrahedron, the cube, and the dodecahedron, considered in terms of their vertices and edges (ignoring the faces), are all cubic graphs, and the remaining two solids are regular graphs but not cubic. Inexplicably, the idea of graph theory had to wait nearly another two millenia after Plato's discovery for a systematic development of this subject; even then, it was by a shear happenstance that the idea sprang up. There were seven bridges across the river that flowed through the town of Königsberg. The Sunday strollers in the town always wondered if it was possible to cross all the seven bridges without crossing any bridge more than once. This problem ultimately got conveyed to the great mathematician Euler, who analyzed the problem by sketching a schematic diagram of the placements of the bridges — relative to the banks of the river and to each other — and proved conclusively that the stroller's conjecture was indeed mathematically impossible. Euler's approach to solving the problem marked the rite of passage for graph theory to become a serious topic of mathematical study.

1.1 Basics of Graph Theory

Definitions

A **graph** G is an ordered pair of disjoint sets (V, E) such that E is a collection of 2-subsets of V: V is the set of **vertices** and E the set of **edges** of G. The **order** of G is simply the number of vertices, $|V|$. A graph of finite order is called a **finite graph**. In this study, all graphs are assumed to be finite. The **weight** of G, denoted by $w(G)$ or simply by w, is the number of edges, $|E|$.

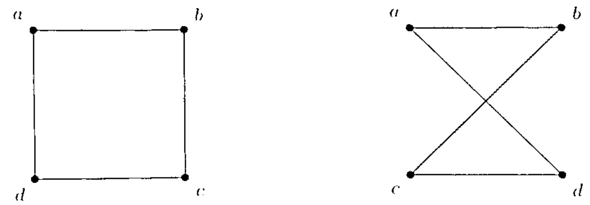
The edge $\{x, y\}$ is said to **join** the vertices x and y and is denoted by xy. The edge xy is the same as yx. The vertices x and y are the **endvertices** of xy. If $xy \in E$, then x and y are **adjacent** or **neighboring vertices** of G and are said to be **incident** with the edge xy. Two **adjacent edges** have exactly one common endvertex. The **complement** of $G = (V, E)$, denoted $\overline{G}$, is the graph on the vertex set V such that for any distinct vertices x and y in V, xy is an edge in $\overline{G} \iff xy \notin E$.

There are structures similar to graphs called pseudographs. For example, a directed graph is one in which the edges are taken as a set of ordered pairs (x, y) of vertices. In such a pseudograph, exactly one of the ordered pairs (x, y) or (y, x) is chosen as an edge. If an ordered pair (x, x) is allowed as an edge, it is called a **loop**. Sometimes weights are assigned to edges to get what we call **weighted graphs**.

Even though we have defined a graph as a pair (V, E), we usually do not think of a graph in those terms. Instead, we draw a diagram in which vertices are represented by dots (in bold) and edges by line segments (not necessarily straight). For more discussion on different drawings of graphs, see the Appendix. A diagram of a graph is only intended to convey the incidence relation between vertices and edges in the graph and has no other geometrical significance. The same graph can usually be drawn in many different ways that may appear quite different from each other. Consider the following example.

Example 1:

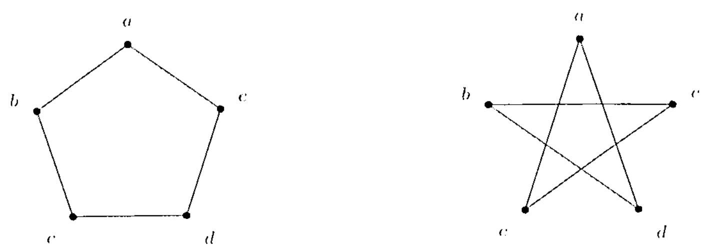
The following two diagrams both represent the graph $G = (V, E)$, where $V = \{a, b, c, d\}$ and $E = \{ab, bc, cd, da\}$.



Naturally the question arises: How can one tell by looking at two diagrams whether they represent the same graph or not? To answer this question, we introduce the notion of an isomorphism of graphs. Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are said to be **isomorphic** if there is a bijection $f : V_1 \to V_2$ such that $\forall x \forall y [xy \in E_1 \iff f(x)f(y) \in E_2]$. Such a bijection is called an **isomorphism** from G_1 onto G_2. If no isomorphism exists from G_1 onto G_2, then the G_1 and G_2 are **nonisomorphic**. An isomorphism from a graph G onto itself is called an **automorphism** of G. The set of automorphisms of a graph G, denoted by $\mathcal{A}(G)$, forms a group under composition (see Appendix for more information on groups).

Example 2:

The following two diagrams show a graph and its complement side-by-side.



Though the two diagrams appear quite different, the two graphs are, in fact, isomorphic.

Definitions

The **degree** of a vertex $x \in V$, denoted $deg(x)$, is defined as the number of vertices that are joined to x. A **pendant vertex** is of degree one. A vertex of degree zero is called an **isolated vertex**. A graph G is said to be **k-regular** if each vertex of G has degree k. 3-regular graphs are called **cubic graphs**.

Theorem 1.1 (Handshaking Lemma). *In a graph $G = (V, E)$, $\sum_{x \in V} deg(x) = 2|E|$.*

Proof. Each edge contributes a count of two towards the sum of degrees. Thus $\sum_{x \in V} deg(x) = 2|E|$. □

Corollary 1.2. *In a finite graph, the number of vertices of odd degree is always even.*

If $G = (V, E)$ and $G' = (V', E')$ are graphs such that $V' \subset V$, and $E' \subset E$, then G' is said to be a **subgraph** of G. If $G = (V, E)$ is a graph and $x \in V$, the subgraph obtained by deleting x (and all edges that contain x) is denoted by G/x. Similarly, if $A \subset V$, then G/A is the subgraph obtained from G by deleting all the vertices in A (along any edge incident with at least one vertex in A).

Two vertices x and y of a graph G are called **similar** and we write $x \sim y$ if there exists $f \in \mathcal{A}(G)$ such that $f(x) = y$. Obviously, for x and y to be similar, it is necessary that the degree of x be same as that of y. In particular, an isolated vertex can only be similar to an isolated vertex and a pendant vertex only to a pendant vertex. Similarity of vertices is an equivalence relation on V, and so it partitions V into equivalence classes called the **similarity classes**. The number of similarity classes of pendant vertices of G is denoted by $scp(G)$.

Theorem 1.3. *If two graphs are isomorphic, then the graphs resulting from removing their pendant vertices are also isomorphic.*

Proof. Suppose $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic graphs. Let $P_1 \subset V_1$ and $P_2 \subset V_2$ be the sets of all pendant vertices in G_1 and G_2 and let $f : V_1 \to V_2$ be an isomorphism of G_1 and G_2. Since an isomorphism maps a pendant vertex to only a pendant vertex, f is also an isomorphism from P_1 to P_2 as well as from V_1/P_1 to V_2/P_2. Therefore, the graphs resulting from removing the pendant vertices of G_1 onto G_2 are isomorphic. □

Definitions

A **walk** in a graph G is defined as an alternating sequence of vertices and edges, such as

$$W: x_0, x_0x_1, x_1, x_1x_2, x_2, x_2x_3, x_3, \ldots, x_{k-1}, x_{k-1}x_k, x_k.$$

Such a walk is briefly written as $W: x_0x_1x_2x_3 \ldots x_{k-1}x_k$ and is often referenced as an x_0-x_k walk. The **length** of W is the number of edges in W, or k. A walk of length 0 is called a **trivial walk**. If $x_0 \neq x_k$, the walk is said to be **open**. If $x_0 = x_k$, the walk is said to be **closed**. If no edge is repeated, the walk is called a **trail**. If no vertex is repeated, the walk is called a **path**. A closed trail is called a **circuit** and a closed path is called a **cycle**. P_n denotes a path of length n and C_n denotes a cycle of length n. The shortest cycle possible is C_3. A graph is said to be **connected** if there exists a path between any two vertices. A graph is said to be **disconnected** if it is not connected. By a **component** of a graph G, we mean a connected subgraph of G which is not properly contained in any connected subgraph of G.

Definition 1 A connected graph that contains no cycles is called a tree. By a **subtree** S of a tree T, we mean a subgraph S of T that is also a tree.

Theorem 1.4. *Any tree $T = (V, E)$ with $|V| \geq 2$, has at least two pendant vertices.*

Proof. Since $|V| \geq 2$, $\exists x, y \in V$ such that $x \neq y$. Since T is connected, there is a path p between x and y. Let p_0 be a longest path containing the path p (such a path will exist because T is finite). Then each of the endpoints of p_0 must have degree 1. □

Theorem 1.5. *If x is a pendant vertex in a tree T, then the T/x is a subtree of T.*

Theorem 1.6. *[6] For any tree $T = (V, E)$, $|V| = |E| + 1$.*

Proof. We prove this theorem by inducting on the number of vertices in T. If $|V| = 1$, then clearly $|E| = 0$ and thus the equation $|V| = |E| + 1$ holds in this case. Now assume that there exists a positive integer n such that the theorem holds for all trees having n vertices. Let T be a tree on $n + 1$ vertices. Then T has at least two pendant vertices. Let x be a pendant vertex in T. Then T/x is a tree on n vertices, and by the induction hypothesis the theorem holds for T/x. Since T has exactly one more vertex and one more edge than T/x, the theorem holds for T as well. Hence for any tree T, $|V| = |E| + 1$. □

Definitions

If a trail contains all the edges in a graph, it is called an **Euler trail** or an **Euler circuit**, depending on if it is open or closed. If a path contains all the vertices in a graph, it is called a **Hamilton path** or a **Hamiltonian cycle**, depending on if it is open or closed. A graph that contains a Hamilton cycle will be referenced as a **Hamilton graph** in this paper. The **girth** of a graph G is the length of the shortest cycle in G and is denoted by g. A **k-g graph** is a k-regular graph whose girth is g. If a graph contains no cycle, then we say that the girth of G is infinite. For given k and g, a k-g graph on the least number of vertices possible is called a k-g **cage**. Another notation that is used to indicate a k-g graph is (k, g).

