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The Role of Achromatic coloring for Determining Molecular Complexity

[1] Nishanth Sugathan, [2] Sarika S G, [3] Rajasree A S
[1] [2][3] Department of Mathematics, Amrita Vishwa Vidyapeetham, Amritapuri, India
[1] nishanthsugathan7@gmail.com,[2] sarikasg@am.amrita.edu, [3] rajasreeas63307@gmail.com

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Abstract—***Achromatic coloring is the process of coloring a graph's vertex so that each pair of distinct colors may be seen on the endpoints of at least one edge. The term "achromatic number" refers to the most colors need to color a graph. This paper explores the achromatic number of the central, middle, splitting, and shadow graphs of various graphs. t also explores in the field of chemistry to find the complexity of a chemical compound.***

Index Terms— ***achromatic coloring, central graph, splitting graph, middle graph, shadow graph, chemical graph theory***

I. INTRODUCTION

The graphs we take into consideration here are straightforward, undirected, finite, and have vertex $V(G)$ and edge $E(G)$. Let C be the colors used to color the vertex $V(G)$, it is said to be vertex coloring such that no two adjacent vertices share a common color. A complete coloring is a vertex coloring in which every pair of colors appear on at least one pair of adjacent vertices [3]. An achromatic coloring of a graph G is a complete coloring and the maximum number of colors used to color a graph G is called the achromatic number. The achromatic number was defined and studied by Harary, Hedetniemi and Prins [1]. Chemical graph theory is a branch of mathematics which combines chemistry and mathematics to model physical and biological properties of a chemical compound. It was introduced by Alexandru Balaban, Ante Graovac, Ivan Gutman in 1988. Some chemical applications: Molecular graphs, Topological indices, chemical reaction networks, spectral graph theory[13][12].

II. BASIC TERMINOLOGY

Definition 2.1 Central graph
The process of creating a new vertex on each Edge of a graph to join all pairs of previously non-adjacent vertices results in the creation of the central graph [1].

Definition 2.2 Graph coloring and chromatic number

When labels named colors are assigned to graph elements under specific restrictions is called graph coloring. The chromatic number, represented by the symbol $\chi(G)$., is the bare minimum of colors needed to color a graph [5].

Definition 2.3 Achromatic coloring and achromatic number

A proper vertex coloring known as achromatic coloring assigns any two different colors to a pair of neighboring vertices. A graph's achromatic number, which is represented by $\chi_A(G)$, is the most colors required to color it.

Definition 2.4 Cycle graph

The symbol for a cycle graph is C_n, and it is a simple graph with n vertices in which each vertex is connected to its two neighboring vertices [3].

Definition 2.5 Middle graph

The middle graph $M(G)$ is obtained by adding a new vertex to edge G, where two vertices are adjacent to one another in the graph G if and only if they are also adjacent to one another in G [1].

Definition 2.6 Splitting graph

By adding a vertex to each corresponding vertex in G, where $N[V] = N[V']$, the splitting graph S'(G)is created [11].

Definition 2.7 Shadow graph

By creating 2 copies of G, G' and G'', connecting each vertex of V' to V'' neighbors, the shadow graph is created [11].

III. RESULTS

In this section we discuss the achromatic coloring of bull graph, bow-tie graph, diamond graph, star graph and their related graphs.

A. BULL GRAPH

The bull graph is a straightforward five-vertex diagram with one additional vertex situated between two of the triangle's vertices.

Theorem 3.1

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The central graph of a bull graph's achromatic number is $C(\chi_A(G)) = 4$.

