

## Iconographic analysis of piperdone derivatives and extension towards Complete Tripartite Graph accepting Continuous Monotonic Decomposition

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### Abstract

In this present investigation 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone has been synthesised and it has been characterised on the basis of elemental analysis and NMR spectral analysis. Several complex compounds have been discussed in graph theory. This is a new concept in which Complete Tripartite Graph  $K_{2,3,m}$  of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone can be literally explained and also accepts the Continuous Monotonic Decomposition rule in chemistry dictionary. This representation has been done to identify the possibility of the prolonging chemical reactions scheme. A complete picturization of the compound has been schematically icono-graphed. The nature of bonding and structural features of piperdone derivatives has been revealed through the Complete Tripartite Graph accepts Continuous Monotonic Decomposition. Thus the objective measures of our research efforts are made ease in identifying the reaction mechanism in terms of p vertices and e edges.

**Keywords:** Piperdone, Semicarbazone, NMR, CTG, CMD, Graph Labelling

### 1. INTRODUCTION

The heterocyclic compound is the precursor of the organic synthesis and also exhibits wider production methodologies are Aldehyde oxidation of Semicarbazone and thiosemicarbazone derivatives was used for the production of 1,2,4-triazole, 1,3,4-oxidiazole and 1,2,4-thiadiazole by metal salts was also reported earlier[1-3]. The

electrochemical work of 2-formylpyridine thiosemicarbazone was also synthesised and extended its studies by the irreversible electrochemical subjection under zero positive sweep peak. The cleavage of N-N single bond reduction and followed by the production of imine formation was carried out by the concepts of 4 electrons transfer mechanism. Several methods of electrochemical subjection like Coulometric, Polarographic measurements were also reported through the oxidation and reduction mechanism, to distinguish their unique structure of the biological activity their redox properties and its metal complexities[4-6]. Several techniques in the five membered Heterocycles of sulphur substituted, Nitrogen substituted heterocycles were also synthesised by standard methods of reaction between DMAD with amides and esters of dicarboxylic acids[7-9]. Further the formulating their reaction are also profound a wider application in microwave irradiation in converting a classical organic synthetic procedure into well promoted new trend of reactions and to gain a maximum yield. In this research work, the compound N-hydroxy-3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone has been arranged Complete Tripartite Graph(CTG)  $K_{2,3,m}$  accepts Continuous Monotonic Decomposition(CMD) of  $H_1, H_2, \dots, H_{(5n+7)/2}$  if and only if  $m=(5n^2+16n+3)/8$  when  $n$  is odd and CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  if and only if  $m=(5n^2+14n)/8$  when  $n$  is even  $\forall n \in N$ . An extensive research analysis has been done on the graph theory by the Gallian. Thus the graph labelling is one of the innovative research areas and emerging out in various fields with new ideas and technologies. But no graph theory has been proved for the compound 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone is under the CTG accepting CMD of two dissimilar mode of arrangement. This work has been carried out for not only its mathematical importance but also its wide range of application arising from the chemistry dictionary. All graphs are finite simple and peculiar mode of compound pattern either in atomic or in molecular form. A useful graph theory survey analysis has been done for the prediction of chemical reaction mechanism of the 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone and it has been initiated by the pattern of CTG accepts CMD by comparing two different forms in which it obeys the same order of the reaction mechanism.

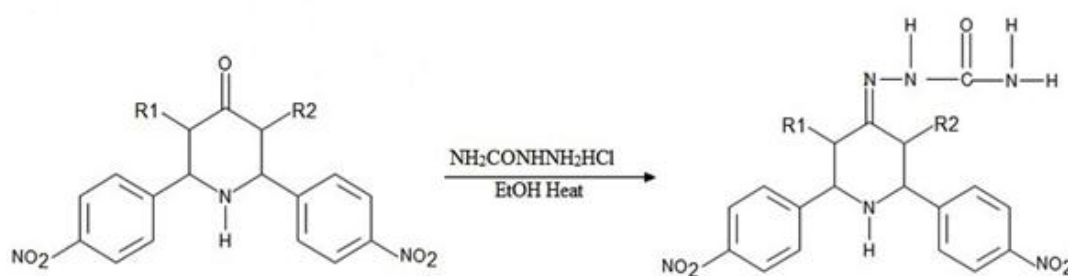
## 2. MATERIALS AND METHODS

The analytical grade of chemicals were utilised for the preparation of compounds. Noller and Balliah[1] have synthesised 2,6-diaryl-4-one. The product purity was determined by its melting point in open capillaries and is uncorrected. The synthesised product whose structural confirmation is done with the spectral features is reported in wave number( $\text{cm}^{-1}$ ).  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on variant Hg-Spectrophotometer at 360  $\text{H}_2$  in  $\text{CDCl}_3$  using TMS as internal standard.