The **distance** between vertices x and y in a graph, denoted $d(x, y)$, is the length of the shortest path between x and y. If there is no path between x and y, then $d(x, y) = \infty$. The **eccentricity**

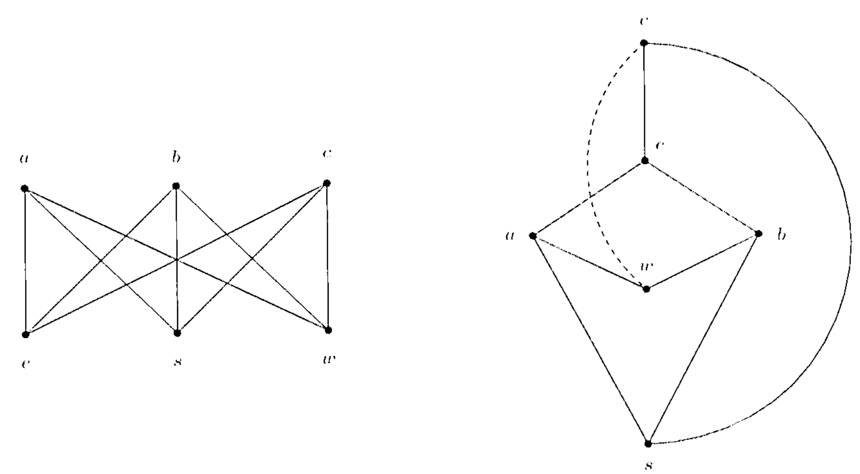
$\epsilon(x)$ of a vertex $x \in V$ is $max\{d(x,y) : y \in V\}$. The diameter $diam(G)$ of G is $max\{\epsilon(x) : x \in V\}$. The **radius** of G, $rad(G)$, is $min\{\epsilon(x) : x \in V\}$. Any $x \in V$ for which $\epsilon(x) = rad(G)$ is called a **center** of G. A graph G can have several centers. For example, a path of even order has two centers and a cycle has all its vertices as centers.

1.2 Some Examples of Graphs

Example 3 (The utility graph):

Suppose each of three houses a, b, c is to be hooked up with each of three utilities e, s, and w (e for electricity, s for sewage, and w for water). In the figure below, each of the two diagrams encodes the adjacency relationship between the houses and utilities completely; however, the left diagram shows too many edge-crossings because of a poor placement of the houses relative to the utilities. The right diagram contains only one edge-crossing. It can be proved that any placement of the six vertices of the utility graph in the plane will always have at least one edge-crossing. The following two diagrams are isomorphic as graphs, but not geometrically or topologically isomorphic.

Figure 1: The utility graph



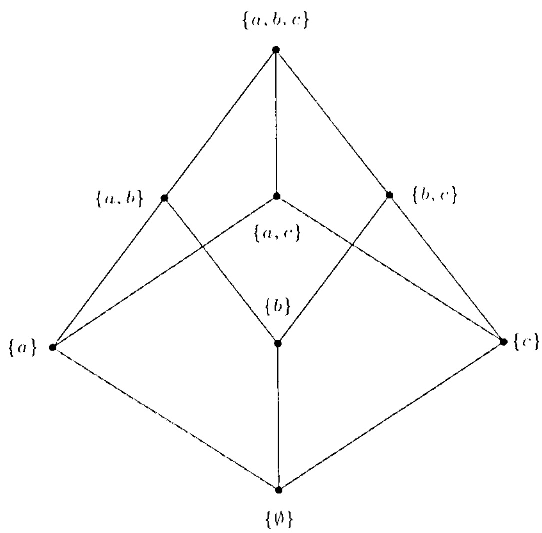
What is an isomorphism?

In set theory, two sets X and Y are said to be isomorphic (equivalent) if there is a bijection from X onto Y. The rationals $\mathbb{Q}$ and the integers $\mathbb{Z}$ are isomorphic as sets. However, they are not isomorphic as additive groups nor are they as linearly ordered sets. Similarly, the integers $\mathbb{Z}$ and the positive integers $\mathbb{Z}^+$ are isomorphic as sets but not as ordered sets (e.g., $\mathbb{Z}^+$ is well-ordered whereas

$\mathbb{Z}$ is not). In classical geometry, we consider two objects are isomorphic (identical, congruent) if it is possible to move one of them by a rigid transformation (translation, rotation, reflection) to occupy exactly the same place as the other. In topology, two objects are said to be isomorphic (homeomorphic, topologically equivalent) if there is a continuous bijection from one onto the other with its inverse also continuous. For example, the boundary of a square is homeomorphic to any simple enclosed curve (e.g. a circle or an ellipse). In graph theory, two graphs are isomorphic if there is an adjacency-preserving bijection between the vertices. Thus, whether two objects are isomorphic or not does not depend on the objects alone, but also on the categories in which choose to we place them.

Example 4:

Call two subsets S and T of the set $X = \{a, b, c\}$ neighbors if $|S \Delta T| = 1$, where $S\Delta T = |S \cup T| - |S \cap T|$. This defines an adjacency relation on the eight subsets of X which is encoded in the following diagram.



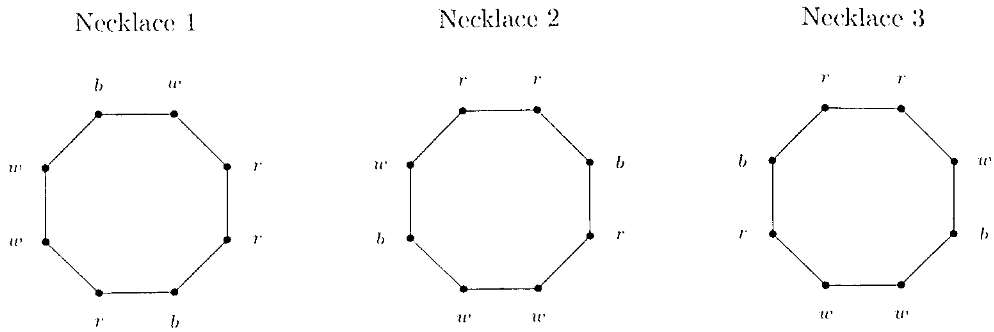
The preceding graph contains the Hamiltonian cycle $\{\emptyset\} \to \{a\} \to \{a, b\} \to \{b\} \to \{b, c\} \to \{a, b, c\} \to \{a, c\} \to \{c\} \to \{\emptyset\}$.

Definition

A function f from a set X to a set Y is called a **coloring** of X and the elements of Y are called the colors.

Example 5 (The necklace problem):

Suppose we want to string a necklace with eight beads, each of which can be any one of three given colors, say red, blue and white (or simply r, b, w). Mathematically, we will think of such a necklace as a regular octagon, with its vertices considered as beads. Naturally the question arises: How many such different necklaces are possible? The answer to this question depends on what we mean by "different" necklaces.



The preceding diagrams illustrate three possible colorings of the necklace. Necklace 2 is obtained by rotating Necklace 1, and Necklace 3 by turning over Necklace 2. Are we to consider Necklaces 1 & 2 the same? Should we consider all three necklaces the same? We now answer these questions systematically.

Let X represent the set of vertices and Y the set of colors. If the vertices of the octagon are labeled, then there are 3^8 different necklaces, because there are that many functions from X to Y. Now suppose we consider two colorings, f and g, to be the same if there exits a rotation α of the octagon such that $f = g \circ \alpha$. This relationship between f and g is an equivalence on the set of 3^8 colorings, and it can be shown that there are exactly 834 equivalence classes. Thus, modulo the rotation group of the octagon, there are 834 different necklaces. Lastly, if we permit both rotations and reflections to define the equivalence relation on the set of 28 colorings, we can show that there are only 498 different necklaces. To learn more about how we calculated these numbers, see the Appendix.

In this thesis, we study two special categories of graphs called *cubic graphs* and *trees*. Both of these categories have been extensively studied. As in any branch of mathematics, there are an untold number of open problems relating to them. The great mathematician Arthur Cayley (1821-1895) forged a singularly powerful method applying group theory (another prominent area of knowledge in mathematics) to build cubic graphs of as high a girth as one may desire. It is to be noted that Cayley's method begins by first constructing a cubic tree and then obtains a cubic graph from the tree. In addition, we will also explore the concept of weight distribution at the vertices of a tree and the existence of a special vertex (sometimes two) in a tree called the centroid(s). Together, these concepts will help us to construct an algorithm for counting a specific type of trees that represents the 2-d graphs of alkane molecules.

2 Cubic Graphs

Recall that a cubic cage of girth g is a cubic graph of girth g with the least possible number of vertices. Cubic graphs have been studied extensively by many famous mathematicians. Molecular biologist and Nobel laureate Joshua Lederberg found important applications of cubic graphs to describe molecular structures.

By the Handshaking Lemma, the number of vertices in a cubic graph must necessarily be even. A cubic graph on $2n$ ($n \geq 2$) vertices can easily be constructed by starting with a regular $2n$-gon and then joining each vertex to the one directly opposite to it. However, such a graph will always have girth $g \leq 4$. The following is an outstanding open problem in cubic graphs:

For each given positive integer g, determine the order of a cubic cage of girth g.

So far this problem has been settled for $3 \leq g \leq 12$. For higher values of g, only bounds are known. We now give examples of some cubic cages and Hamiltonian cubic graphs. Figure 2 is a cubic cage of girth three; the complete bipartite graph $K_{3,3}$, which was shown in Figure 1, is a cubic cage of girth four. The Peterson graph (Figure 8) is a cubic cage of girth five. Figure 5 is a cubic cage of girth six on 14 vertices.

Figure 2: (3,3) cage

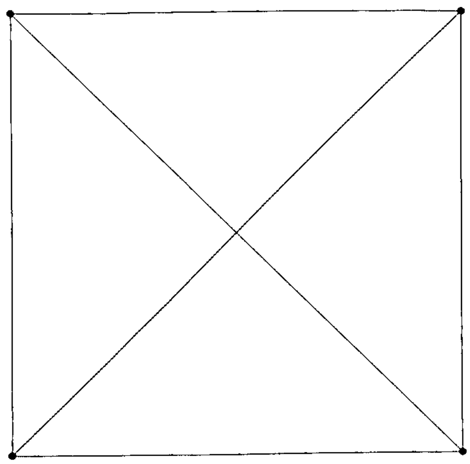


Figure 3: A (3,4) graph on eight vertices—a cube

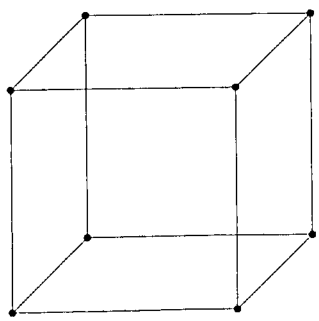


Figure 4: A (3,6) Hamiltonian graph on 16 vertices

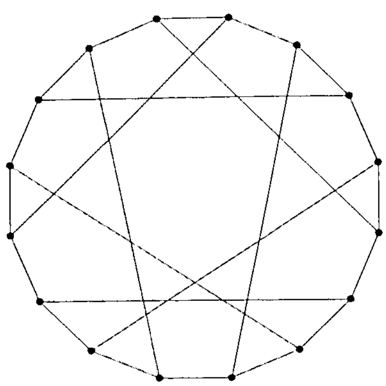
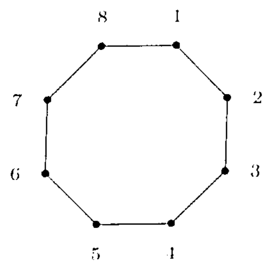


Figure 3 is a cubic graph on eight vertices of girth four. Since $K_{3,3}$ is a cubic cage of girth four but has only six vertices, the cube is not a cage.