Proof

Let [V_1, V_2, V_3, V_4, V_5] be the vertices of the bull graph G, V_1, V_2, V_3 forms a triangle K_3. To take central of a bull graph G introduce [u_1, u_2, u_3, u_4, u_5] where u_1 is introduced to the edge between V_1 and V_2, u_2 to the edge between V_2 and V_3, u_3 to the edge between v_1 and v_3,u_4 to the edge between V_2 and V_4, u_5 to the edge between $V_3$and V_5. Then join the non-adjacent vertices [V_4, V_1], [V_4, V_3], [V_4, V_5], [V_5, V_1] and [V_5, V_2] with an edge. Consider $\{C_1, C_2, C_3\ldots\}$ be the colors used to color the central of the bull graph $C(G)$, assign C_1, C_2, C_3 to the vertices of $K_3(V_1, V_2, V_3)$ C_4 to either v_4 or v_5, then assign colors to the rest of the vertices according to achromatic coloring to get the distinct pair of colors. The maximum number of colors used is 4

Illustration

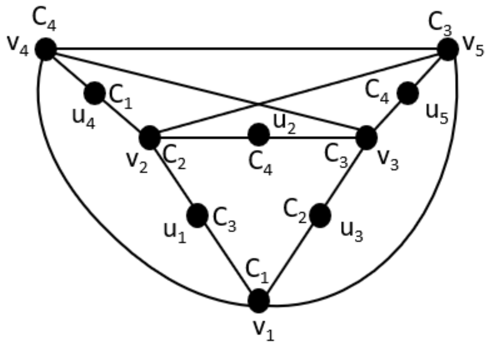


Figure 1: $C(\chi_A(G)) = 4$.

Figure 2: $M(\chi_A(G)) = 4$

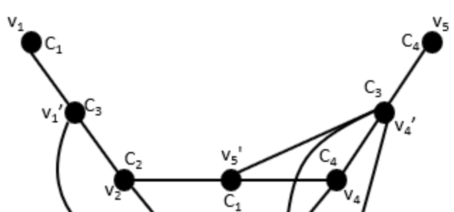
Theorem 3.2

The achromatic number for a bull graph's middle graph is 4.

Proof

Let V_1, V_2, V_3, V_4, V_5 be the bull graph's vertices. To get the middle graph M(G) we introduce a new vertex set V_i' ;(i=1,2,3…) subdivide the edges V_1V_2, V_2V_3, V_3V_4, V_4V_5, Join the new vertices according to the adjacency of the original graph G. Allot the colors $\{C_1, C_2, C_3\ldots\}$. Set the colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4 respectively. Then assign colors to the rest of the vertices according to achromatic coloring to obtain each of the color pairs. The maximum number of colors used is 4

Illustration



Theorem 3.3
The achromatic number is 5 for the shadow graph of a bull graph.

Proof

The vertices for the bull graph G are given as V_1, V_2, V_3, V_4, V_5. To get the shadow graph we take two copies of G, G' and G''. V' is the vertex set of G' and V'' is the vertex set of G''. The neighbors of the relevant vertex u should be connected to each vertex V'. Let $C = \{C_1, C_2, C_3\ldots\}$ be the colors. Allot the colors C_1, C_2, C_3, C_4, C_5 to the vertices V_1', V_2', V_3', V_4', V_5' respectively. Then allot rest of the colors to the remaining vertices according to achromatic coloring to get all the distinct pairs of colors. The maximum number of colors used is 5.

Illustration

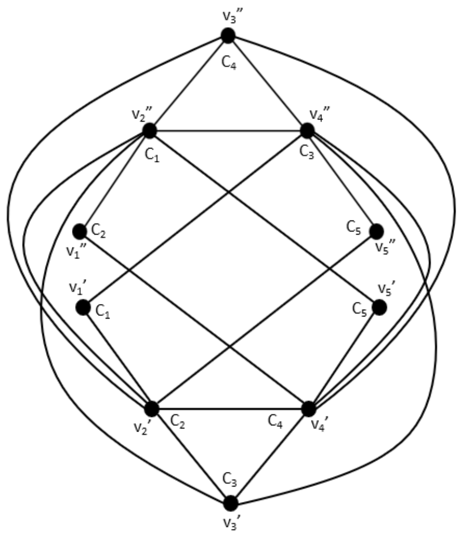


Figure 3: $\chi_A(G) = 5$.

Theorem 3.4

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The achromatic number is $S'(\chi(G)) = 5$ for the bull graph's splitting graph.