### 2.1. Synthesis of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone

The compound is synthesised by the proper mixture of piperidin-4-one(1gm,0.0027mol), Semicarbazide hydrochloride(0.316,0.0027mol) and sodium acetate(0.75gm) were dissolved in ethanol(40ml) and refluxed for two hours on a

steam bath and cooled. The products were separated and filtered with water and recrystallised from ethanol. The separated solids are now transformed to the final product of 97.7% of purity level with repeated recrystallisation is done using ethanol. The synthesised product is separated and the corresponding physical data and the chemical reaction of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone whose melting point is 156 and its yield 86.23% is depicted in figure 1.



**Figure 1: Reaction Scheme 1**

## 2.2. Complete Tripartite Graph $K_{2,3,m}$ accepting CMD

Theorem:

A Complete Tripartite Graph(CTG)  $K_{2,3,m}$  accepts Continuous Monotonic Decomposition(CMD) of  $H_1, H_2, \dots, H_{(5n+7)/2}$  if and only if  $m = (5n^2 + 16n + 3)/8$  when  $n$  is odd and CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  if and only if  $m = (5n^2 + 14n)/8$  when  $n$  is even  $\forall n \in N$ .

Proof: Assume that a Complete Tripartite Graph  $K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+7)/2}$  when  $n$  is odd and CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  when  $n$  is even  $\forall n \in N$ .

We have  $q(K_{2,3,m}) = 5m + 6 \forall m \in N$

We know that  $G$  accepts CMD  $H_1, H_2, \dots, H_n$  iff  $q(G) = n(n+1)/2, \forall n \in N$

Case 1: when  $n$  is odd

$K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+7)/2}$  iff  $q(K_{2,3,m}) = ((5n+7)/2(5n+7)+1)/2$  when  $n \in N$  is odd

$q(K_{2,3,m}) = (5n+7)(5n+9)/8$  for all  $n \in N$  is odd

i.e.,  $q(K_{2,3,m})$  must be a member of the sequence 1,3,6,10,15,21.....,  $k(k+1)/2$  for all  $n \in N$  is odd

i.e.,  $(5n+7)(5n+9)/8 = k(k+1)/2$  for some  $k \in N$  and for all  $n \in N$  is odd

i.e.,  $k = (5n+7)/2$  for all  $n \in N$  is odd

Also,  $K_{2,3,m}$  accepts CMD if and only if  $q(K_{2,3,m})$  is one among the members of the sequence given.

i.e.,  $5m+6$  should be one of these values

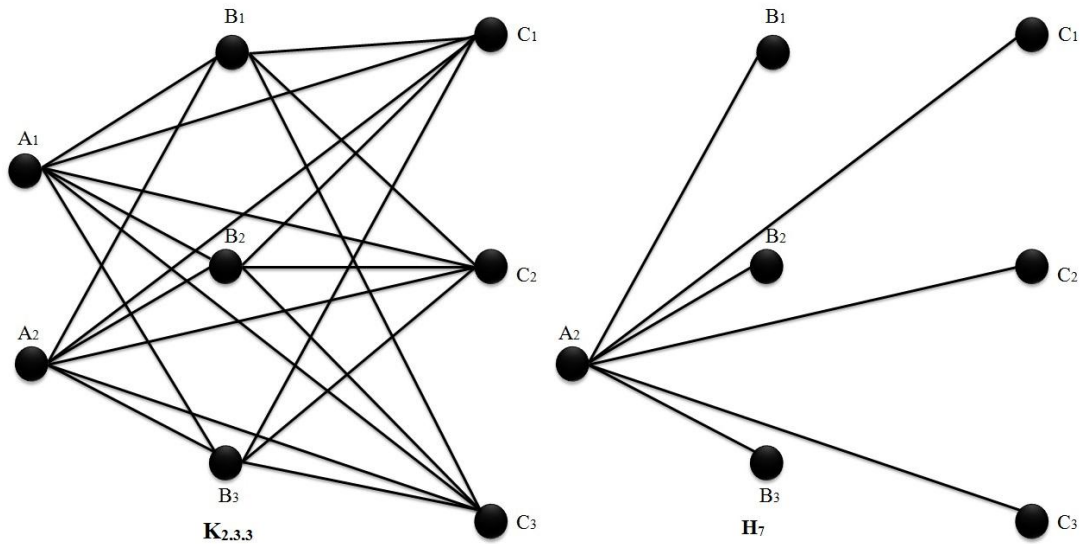
i.e.,  $5m+6 = k(k+1)/2$  for some  $k \in N$