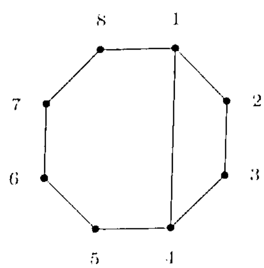
2.1 LCF Notation

In 1965, American Nobel Prize winner Joshua Lederberg first developed a simplified notation for constructing cubic Hamiltonian graphs by starting with a Hamiltonian cycle [8]. The idea was later refined by Harold Coxeter in 1981 and Robert Frucht in 1976, thus deriving the name LCF notation. To use this notation, one starts with a Himiltonian cycle and then adds more edges to it according to a suitable scheme. **Let us explain the LCF notation $[3, -3]^4$.**

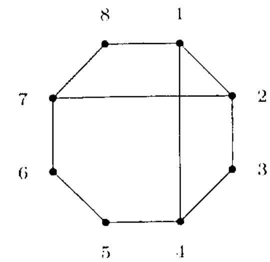
Step 1: Start with a Hamiltonian cycle on eight vertices (the LCF notation has two numbers within the brackets and superscript four, $2x4 = 8$). Label the vertices one through eight.



Step 2: The first entry in the LCF notation is three, so join vertex one to four $(1 + 3)$.

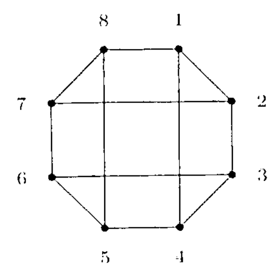


Step 3: Next join vertex two to seven ($2 - 3 = 7(mod\ 8)$).



Final Steps:

The superscript four in the LCF notation indicates that this pattern of adding three then subtracting three is repeated four times. If you reach a vertex that is already of degree three, skip that step in the pattern (don't create a loop). Once all of the vertices are of degree three, we have finished constructing the cubic graph described by the given LCF notation.



Below are two additional examples of graphs and their LCF notation.

Figure 5: A (3,6) cage with LCF notation $[-5, 5]^7$

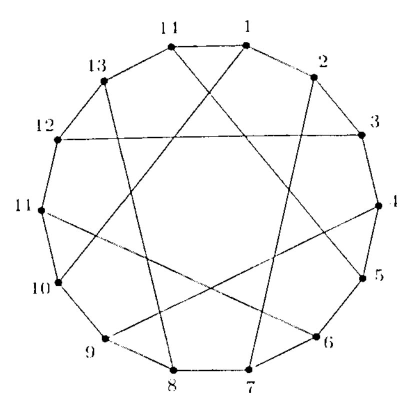
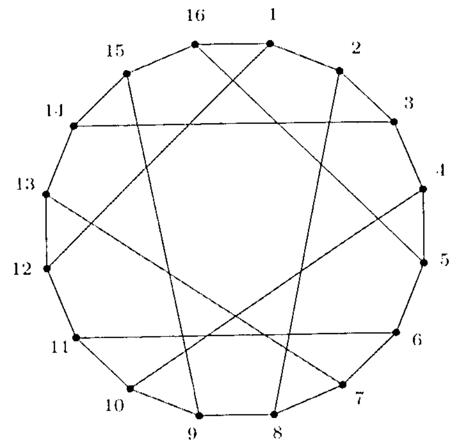


Figure 6: A (3,6) graph on 16 vertices with LCF notation [-5,6,-5,6,-5,5,6,-6,6,-6,-5,5,-6,5,-6,5]

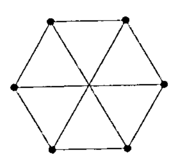


2.2 Construction of Cubic Graphs

While constructing a cubic graph is not difficult, discovering cubic cages is a fiendishly difficult problem. The following four constructions are examples of different ways to construct cubic graphs of varying girths. Though not all of these constructions produce cages, but they outline techniques taht yield graphs of higher girths.

Construction 1: For $n \geq 2$, take $2n$ equally spaced vertices on a circle and label them one through $2n$. For each i, $1 \leq i \leq 2n$, join the vertex i with $i-1$, $i+1$, and $i+n$. This gives a cubic graph of girth at most four. In this and all other similar constructions that follow, the arithmetic on the numbered vertices is *mod n*.

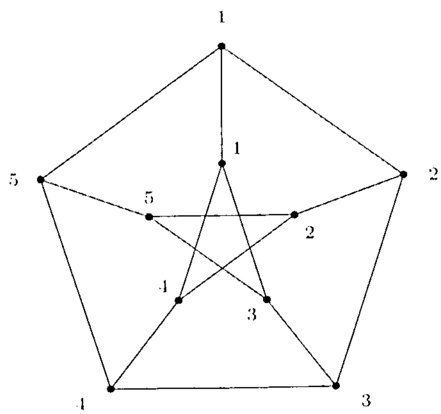
Figure 7: Construction 1 with $2n = 6$



Construction 2: Take two concentric circles. Choose n ($n \geq 5$) equally spaced vertices on the outer circle and label them one through n. Take the corresponding n vertices on the inner circle and label each with the same number assigned to its corresponding one on the outer circle. Join each vertex i on the outer circle to vertices $i+1$ and $i-1$ on that circle. Next, choose a positive integer k relatively prime to n, $1 < k < n$. On the inner circle, join vertex i to both vertices $i+k$ and $i-k$.

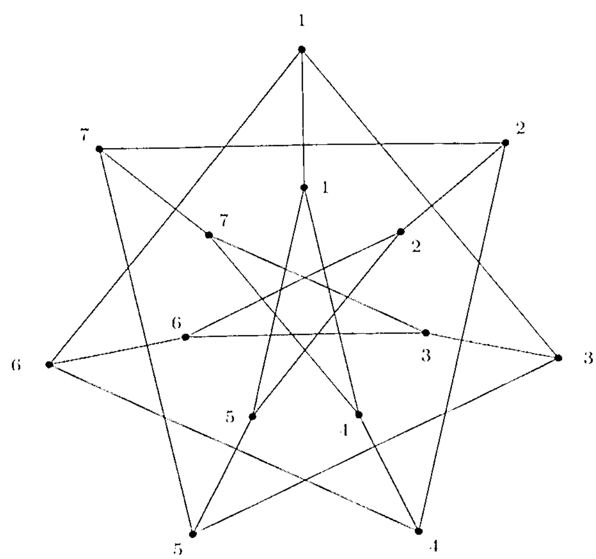
Finally, join each vertex i on the outer circle to the corresponding vertex i on the inner circle. This construction coded as $[n/1, n/k]$ yields a cubic graph.

Figure 8: Peterson graph [5/1,5/2]



In Figure 9, each vertex i in the outer circle is joined to $i + 2 (\mathrm{mod}\ 7)$ and each vertex i in the inner circle is joined to $i + 3 (\mathrm{mod}\ 7)$.

Figure 9: [7/2,7/3]

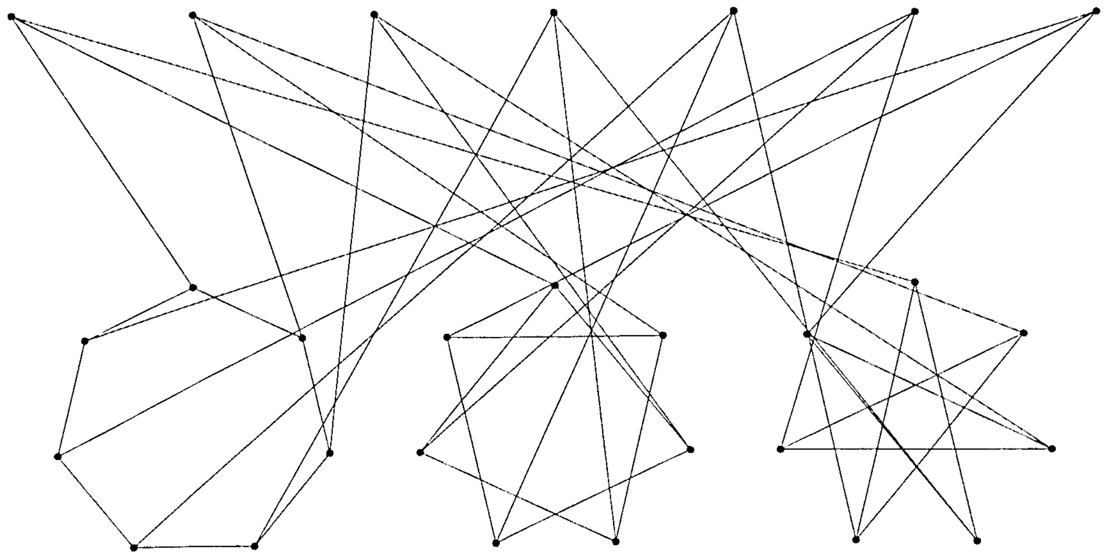


Construction 3: This construction is coded as $[n/0, n/1, n/b, n/c]$. The code indicates that we take n vertices on each of four concentric circles. While the meaning of $n/a, n/b, n/c$ is clear, $n/0$

means that no two vertices on the outermost circle are to be joined to each other. Each vertex on the outermost circle is joined to each of its three corresponding vertices on the three inner circles. No edge is drawn from a vertex on one inner circle to another on the other inner circle.

In Figure 10, the top line of vertices has no two vertices joined to each other.

Figure 10: [7/0, 7/1, 7/2, 7/3]



Construction 4: This construction of cubic graphs is given in Dr. Norman Biggs' paper *Constructions of Cubic Graphs with Large Girth* and utilizes permutation groups (see the Appendix for more information on group theory) [1]. Suppose X is a set and S is a set of permutations of X that is closed under inversions and does not contain the identity. The set S generates a subgroup $\langle S \rangle$ of the symmetric group $Sym(X)$ of X contains all the permutations of X. A **Cayley graph** $Cay(S)$ is defined to be the graph whose vertices $x, y \in \langle S \rangle$, with x and y being joined by an edge if $yx^{-1} \in S$. If $S = \{\alpha_1, \alpha_2, \ldots, \alpha_k\}$, the vertex x is adjacent to $\alpha_1 x, \alpha_2 x, \ldots, \alpha_k x$. Since S is closed under inversions, yx is also included in $Cay(S)$; thus xy is not a directed edge.