Proof

Let V_1, V_2, V_3, V_4, V_5 be the vertices of the bull graph. To get the splitting graph $S'(G)$, take the vertices V_i' ;(i=1,2,3…), neighborhood set of V' is equal to the neighborhood of V''. Let {C_1, C_2, C_3…} be the colors. Set the colors C_1, C_2, C_3, C_4, C_5 to the points V_1, V_2, V_3, V_4, V_5 respectively. Then assign color C_5 to V_1', V_2' and C_1 to V_3', V_4' and C_2 to V_5'. The maximum number of colors used is 5.

Illustration

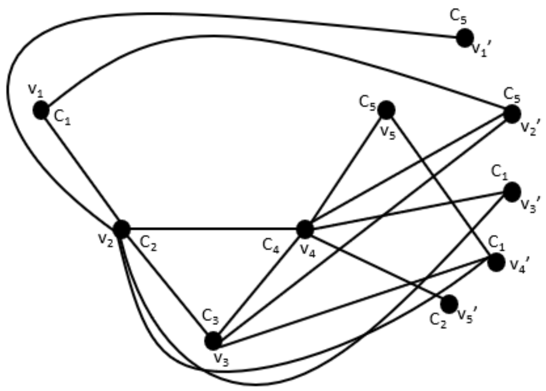

Figure 4: $S'(\chi(G)) = 5$.

B. BOW-TIE GRAPH

A planar undirected graph with 5 vertices and 6 edges is known as a bow-tie graph (also known as a butterfly graph). By connecting two copies of the cycle graph C_3 at a common vertex, it can be created.

Theorem 3.5

The achromatic number of a bow-tie graph's central graph is $C(\chi_A(G)) = 5$.

Proof

Let V_1, V_2, V_3, V_4, V_5 be the vertices of the bow-tie graph, v_5 is a common vertex for the cycle graph [$V_1 V_2 V_5$] and [$V_3 V_4 V_5$]. To get the central graph of the butterfly graph let the vertices u_i ;(i = 1,2, 3…) subdivide the edges V_1V_2, V_1V_5, V_2V_5, V_4V_5, V_4V_3, V_3V_5 and link every vertex of G that isn't neighboring. Consider the colors {C_1, C_2, C_3…}. Assign the colors C_1, C_2, C_3, C_4, C_5 to the vertices v_1, v_2, v_3, v_4, v_5, then assign colors to the rest of the vertices according to achromatic coloring to obtain all color-contrasting pairs. The maximum colors used is 5.

Illustration

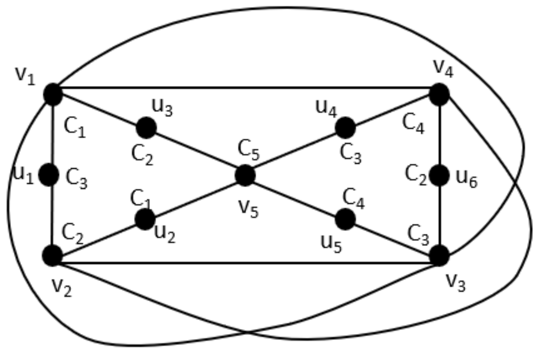

Figure 5: $C(\chi_A(G)) = 5$

Theorem 3.6

The achromatic number of bow-tie's middle graph M(G) is 5.

Proof

Let G be a graph with vertex $V(G)$. To acquire the middle graph M(G) we introduce a new vertex set V_i' ;(i=1,2,3…) subdivide the edges V_1V_2, V_2V_3, V_3V_4, V_4V_5, Join the new vertices according to the adjacency of the original graph G. Consider the colors {C_1, C_2, C_3…}. Set the colors C_1, C_2, C_3, C_4, C_5 to the vertices V_1, V_2, V_3, V_4, V_5 respectively. Assign colors to rest of the vertices according to achromatic coloring to get all the distinct pair of colors. The maximum number of colors used is 5.