i.e.,  $5m+6 = (5n+7)(5n+9)/8$

i.e.,  $m = (25n^2+80n+15)/8 \forall n \in N$  and  $n$  is odd

The first few values of  $m$  are 3,12,26,45.....

Example 2.1



**Figure 2: Pictorial representation of  $K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+7)/2}$  iff  $q(K_{2,3,m}) = ((5n+7)/2(5n+7)+1)/2$  when  $n \in N$  is odd**

Case 2: when  $n$  is even

$K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  iff  $q(K_{2,3,m}) = ((5n+6)/2(5n+6)+1)/2$  when  $n \in N$  is even

$q(K_{2,3,m}) = (5n+6)(5n+8)/8$  for all  $n \in N$  is even

i.e.,  $q(K_{2,3,m})$  must be a member of the sequence 1,3,6,10,15,21.....,  $k(k+1)/2$  for all  $n \in N$  is even

i.e.,  $(5n+6)(5n+8)/8 = k(k+1)/2$  for some  $k \in N$  and for all  $n \in N$  is even

i.e.,  $k = (5n+6)/2$  for all  $n \in N$  is even

Also,  $K_{2,3,m}$  accepts CMD if and only if  $q(K_{2,3,m})$  is one among the members of the sequence given.

i.e.,  $5m+6$  should be one of these values

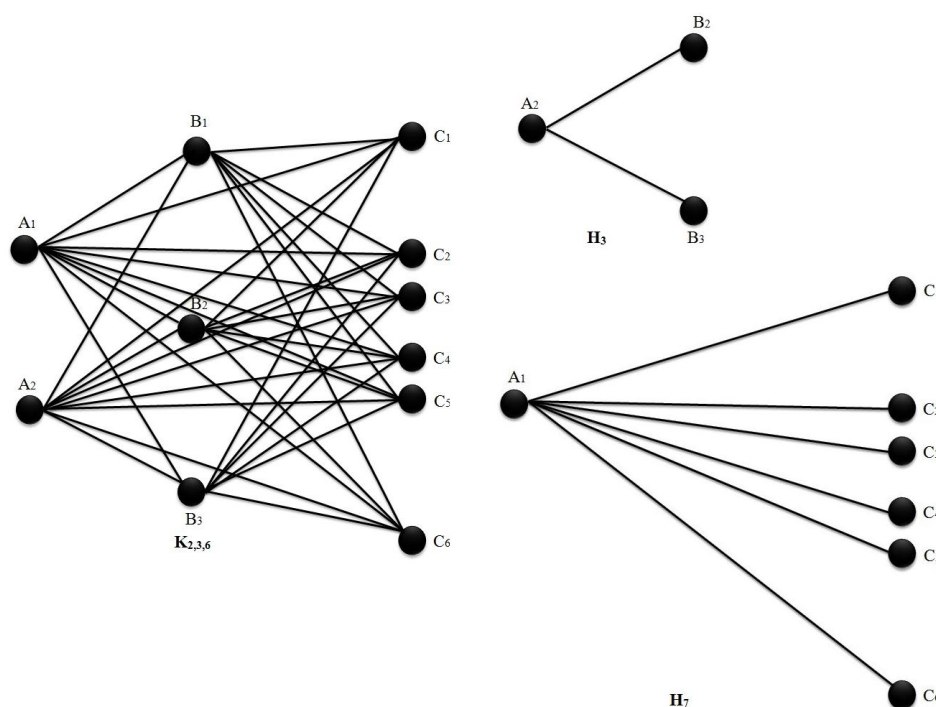
i.e.,  $5m+6 = k(k+1)/2$  for some  $k \in \mathbb{N}$

i.e.,  $5m+6 = (5n+6)(5n+8)/8$

i.e.,  $m = (5n^2+14n)/8 \forall n \in \mathbb{N}$  and  $n$  is even

The first few values of  $m$  are 6,17,33,54.....