Any cycle of length r in $Cay(S)$ can be constructed from:

$$x, \omega_1 x, \omega_2\omega_1 x, \ldots, \omega_r \cdots \omega_2\omega_1 x.$$

where each $\omega_i \in S$, $\omega_r \cdots \omega_2\omega_1$ is the identity permutation: $\omega_i \neq {\omega_{i+1}}^{-1}$ $(1 \leq i \leq r-1)$ and $\omega_r \neq {\omega_1}^{-1}$. If this condition holds, we say that $w_r \cdots w_2 w_1$ is an **identity word**. To find the girth of a Cayley graph, you must find the shortest identity word.

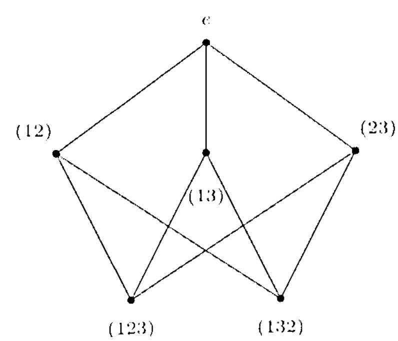
Using this construction, there are two kinds of generating sets S that construct cubic Cayley graphs.

- Type 1: $S = \{\alpha, \beta, \gamma\}$, where all three generators are involutions (elements of order two).

- Type 2: $S = \{\alpha, \delta, \delta^{-1}\}$, where α is an involution and δ is not.

Example 6:

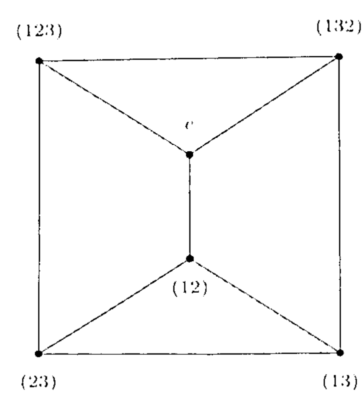
The sets $X = \{1, 2, 3\}$ and $S = \{(12), (13), (23)\}$ produce a Cayley graph of Type 1. In this example, $\langle S \rangle = \{e, (12), (13), (23), (123), (321)\} = Sym(X)$ are the six vertices of this graph. The full graph is shown below:



Here, a shortest identity word is $(13)(23)(13)(12)$. Therefore the girth of the graph is four.

Example 7:

The sets $X = \{1, 2, 3\}$ and $S = \{(12), (123), (321)\}$ give a Cayley graph of Type 2. In this example, $\langle S \rangle = \{e, (12), (123), (132), (13), (23)\} = Sym(X)$ as well.



Here, a shortest identity word is $(123)^3$. Therefore the girth of the graph is three.

Under this construction, we begin to see a clearer connection between cubic graphs and trees. When we begin to construct cubic graphs in this manner, their formation first looks like trees. Eventually, the construction tells us how to connect vertices in such a way that we achieve a given girth and eventually complete the cubic graph. In our examples, our starting vertex is e, which we say is at level zero. Next, we join e with each element in S, and these vertices are said to be at level one. So far, we have a tree of height one with three pendant vertices. From there, our edge relationships tell us how to continue to add vertices or join existing ones. If our graph is currently still a tree at height k, then the girth $g \leq 2k+1$. To achieve $g > 2k+1$, we necessarily need some vertices at the level $k+1$.

Figure 11: Diagram of Example 6 showing beginning tree structure

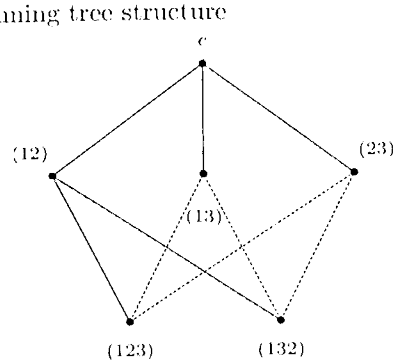
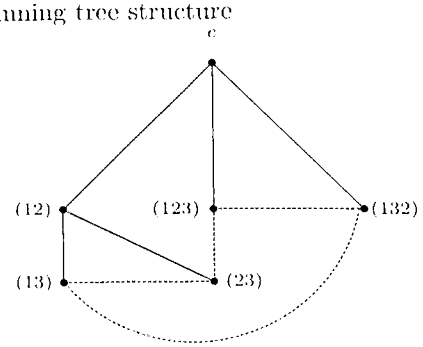


Figure 12: Diagram of Example 7 showing beginning tree structure



2.3 Cubic Cages

2.3.1 Bounds on the Order of Cubic Cages

Let x be a vertex in a cubic graph G with odd girth g. We know that x must have three neighbors, and each of those vertices must have two additional unique neighbors for $g \geq 5$. This pattern would continue until we reached a level where we would then join two existing vertices to create the desired odd girth.

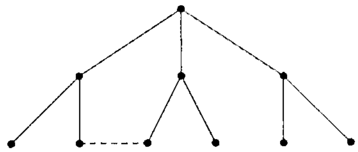


Figure 13: Beginnings of cubic graph with $g = 5$

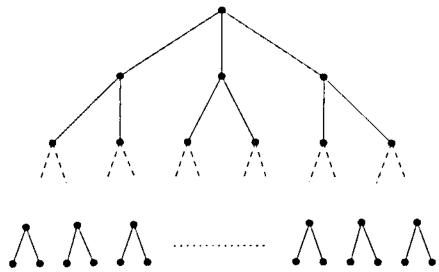


Figure 14: Adding levels of unique neighbors

This pattern of adding unique neighbors generates a formula for the smallest number of vertices possible for a cubic graph of odd girth. The final row would have $\frac{g-3}{2}$ unique neighbors.

Formula 1 (Lower bound for cubic cages with odd girth).

$$\begin{aligned} 1 + 3 + 3 \cdot 2 + 3 \cdot 2^2 + \cdots + 3 \cdot 2^{\frac{g-3}{2}} &= 1 + 3(1 + 2 + 2^2 + \cdots + 2^{\frac{g-3}{2}}) \\ &= 3 \cdot 2^{\frac{g-1}{2}} - 2 \end{aligned}$$

Similarly, by starting with two vertices, a formula can be derived for the lower bound of cubic cages with even girth.

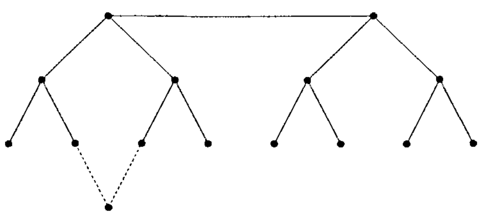


Figure 15: Beginnings of cubic graph with $g = 6$

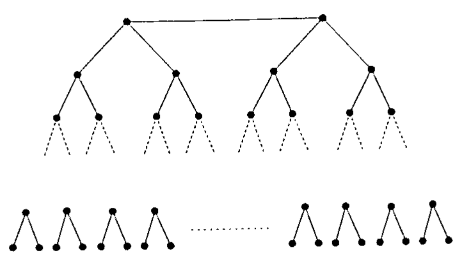


Figure 16: Adding levels of unique neighbors

Formula 2 (Lower bound for cubic cages with even girth).

$$2 + 2^2 + 2^3 + \cdots + 2^{\frac{g}{2}} = 2^{\frac{g+2}{2}} - 2$$

Since one can almost never achieve a cubic cage at these lower bounds and the number of vertices must always be even, we can assume the following formulas to calculate the lower bound $v_0(g)$ of a cubic cage with girth g.

Formula 3 (Lower bound for cubic cages).

$$v_0(g) = \begin{cases} 3 \cdot 2^{\frac{g-1}{2}} & \text{if } g \text{ is odd} \\ 2^{\frac{g}{2}} & \text{if } g \text{ is even} \end{cases}$$

Using the same construction, the upper bound $\lambda(g)$ could similarly be established so that $\lambda(g) = 3 \cdot 2^g - 2$, but an improved bound has also been proved [1].

Formula 4 (Upper bound for cubic cages).

$$\lambda(g) = 2^g$$

2.3.2 Known Cubic Cages

The problem of constructing a cubic cage of a given girth g has intrigued mathematicians for years. While cages of girths three through eight are relatively simple to construct, many papers have been published on the construction of cubic cages with larger girth. Below is a table listing the known cubic cages and the best bounds for the given girths for which cages are not known. Because cages with increasingly large girths require a large number of vertices, not all of the following table's values have been proved to be the best cages possible, but rather are the current-best.

Table 1 is from the online table populated by Gordon Royle and the 2011 *Dynamic Cage Survey* published by Geoffrey Exoo and Rober Jajcay. The function $v_3(g)$ is the upper bound for the cubic cage of girth g. The number indicates the number of graphs known to meet the given upper bound. Numbers with a "+" next to them are not known to be exact. Some current-best cages of girth larger than 22 have been omitted.

Table 1: Cubic cages of small girth [3]

Cage	$v_0(g)$		Best-Known	$v_3(g)$	Number	Reference
(3,3)	6	*	4	4	1	K_4
(3,4)	4		6	6	1	$K_{3,3}$
(3,5)	12	*	10	10	1	Peterson
(3,6)	8		14	14	1	Heawood
(3,7)	24		24	22	1	McGee graph
(3,8)	16		30	30	1	Tutte's 8-cage
(3,9)	48		58	46	18	Brinkmann/McKay/Saager
(3,10)	32		70	62	3	O'Keefe/Wong
(3,11)	96		112	94 [112]	1	McKay/Myrvold-Balaban
(3,12)	64		126	126	1	Generalized hexagon
(3,13)	192		272	190 [202]	1+	McKay/Myrvold-Hoare
(3,14)	128		384	254 [258]	1+	McKay-Exoo
(3,15)	384		620	382	1+	Biggs
(3,16)	256		960	510	1+	Exoo
(3,17)	768		2176	766	1+	Exoo
(3,18)	512		2640	1022	1+	Exoo
(3,19)	1536		4324	1534	1+	H(47)
(3,20)	1024		6048	2046	1+	Exoo
(3,21)	3072		16028	3070	1+	Exoo
(3,22)	2048		16206	4094	1+	Whitehead S(73)

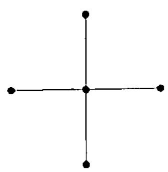
3 Isomers of Alkanes

The study of chemistry deals with molecules and their structures. Molecules are the basic element of chemical compounds. They are formed by atoms which are held together by chemical bonds. While molecules are 3-d chemical structures, some can be easily represented by 2-d mathematical graphs. All molecules are undirected and connected graphs. While not all molecules are trees, we will limit our study to those that are.