Illustration

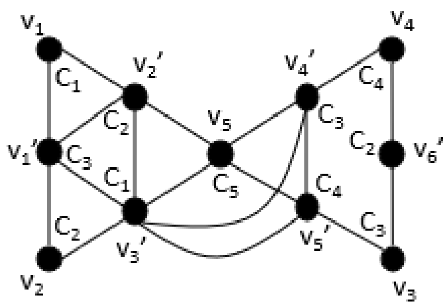

Figure 6: $M(\chi_A(G)) = 5$

Theorem 3.7

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For the shadow graph of a bow-tie graph, the achromatic number is 5

Proof

Suppose that G is a bow-tie graph with vertices V_1, V_2, V_3, V_4, V_5. To get the shadow graph we take two copies of G: G' and G''. V ' is the vertex set of G' and V'' is the vertex set of G''. Connect each vertex V' to its corresponding vertex V'' neighbors. Consider the colors $C = \{C_1, C_2, C_3\ldots\}$. Assign colors C_1, C_2, C_3, C_4, C_5 to the vertices V_1', V_2', V_3', V_4', V_5' respectively. Then assign C_5 to V_5'' and assign colors to the rest of the vertices to get a distinct pair of colors. The maximum number of colors used is 5.

Illustration

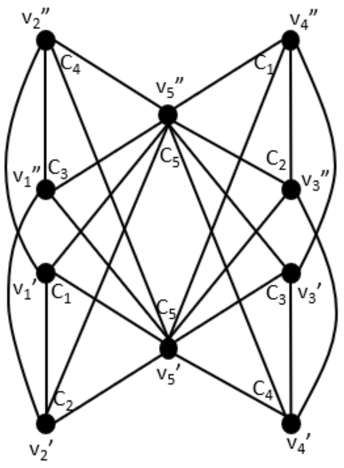


Figure 7: $\chi_A(G) = 5$.

Theorem 3.8

For the splitting graph of a bow-tie graph, the achromatic number is $S'(\chi(G)) = 4$.

Proof

Provide the graph G, where V is the vertices of G. To get the splitting graph $S'(G)$, take the vertices V_i' ;(i=1,2,3…), neighborhood set of V' is equal to the neighborhood of V''.Consider the colors $\{C_1, C_2, C_3\ldots\}$. Assign the colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4, V_5 respectively. Assign colors to rest of the vertices according to achromatic coloring to get all the distinct pair of colors. The maximum number of colors used is 4.

Illustration

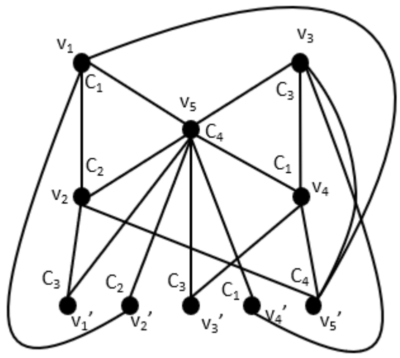


Figure 8: $S'(\chi(G)) = 4$.

C. DIAMOND GRAPH

An undirected planar graph with 4 vertices and 5 edges is called a "diamond graph." It is a K_4 graph with all edges present except for one.

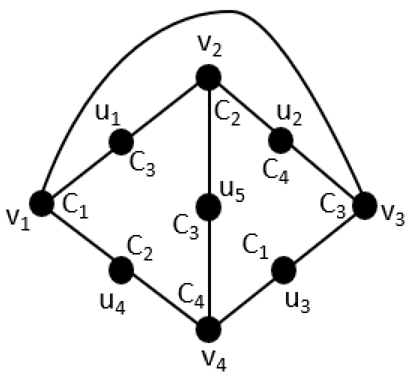
Theorem 3.9

Achromatic number for the diamond graph's central graph is $C(\chi_A(G)) = 4$.