Example 2.2



**Figure 3: Pictorial representation of  $K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  iff  $q(K_{2,3,m}) = ((5n+6)/2(5n+6)+1)/2$  when  $n \in \mathbb{N}$  is even**

Conversely,

Suppose that  $K_{2,3,m}$  is a complete tripartite graph with  $m = (5n^2+16n+3)/8$  when  $n$  is odd and  $m = (5n^2+14n)/8$  when  $n$  is even  $\forall n \in \mathbb{N}$ .

We know that  $q(K_{2,3,m}) = 5m+6$

Case 1:

i.e., when  $m = (5n^2+16n+3)/8$ ,  $n$  odd

$$q(K_{2,3,m}) = 5((5n^2+16n+3)/8)+6$$

$$= (5n+7)(5n+9)/8$$

$$= ((5n+7)/2)((5n+7)/2+1))/2 \text{ is of the form } [k(k+1)/2]+1, \forall k \in \mathbb{N}.$$

This implies that  $K_{2,3,m}$  being a connected simple graph, can be decomposed into  $H_1, H_2, \dots, H_k \forall k \in N$

i.e  $K_{2,3,m}$  can be decomposed into  $H_1, H_2, \dots, H_{(5n+7)/2}$  for  $n$  is odd

Case 2:

$$\begin{aligned} m &= (5n^2+14n)/8, n \text{ even} \\ q(K_{2,3,m}) &= 5((5n^2+14n)/8)+6 \\ &= (5n+6)(5n+8)/8 \\ &= ((5n+6)/2)((5n+6)/2+1))/2 \text{ is of the form } [k(k+1)/2]+1, \forall k \in N. \end{aligned}$$

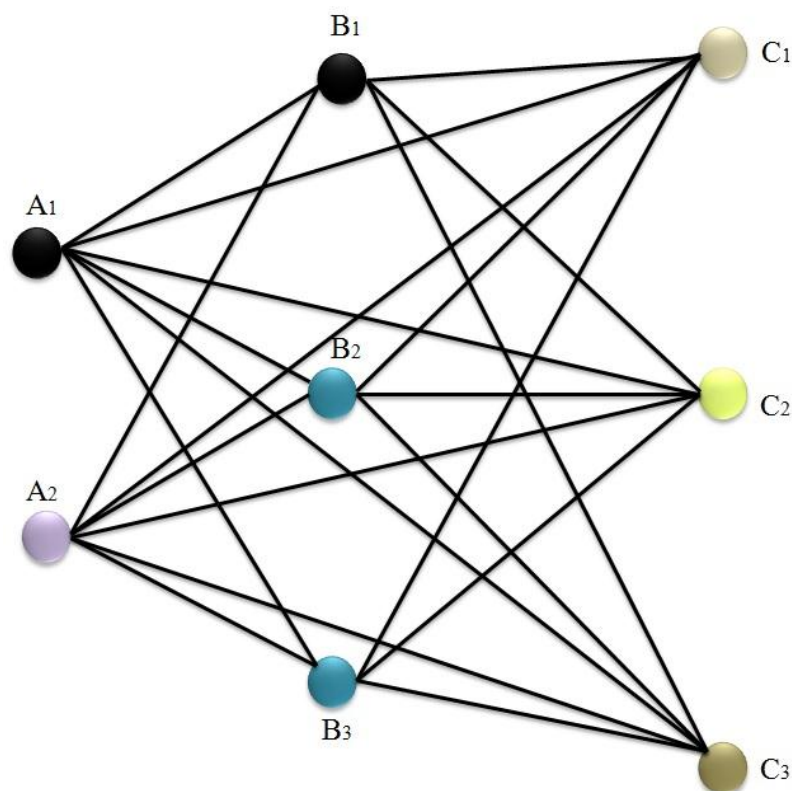
This implies that  $K_{2,3,m}$  being a connected simple graph, can be decomposed into  $H_1, H_2, \dots, H_k \forall k \in N$

i.e  $K_{2,3,m}$  can be decomposed into  $H_1, H_2, \dots, H_{(5n+6)/2}$  for  $n$  is even