Let M_1 and M_2 represent the graphs of two molecules with exactly the same atoms. If M_1 and M_2 are non-isomorphic, then M_1 and M_2 are called **isomers**. The molecules that we are particularly interested in are called alkanes. **Alkanes** are molecules consisting of only carbon and hydrogen atoms and that have only single bonds and no cycles. Therefore, each alkane can be represented by a tree. Any vertex corresponding to a carbon atom must have degree four and any vertex corresponding to a hydrogen atom must have degree one.

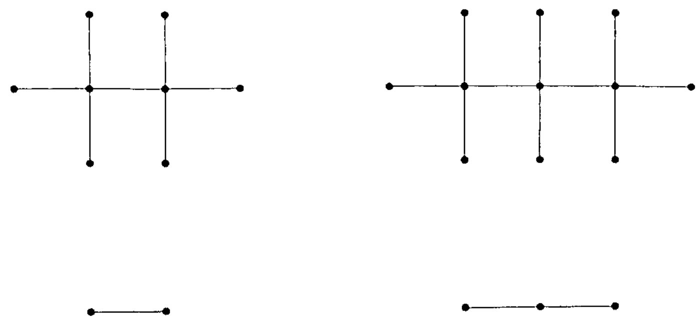
To graph these molecules, each atom is represented by a vertex and each bond is represented by an edge. Therefore, all carbon vertices must be of degree four and all hydrogen vertices must be of degree one.

Figure 17: C_1H_4 (methane) is the most basic alkane.



Because all hydrogen atoms in the graphs of alkanes are pendant vertices, Theorem 1.3 allows us to study just the underlying structure of the carbon atoms. For example, Figure 18 illustrates the graphs of C_2H_6 and C_3H_8 molecules, comparing the true structure of the molecules to the underlying structure of the carbon atoms.

Figure 18: C_2H_6 & C_3H_8



Since removing the hydrogen atoms, or pendant vertices, simplifies the appearance of the graph, from now on we will illustrate alkane graphs using only the underlying structure of the carbon atoms. If you want to construct the true graph of a molecule given the underlying carbon structure, join a hydrogen atom (or pendant vertex) to each carbon atom in the underlying graph until each carbon atom is of degree four.

Suppose an alkane has c carbon atoms. How many hydrogen atoms (h) must also be present?

Let $G = (V, E)$ be the graph of the alkane such that $|V| = v$, $|E| = e$, $x_k \in V$, and G is a tree. Define c as the number of carbon atoms and h as the number of hydrogen atoms in the molecule. According to Theorem 1.1, $\sum_{k=1}^{v} x_k = 2e$. Since the degree of each carbon atom is four and the degree of each hydrogen atom is 1, $\sum_{k=1}^{v} n_k = 4c + h$. But this value is also equal to $2e$. By Theorem 1.6, $v = e + 1$. Since the atoms of a molecule are the vertices in it's graph, $v = c + h$. Therefore $c + h = e + 1$ or $e = c + h - 1$. Combining the two theorems gives the following formula.

Formula 5.

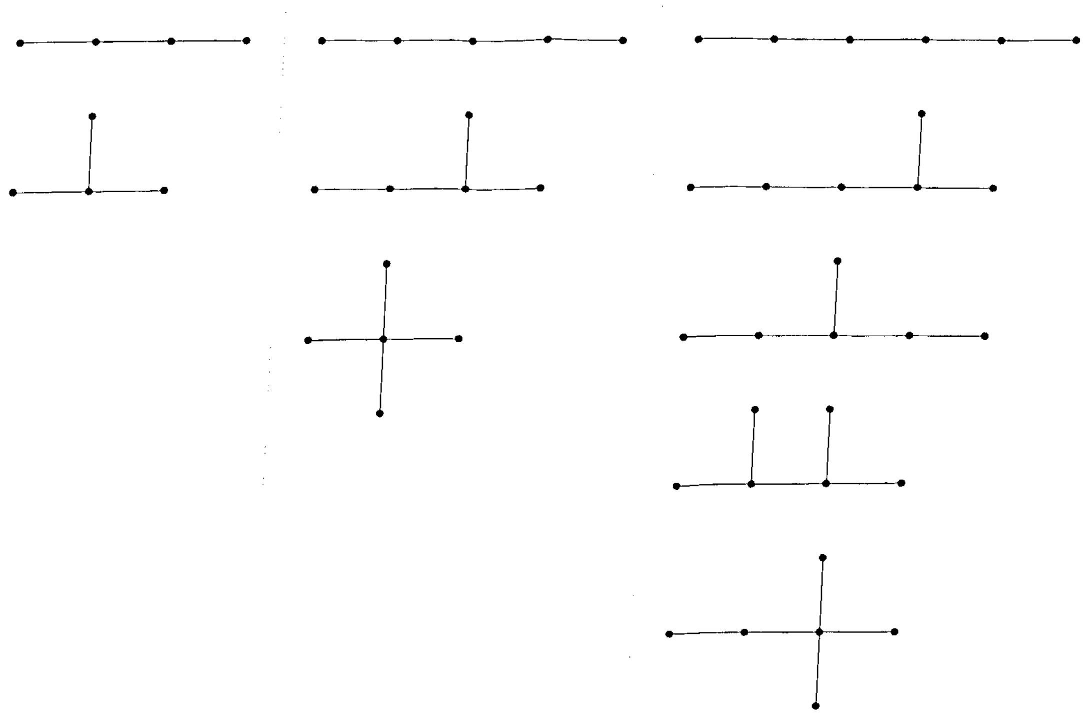
$$4c + h = 2(c + h - 1)$$

$$4c + h = 2c + 2h - 2$$

$$2c + 2 = h$$

Figure 19 sketches the different isomers of alkanes with four to six carbons. The isomers of alkanes with two and three carbons were illustrated in Figure 18.

Figure 19: Isomers of alkanes with four to six carbons



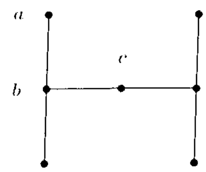
Because the graphs of the underlying carbon structure of alkanes with no cycles are trees, it is relatively simple to count how many isomers there are for such alkanes with a small number of carbons. All you must do is draw all possible nonisomorphic trees on v vertices. As v increases, it becomes increasingly difficult to draw all the nonisomorphic trees on v vertices. An important connection between the study of graph theory and chemistry is knowing how many isomers exists with no cycles for a certain alkane. In this paper, $\tau(n)$ denotes the number of nonisomorphic trees on n vertices with a maximum degree of four.

3.1 Rooted Trees

A **rooted tree** is a particular embedding of a tree that emphasizes how the vertices stem off from a single vertex, called the **root**. The degree of the vertex used as the root is called the **root degree**. Any vertex in a tree can be chosen as a root for a particular embedding of a rooted tree. Once a vertex is chosen, the tree is drawn by **hanging** the branches of that tree from the root. The number of unique hangings that can be drawn for a given tree depends upon the number of similarity classes of the vertices.

Example 8 (Rooted tree hung from three different vertices):

The following graph has three similarity classes of vertices and therefore can be hung as a rooted tree in three different ways.



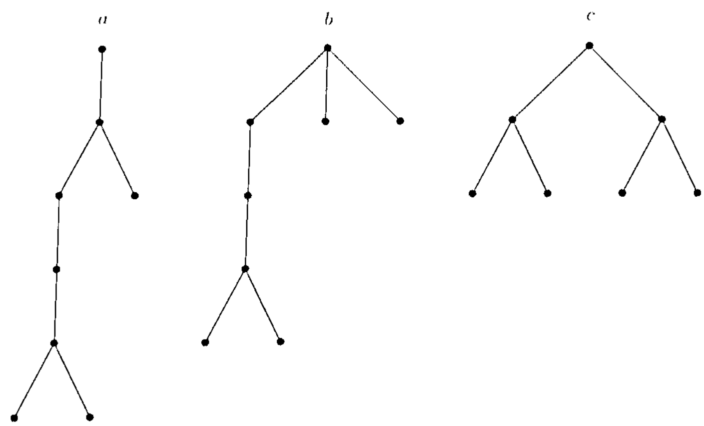
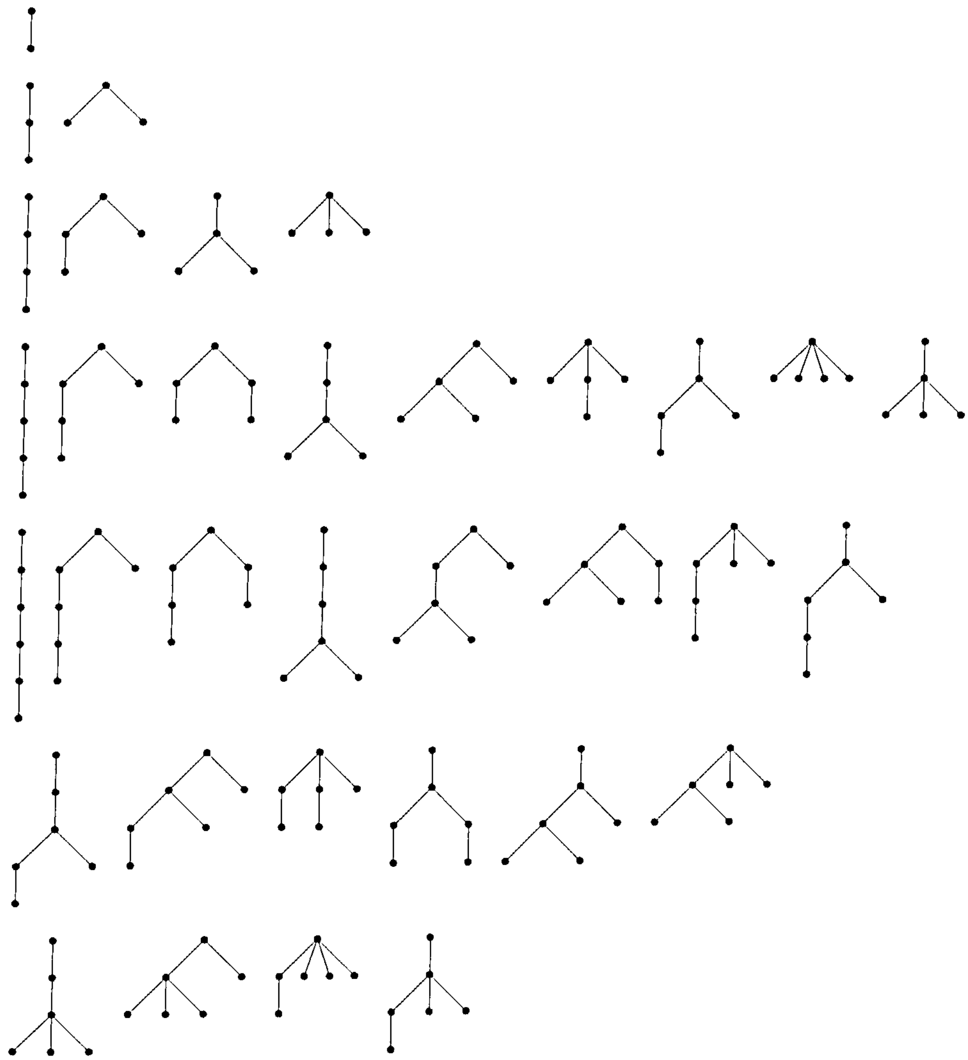


Figure 20 shows the unique rooted trees produced by hanging the various isomers of alkanes with two to six carbon atoms.