Proof

Let V_1, V_2, V_3, V_4 be the vertices of the diamond graph G. $V_4 V_2$ is the edge that divides the graph into two cyclic graphs K_3. To get the central graph of the diamond graph let the vertices u_i;(i= 1, 2, 3…) subdivide the edges V_1V_2, V_2V_3, V_3V_4, V_4V_1, V_4V_2 and join all the non-adjacent vertices in G. Consider the colors $\{C_1, C_2, C_3\ldots\}$.Assign the colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4 then assign colors to the rest of the vertices according to achromatic coloring to obtain all the different color pairs. The maximal colors used is 4.

Illustration



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Theorem 3.10

Figure 9: $C(\chi_A(G))$ = 4.

Achromatic number is 4 for the middle graph of the diamond graph $M(G)$.

Proof

A diamond graph G with vertices (V_1, V_2, V_3, V_4). To get the middle graph $M(G)$,we introduce a new vertex set V'(G) to the edges V_1V_2, V_2V_3, V_3V_4, V_1V_3. Join the new vertices according to the adjacency of the original graph G. Consider the colors C = {C_1, C_2, C_3…}. Assign colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4 respectively, then assign colors to the rest of the vertices according to achromatic coloring to get distinct pair of colors. The maximum number of colors used is 4.

Illustration

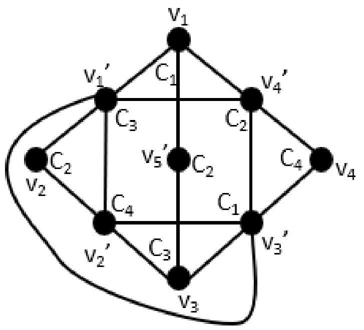

Figure 10: M($\chi_A(G)$) = 4.

Theorem 3.11

Achromatic number of diamond graph's shadow graph is 3.

Proof

G is the diamond graph with vertices V(G). To get the shadow graph we take 2 copies of G: G' and G'', where V' is the vertex set of G' and V'' is the vertex set of G''. Connect each vertex V' to its corresponding vertex V's neighbors. Consider the colors C = {C_1, C_2…}. Assign colors C_1, C_3 to the vertices V_1, V_3 respectively and C_2 to V_2 and V_4. Similarly allot the colors to V'' set. The maximum colors used is 3.

Illustration

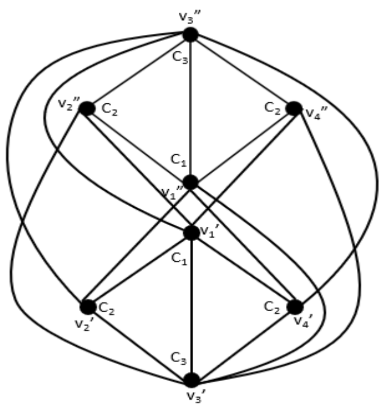

Figure 11: $\chi_A(G)$ = 3.

Theorem 3.12

The achromatic number for a splitting diamond graph is $S'(\chi(G)) = 4$.

Proof

Consider a graph G with vertex V(G). To get the splitting graph $S'(G)$, take the vertices V_i' ;(i=1,2,3…). Neighborhood set of V' is equal to the neighborhood of V''.Consider the colors {C_1, C_2, C_3…}. Assign the colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4 respectively. Assign colors to rest of the vertices according to achromatic coloring to get all the distinct pair of colors. The maximum number of colors used is

Illustration

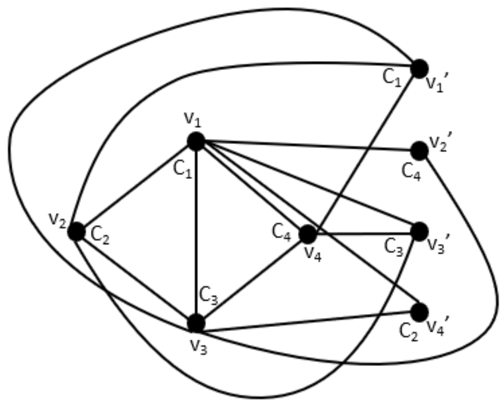

Figure 12: $S'(\chi(G)) = 4$.

D. STAR GRAPH

A star diagram S_n is a fully connected bipartite graph $K_{1,\ n}$ with n leaves and one internal node.

Theorem 3.13

A star graph whose central graph's achromatic number is $C(\chi_a(S_n)) = n + 1, n \geq 3$.

Proof:

Let V_1, V_2, V_3, V_4 be the vertices of the star graph G, where V_4 is the internal node and V_1, V_2, V_3 are the leaves. To acquire the central graph $C(G)$ let the vertex u_i;(i=1,2, 3...) subdivide the edges v_1v_4, v_2v_4, v_3v_4 and join all the non-adjacent vertices in G. consider the colors {C_1, C_2, C_3…}.Assign the colors C_1, C_2, C_3, C_4 to the vertices V_1, V_2, V_3, V_4. Then assign colors to the rest of the vertices according to achromatic coloring. The most colors that can be used are n+1.

Illustration

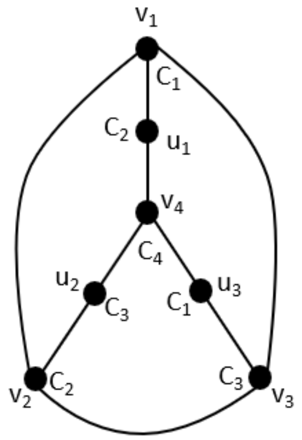

Figure 13: $C(\chi_A(S_3)) = 4$

Theorem 3.14

Middle graph of a star graph S_n ($n \geq 3$), the achromatic number is 4.

Proof

Let G be the star graph with vertex set V(G) = {V_1, V_2, V_3, V_4}, where V_1 is the internal node and V_2, V_3, V_4 be the leaves. To get the middle graph $M(G)$we introduce vertex V_i' (i = 1, 2…) to the edges. Join the new vertices according to the adjacency of the original graph G. Consider the colors C = {C_1, C_2, C_3…}. Assign the colors C_1 to V_1, C_2, C_3, C_4 to V_2, V_3, V_4 respectively, assign colors to the rest of the vertices according to achromatic coloring to get all the distinct pair of colors. The maximum number of colors used is 4.

Illustration

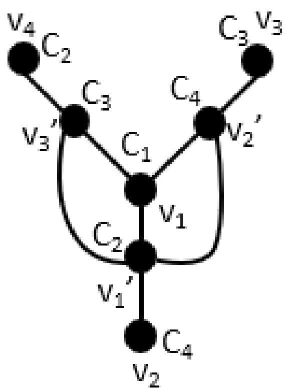

Figure 14: $M(\chi_A(G)) = 4$.

Theorem 3.15

Shadow graph of a star graph S_n ($n \geq 3$), the achromatic number is 2.

Proof

Suppose G be a graph with vertices $V(G)$, where V_1 is the internal node and V_2, V_3, V_4 be the leaves. To get the shadow graph we take 2 copies of G: G' and G'', where V' is the vertex set of G' and V'' is the vertex set of G''. Connect each vertex V' to its corresponding vertex V's neighbors. Consider the colors C = {C_1, C_2…}. Allot the color C_1 to V_1 and V_1', C_2 vertices V_2, V_3, V_4, V_2', V_3', V_4'. The maximum colors used is 2.

Illustration

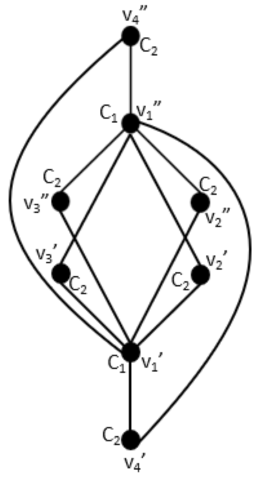

Figure 15: $\chi_A(G) = 2$.

Theorem 3.16

For the splitting graph of a star graph, the achromatic number is $S'(\chi(G)) = 2$.

Proof

Consider a graph with vertex set V(G). To get the splitting graph $S'(G)$, take the vertices Vi' ;(i=1,2,3…). Neighborhood set of V' is equal to the neighborhood of V''.Consider the colors {C_1, C_2, C_3…}. Assign the color C_1 to the vertices V_1' and V_1", then assign C_2 to the rest of the vertices. The maximum number of colors used is 2.