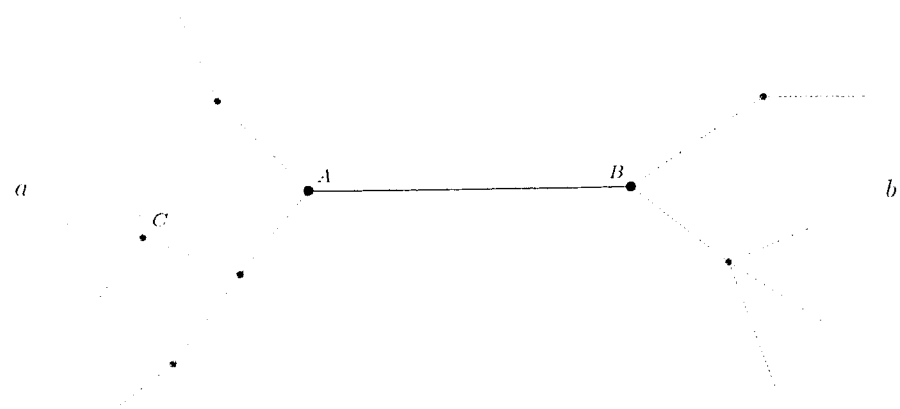
Figure 20: Rooted tree embeddings of Figure 19



Because the graphs of alkanes only contain vertices of degrees less than or equal to four, we will focus our study of rooted trees on these graphs.

3.2 Centroid(s) of a Tree

For any two distinct vertices x_i and x_j in a tree T, there is a unique $x_i - x_j$ path in T. This property, characterizing trees among graphs, will be useful as we introduce some new concepts, meaningful only for trees and not for graphs in general. Two such concepts are the notions of branches at a given vertex and the existence of a centroid (or centroids) in a tree. Our goal in this section is to formulate these concepts precisely and to develop a coherent theory relating to them. In order to bypass the trivial case, we will only consider the trees that have at least two vertices, and from henceforth the term "tree" will only be used in that sense.

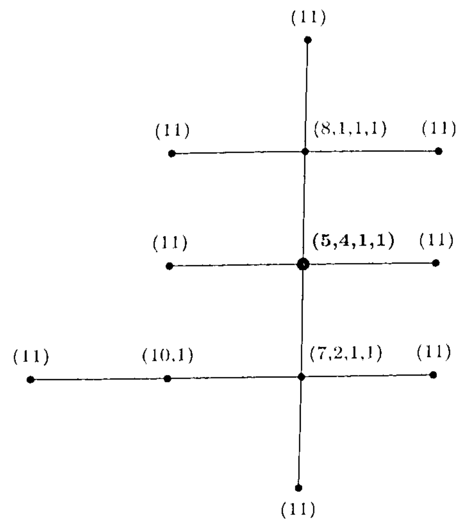


Let A be a fixed vertex in a tree T. The maximal subtree of T having A as an endvertex is called a **branch** of T at A. The number of branches of A must, obviously, equal the degree of A in T. The **weight sequence** of A is the listing in decreasing order of the weights of the branches of A and is usually denoted $(w_1, w_2, \ldots, w_k)$, where $k = deg(A)$. Any given branch of T at A contains a unique neighbor B of A; the directed edge $\overrightarrow{AB}$ is called the **stem** of this branch. A branch at A whose weight is not less than the weight of any other branch at A is called a **principal branch** at A, its weight the **principal weight** at A, and its stem a **principal stem** at A. Of course, there could be several principal branches at A (all of which must necessarily have the same weight). A vertex x_0 of T with the least principal weight is called a **centroid** of T.

Suppose A and B are two neighboring vertices in a tree T. Let a be the total number of edges in all the branches at A, except the branch with the stem $\overrightarrow{AB}$. Similarily, let b denote the total number of edges in all the branches at B except the one with stem $\overrightarrow{BA}$. For convenience, the branch at A with stem $\overrightarrow{AB}$ is denoted by $(AB \rightarrow)$.

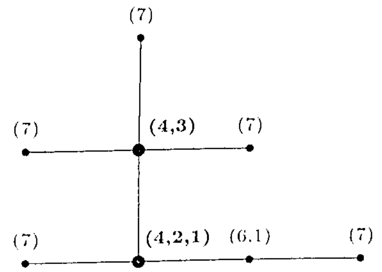
Example 9 (A tree with a unique centroid):

In the following tree diagram, the vertex with principle weight five is the unique centroid.



Example 10 (A tree with a bicentroid):

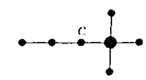
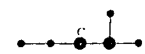
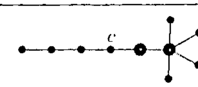
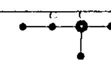
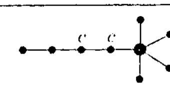
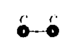
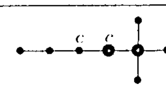
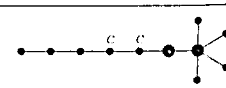
In the following diagram, the tree has two bicentroids, both with principal weight four.



3.2.1 Centers versus Centroids

In the following table, we give examples of trees with all the possible combinations of centers or centroids. The total number of vertices that are centers or centroids varies from one to four.

Table 2: Comparison of centers vs. centroids

Number of Centers	Number of Centroids	Total Number of Vertices	Example
1	1	1	
1	1	2	
1	2	2	
1	2	3	
2	1	2	
2	1	3	
2	2	2	
2	2	3	
2	2	4	

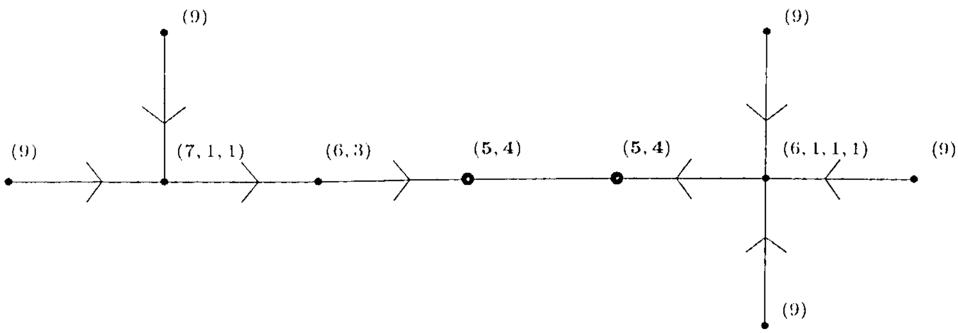
3.2.2 Methods for Finding a Centroid

Method 1

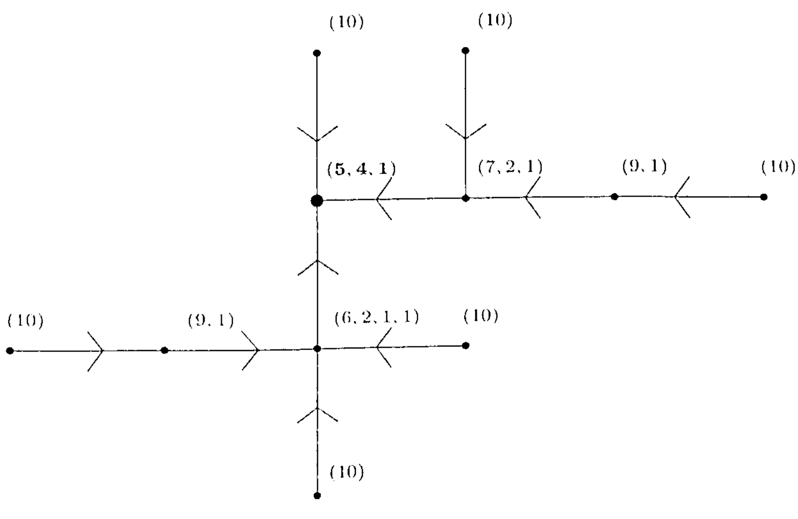
Start with a pendant vertex and travel along a principal branch. Continue moving from vertex to vertex along principal branches until you reach a vertex v_0 with a principal weight $\lceil \frac{w}{2} \rceil$ or less. If the principal weight at v_0 is $\lfloor \frac{w}{2} \rfloor$ or less, then v_0 is the unique centroid of T. If the principal weight at v_0 is $\lceil \frac{w}{2} \rceil > \frac{w}{2}$, then v_0 is one of the bicentroids of T, the other centroid being the neighbor of v_0 on the principal branch of v_0.

Using this method, you can draw a connected graph that shows how you would move along the unique path between any pendant vertex and a centroid.