Illustration

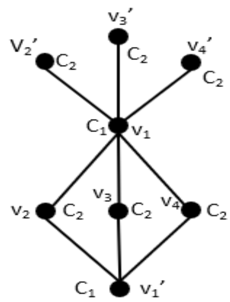

Figure 16: $S'(\chi(G)) = 2$.

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IV. CHEMICAL APPLICATION OF ACHROMATIC NUMBER

The field of mathematics known as chemical graph theory studies the many physical properties of molecules by modelling them. The geometric structures of the compound are connected to some physical characteristics, such the boiling point. In chemistry, a molecule's atoms are represented as its vertices, while its chemical bonds are shown as its edges. The resulting graph is called chemical graph. [13]

The significance of Achromatic number in predicting the complexity of Acetaminophen and Ibuprofen

Acetaminophen is classified as a non-opioid analgesic and antipyretic drug. Acetaminophen is commonly used to treat mild to moderate pain, such as headache, toothache, muscle aches, etc. it is also used to reduce fever associated with cold, flu, and other infections. Similarly, Ibuprofen is also used to relive pain, reduce fever, and alleviate inflammation. Ibuprofen is a non-steroidal anti-inflammatory drug (NSAID). It is a propionic acid derivative and its chemical name is (RS)-2-(4-(2-methylpropyl) phenyl) propanoic acid [14].

This study demonstrates how achromatic number can be used to determine a molecule's complexity and diversity. In this case, achromatic coloring is observed using the drugs acetaminophen and ibuprofen. Here when the achromatic number is higher the drug has a relatively large and complex structure with many functional groups (with many vertices that are connected by edges) and lower the achromatic number indicates that the drug has a lesser complex structure with less functional groups.

Achromatic coloring applied on Ibuprofen and Acetaminophen

Consider the colors $C = \{C_1, C_2, C_3 \ldots\}$ to color Ibuprofen and Acetaminophen. Assign the colors according to achromatic coloring such that no two adjacent vertices have the same color and to get a distinct pair of colors. The most colours that may be used to colour Ibuprofen is 7 and the maximum used to color Acetaminophen is 6.

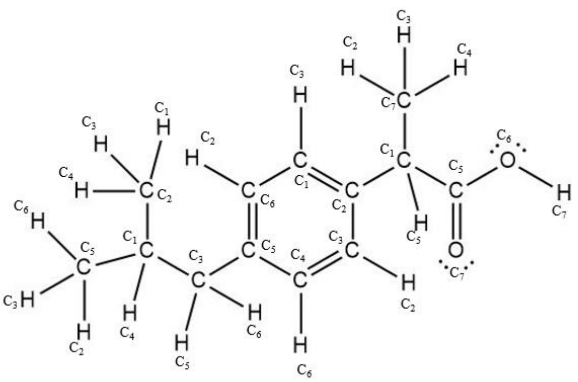

Figure: 17 Achromatic coloring on Ibuprofen

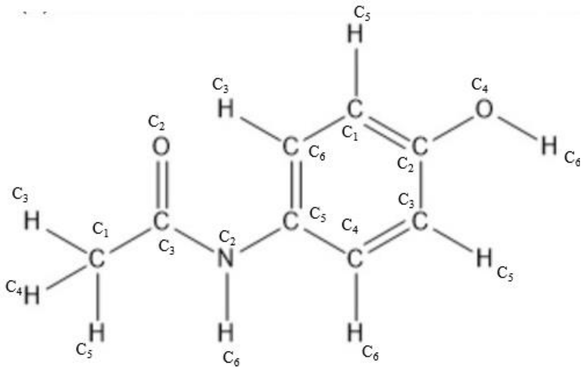

Figure: 18 Achromatic coloring on Acetaminophen

Since Ibuprofen has a higher achromatic number than Acetaminophen, it shows us that Ibuprofen is a much more complex chemical structure than Acetaminophen.

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