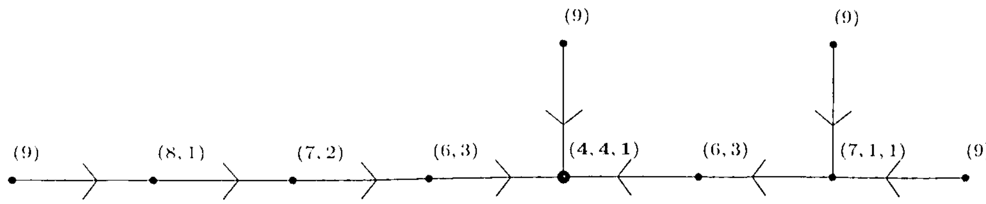
Example 11 (Bicentroids):



Example 12 (Unique centroid with single principal branch):



Example 13 (Unique centroid with multiple principal branches):

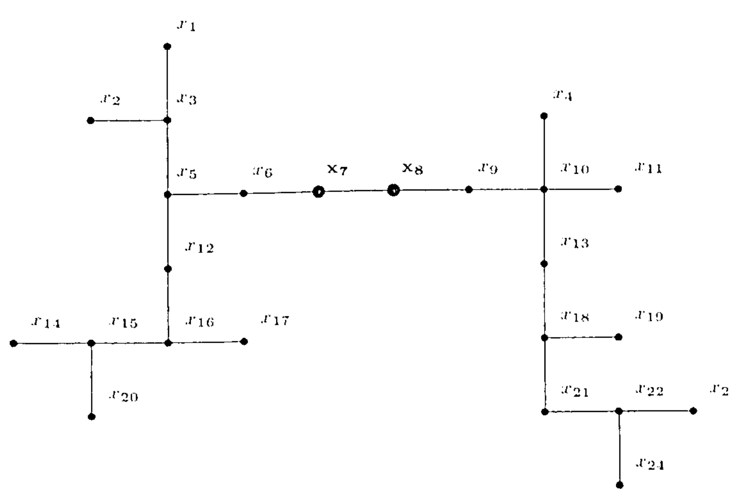


Method 2

In large trees, finding a centroid by Method 1 can take a long time. Method 2 utilizes the same idea of moving along the principal branches, except you start at an interior vertex. A good interior vertex to choose is a center. If you cannot easily locate a center, start at an approximate center and move along the principal branches to find the centroid.

Example 14 (Approximate center):

In the below graph, it appears that one of the longest paths is $x_{20} - x_{24}$, so x_8 is a good approximate center to choose. The weight sequence of x_8 is (12, 11). Moving in the direction of the principal branch takes us to x_7, which has weight sequence (12, 11). Therefore, x_7 and x_8 are the bicentroids of the graph.



3.3 Enumerating Unlabeled Trees

3.3.1 Historical Background

In 1874, the British mathematician Arthur Cayley published *On the Mathematical Theory of Isomers*, the first paper that made a serious connection between graph theory and chemicals. Cayley's goal was to determine a formula for counting the number of isomers of alkanes. He published a table of his calculations for only isomers up to $C_{13}H_{28}$, but his last two calculations were errored. Cayley approached the problem by constructing unlabeled trees from the center vertex or vertices. Constructing trees in this manner is a more cumbersome approach, but focusing instead on the centroid(s) of a graph reduces the task because the tree gets devided into a number of branches more rapidly.

3.3.2 Counting Rooted Trees of Order n

Later the algorithm presented will make use of rooted trees of root degree less than or equal to three. Why restrict to smaller degrees? The reasoning is because an edge will be added to the root, making it of degree less than or equal to four. Let r_n be the number of rooted (unlabeled) trees on n vertices where the root degree is less than or equal to three. Let $r_n(m)$ be the corresponding number when the root has degree m.

Theorem 3.4.

(a) $r_n = r_n(1) + r_n(2) + r_n(3)$

(b) $r_n(1) = r_{n-1}$

Formula 6.

$$r_n(2) = \begin{cases} r_1 r_{2k-2} + r_2 r_{2k-3} + \cdots + r_{k-1} r_k & \text{if } n = 2k \\ r_1 r_{2k-1} + r_2 r_{2k-2} + \cdots + r_{k-1} r_{k+1} + \left[\binom{r_k}{2} + r_k\right] & \text{if } n = 2k+1 \end{cases}$$

This equation for $r_n(2)$ is defined piece-wise in a way that conveniently does not double count when we add branches. This structure makes the equation for $r_n(3)$ even more complicated. In the following formula, a, b, and c are distinct positive integers. The following sums count the number of partitions of $n-1$ into three summands.

Formula 7.

i. $S(a,b,c) = \sum r_a \cdot r_b \cdot r_c$ with the sum taken over all partitions $a+b+c = n-1$

ii. $S(a,a,b) = \sum \binom{r_a+1}{2} r_b$ with the sum over $2a+b = n-1$

iii. $S(a,a,a) = \sum \binom{r_a+2}{3}$ with the sum over $3a = n-1$

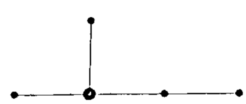
Taking Theorem 3.4 together with Formulas 6 and 7, we can now calculate $r_n(3) = S(a,b,c) + S(a,a,b) + S(a,a,a)$.

Table 3: First few values of r_n

n	$r_n(1)$	$r_n(2)$	$r_n(3)$	r_n
2	1	0	0	1
3	1	1	0	2
4	2	1	1	4
5	4	3	1	8
6	8	6	3	17

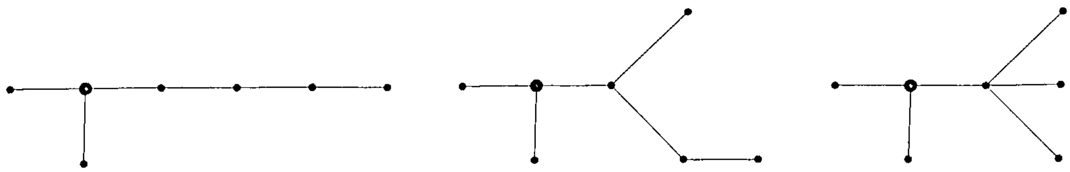
3.3.3 Forming a Tree from a Centroid

Example 15 (Simple weight sequence of a unique centroid):
Suppose (2,1,1) is the weight sequence of the **unique centroid of an unknown tree**. From this weight sequence, we can deduce that the weight of the tree is four and the centroid has three branches. First, join two pendant vertices to the centroid. Last, attach a rooted tree with weight one (by attach, we mean add an edge between the centroid and the root of the tree you are attaching). This produces a tree of weight four such that the centroid has degree sequence (2,1,1).

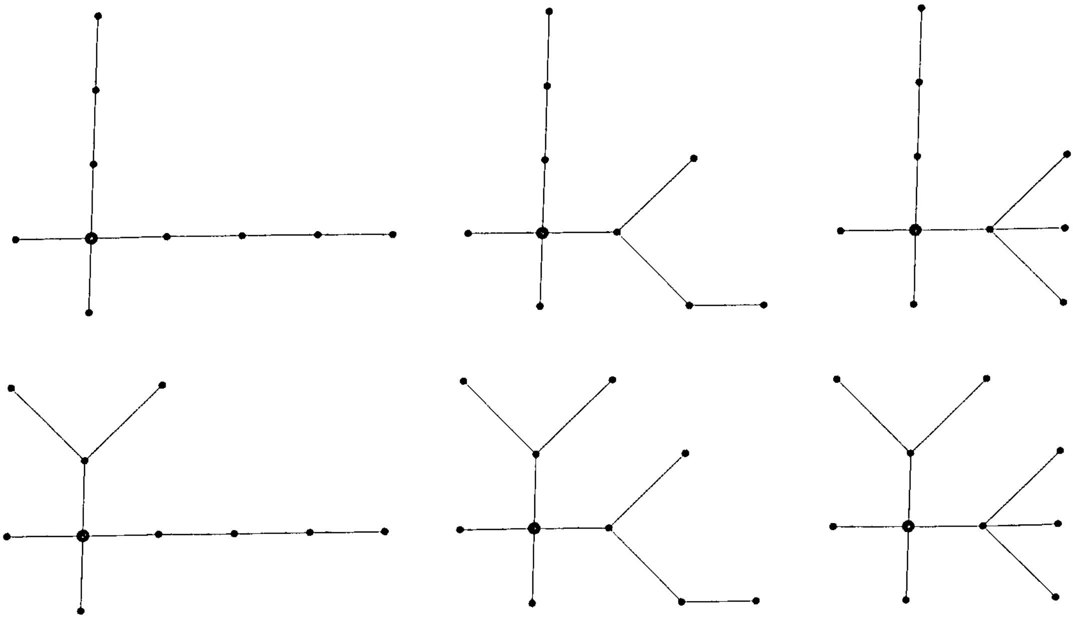


Example 16 (More complex weight sequence of a unique centroid):
Suppose (4,3,1,1) is the weight sequence of the unique centroid of an unknown tree. From this weight sequence, we can deduce that the weight of the tree is nine and that the centroid has four branches. First, join two pendant vertices to the centroid. Next we attach a rooted tree of weight three. There

are three possible rooted trees that we can attach:



Next we attach a rooted tree of weight two. There are two possible trees to attach:



This method produces six nonisomorphic trees of weight nine such that the unique centroid has weight sequence (4,3,1,1).

3.3.4 Algorithm for Counting

We now revisit the original question: how many unlabeled nonisomorphic trees exist on n vertices? The following algorithm can be used to make these calculations and is our original work.

Let $|\tau(n, w(x_i))|$ be the number of nonisomorphic trees on n vertices, where the weight sequence of the centroid is $w(x)$.

Step One: Determine the Possible Centroid Weight Sequences

The possible centroid weight sequences are equivalent to partitions of $n-1$ into four summands, such that the largest summand is of size less than or equal to $\lceil \frac{n-1}{2} \rceil$.

Step Two: Count the Number with Unique Centroids

Let x_i be a unique centroid determined in the previous step.

Formula 8.

$$|\tau(n, w(x_i))| = \begin{cases} r_{w_1} * r_{w_2} * r_{w_3} * r_{w_4} & \text{if none of the terms in the weight sequence are equal} \\ \binom{r_{w_1}+1}{2} * r_{w_3} * r_{w_4} & \text{if only } w_1 \text{ and } w_2 \text{ are equal} \\ r_{w_1} * \binom{r_{w_2}+1}{2} * r_{w_4} & \text{if only } w_2 \text{ and } w_3 \text{ are equal} \\ r_{w_1} * r_{w_2} * \binom{r_{w_3}+1}{2} & \text{if only } w_3 \text{ and } w_4 \text{ are equal} \\ \binom{r_{w_1}+2}{3} * r_{w_4} & \text{if only } w_4 \text{ is different} \\ r_{w_1} * \binom{r_{w_2}+2}{3} & \text{if only } w_1 \text{ is different} \\ \binom{r_{w_1}+3}{4} & \text{if all the terms are equal} \end{cases}$$

The total number of nonisomorphic trees on n vertices that have a unique centroid is equal to $|\tau_u(T)| = \sum_i |\tau(n, w(x_i))|$, where each x_i is a distinct unique centroid.

Step Three: Count the Number of Bicentroids

If $n-1$ is odd, then some graphs of T have bicentroids. The total number of nonisomorphic trees on n vertices that have a bicentroid is:

Formula 9.

$$|\tau_b(n)| = \binom{r_{(n/2)} + 1}{2}$$

Step Four: Calculate the Total Number

Formula 10.

$$|\tau(n)| = |\tau_u(n)| + |\tau_b(n)|$$

Example 17 (Counting the number of nonisomorphic trees on eight vertices):

Let T_8 be a tree on eight vertices.

Step One:

List the unique centroid weight sequences: $x_1 = (3, 3, 1)$, $x_2 = (3, 2, 2)$, $x_3 = (3, 2, 1, 1)$, $x_4 = (2, 2, 2, 1)$

A Appendix

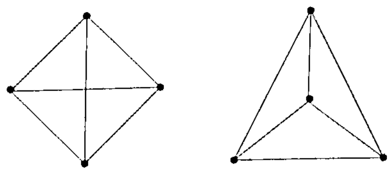
Throughout this paper, several references are made to content included in this Appendix. We felt that the inclusion of an Appendix was necessary to give additional definitions and further explanations that are not integral to the theme of the paper, but still useful in some aspect.

A.1 Planar Graphs

Definition 2 A graph is said to be **planar** if you can draw an embedding of the graph in a plane without edges crossing.

In the introduction, we pointed out that a given graph can usually be drawn in several ways that appear geometrically quite different from each other. A graph **embedding** is a particular drawing of a graph. Example 1 shows two embeddings of a graph. The edges of a graph are said to **cross** if they intersect somewhere that there is not a vertex. In the second embedding in Example 1, the edges wx and yz cross. Observe that $K_{3,3}$ cannot be drawn in a plane without some of its edges crossing. In other words, $K_{3,3}$ is not a planar graph.

Example 18 (Another planar graph):
Of the following two diagrams of the complete graph K_4, the first one is not planar, whereas the second one is planar.



A **complete graph** is a graph where each pair of vertices is joined by an edge. A **bipartite graph** is a graph that has a vertex set made up of two disjoint vertex classes such that no two vertices in the same class are joined by an edge. A bipartite graph G with vertex classes V_1 and V_2 is called a **complete bipartite graph** if $xy \in E(G)$ $\forall x \in V_1$ and $\forall y \in V_2$. $K_{m,n}$ denotes a complete bipartite graph with vertex classes of order m and n.

Figure 21: Complete graph K_5

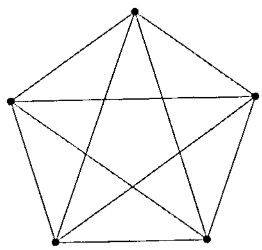
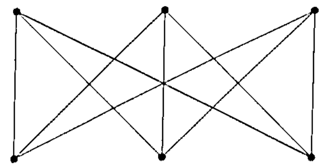


Figure 22: Complete bipartite graph $K_{3,3}$



Theorem A.1. *A graph G is planar iff K_5 and $K_{3,3}$ are not subgraphs of G* [10].

A.2 Group Theory

In a number of constructions in graph theory, we apply another branch of mathematics called group theory. We outline a method where permutation groups are applied to construct cubic graphs of large girth.

A **permutation** p of a set X is a bijection of X onto X. The set of all permutations of a set X is denoted by $S(X)$. A permutation that is its own inverse is called an **involution**. As the bijections of a set onto itself are obviously invertible and the identity function is a permutation, so $S(X)$ is a group. The notation $(x_0, x_1, \ldots, x_k)$, represents a permutation f of $X = \{x_0, x_1, \ldots, x_k\}$, where $f(x_i) = x_{i+1} \forall i < k$ and $f(x_k) = x_1$. Such a permutation is called a cycle (not to be confused with the earlier definition of cycles in graphs). Any permutation of a finite set can be written as a product (composition) of unique disjoint cycle. For $X = \{1, 2, 3, 4, 5, 6\}$, $1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 1$ is a permutation, as is also $(1, 2)(3, 4, 5, 6)$. The permutation $(0)(1) \cdots (k)$, where each element of a finite set is sent to itself, is called the **identity**.

A **binary operation** on a set X is a function $* : X \times X \to Y$, where Y is a set. If $* : X \times X \to X$, we call $*$ a **closed binary operation**. For $x, y \in X$, $*(x, y)$ is written as $x * y$. This notation is called **infix notation**.

Definition 3 A group is a nonempty set G with a binary operation $*$ on G such that

1. for all $x, y \in G$, $x * y \in G$ (closure property)

2. for all $x, y, z \in G$, $x * (y * z) = (x * y) * z$ (associativity)

3. there exists $e \in G$ for $x \in G$ such that $x * e = e * x = x$ (identity element)

4. for all $x \in G$ there exists an $x' \in G$ such that $x * x' = x' * x = e$ (inverse)

A.2.1 Group Actions

A group G is said to **act on a set** X if there is a function $G \times X \to X$, denoted by $(g, x) \to gx$, satisfying

1. $1 * x = x$ for all $x \in X$

2. $gh(x) = g(hx)$ for all $g, h \in G$ and all $x \in X$.

The map $(g, x) \to gx$ is called the **action** and X is the **G-set** of the action. If $|X| = n$, then n is called the **degree** of X (or the degree of the action). A G-set is **faithful** if $g, h \in G$ and $g(x) = h(x)$ for all x implies that $g = h$. If X is a G-set, the **orbit** of an element $x \in X$ under G is the subset Gx of X defined by

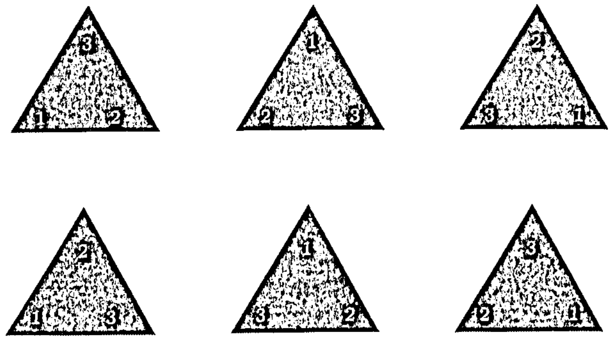
$$Gx = \{gx : g \in G\}.$$

Example 19:
Any subgroup H of the symmetric group $S(X)$ acts faithfully on X in the natural way: $(f, x) \to f(x)$. In particular, the automorphism group $Aut(\Gamma)$ of a graph $\Gamma = (V, E)$ acts on V.

A graph $\Gamma = (V, E)$ is **vertex-transitive** if for any $x, y \in V$, there exits an automorphism τ of Γ satisfying $\tau(x) = y$. Equivalently, Γ is vertex-transitive if there is only one orbit in V. A graph Γ is **symmetric** if for all vertices $w, x, y, z \in V$, such that w and x are adjacent and y and z are adjacent, there is an automorphism τ of Γ for which $\tau(w) = y$ and $\tau(x) = z$. A graph Γ is **distance-transitive** if for all vertices $w, x, y, z \in V$ satisfying $d(w, x) = d(y, z)$, there is an automorphism τ of Γ satisfying $\tau(w) = y$ and $\tau(x) = z$.

A.2.2 Symmetries of a Regular n-gon

By rotating and reflecting a regular n-gon, one can create a group of symmetries. Consider a triangle shaped disc whose corners are numbered that fits perfectly into a mold. The original position of the disc is pictured below in the upper-left spot. From this position, the disc can be rotated and/or reflected (flipped). This gives six possible ways to place the disc into the mold:

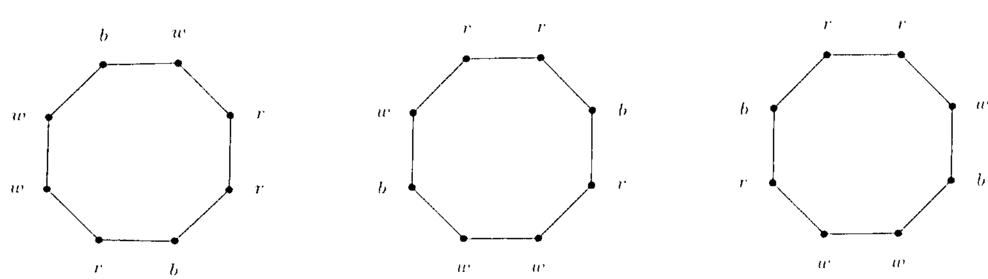


The first three positions (including the identity) are all achieved by rotations only. Using any such rotation three times brings the disc back to the identity. This group of permutations is called the cyclic group of order three. A **cyclic group** is a group of permutations that can be generated by a single element, which we called a rotation. The **order** of a cyclic group is equal to the number of elements in the set X. All six positions can be obtained by either rotating or reflecting the disc. Using a reflection twice brings the disc back to the identity. The whole group of permutations is called the dihedral group of order six. A **dihedral group** is a group of permutations that can be generated by two elements, which we called rotation and reflection. The **order** of a dihedral group is equal to twice the number of elements in X.

A.3 The Necklace Problem

In the introduction, we first discussed the idea of stringing a necklace with eight beads, each of which can be red, white, or blue. For the three necklaces below, we are now able to determine if two necklaces are the same depending upon what group structure we are allowing.

Necklace 1 Necklace 2 Necklace 3



Suppose we allow only a cyclic structure (rotating the necklace on the table). Then Necklace 1 and 2 are the same because you can achieve one coloring from the other by rotating it. On the other hand, Necklace 3 is different because you cannot just rotate the necklace to achieve the same coloring. However, if we allow a dihedral structure (handling the necklaces as pleased), all three necklaces are the same. It's obvious that Necklace 1 and 2 are the same through rotations, but Necklace 3 must be reflected and rotated in order to see that it's also the same.

In this problem, two necklaces are considered the same if you can transform one into another through a function composition of permutations and colorings. Using Polya's Theorem [9], we are able to determine polynomials for counting the number of unique necklaces for the two cases where we allow a cyclic or dihedral group structure. For a group G we can determine the cycle index, which is a polynomial structured in such a way that we can identify the different types of cycles that appear in the permutations in G. Using Polya's theorem, we are able to replace each x_i term in the cycle index with three, since we are using three colors, to obtain the total number of unique necklaces possible under the given permutation group.

Permutation Group	**Cycle Index**	**Unique Necklaces**
Fixed	${x_1}^8$	3^8
Cyclic	$\frac{1}{8}[{x_1}^8 + {x_2}^4 + 2{x_4}^2 + 4x_8]$	834
Dihedral	$\frac{1}{16}[{x_1}^8 + 5{x_2}^4 + 4{x_1}^2{x_2}^3 + 2{x_4}^2 + 4x_8]$	498

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