### 3. RESULTS AND DISCUSSION

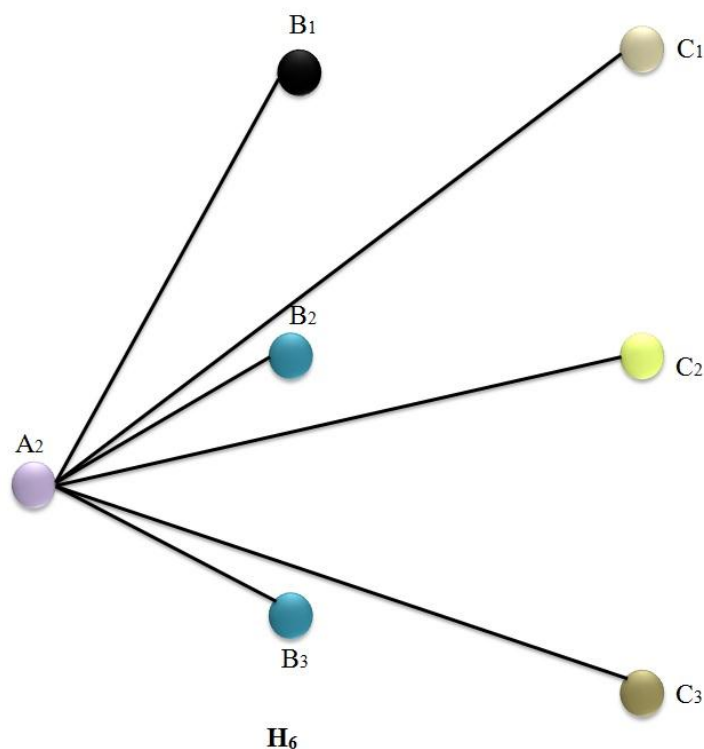
#### 3.1. Complete Tripartite Graph(CTG) $K_{2,3,m}$ accepts Continuous Monotonic Decomposition(CMD) of $H_1, H_2, \dots, H_{(5n+7)/2}$ if and only if $m=(5n^2+16n+3)/8$ when $n$ is odd

The schematic diagram for the compound 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone have been arranged in the pattern of Complete Tripartite Graph(CTG)  $K_{2,3,m}$  accepts Continuous Monotonic Decomposition(CMD) of  $H_1, H_2, \dots, H_{(5n+7)/2}$  if and only if  $m=(5n^2+16n+3)/8$  when  $n$  is odd. We shall argue that with the compound there is a classification of vertex in three positions[5-9]. The left vertices( $A_1, A_2$ ), central vertices ( $B_1, B_2, B_3$ ) and right vertices( $C_1, C_2, C_3$ ) and the link or edge are chosen with proper colours and represented respectively. Having done so the left vertex  $A_1$  and central vertex  $B_1$  holds with same methyl group with black colour. The central vertices  $B_2$  and  $B_3$  are indicated by the nitro aromatic atom with dark aqua in colour mode. Certainly let's proceed with left vertex  $A_2$  with N-H ring atom with lighter purple colour as shown in the figure 1. The right vertices  $C_1, C_2$  and  $C_3$  constitutes a semicarbazone group[9-14]. We have seen that within the right vertex in the position  $C_1$  consists of secondary amine and  $C_2$  holds with carbonyl group and  $C_3$  vertex is represented a primary amine respectively. The colour representations of the right vertex are indicated in the figure 4.



**Figure 4: Pictorial representation of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG  $K_{2,3,3}$**

Consequently there is a positive probability that all the vertices are good when analysis is successful through CTG accepting CMD of  $H_1, H_2, \dots, H_{(5n+7)/2}$  if and only if  $m = (5n^2 + 16n + 3)/8$  when  $n$  is odd ( $n=1$ ). By the theorem the compound undergoes for the decomposition factor of  $H_6$ . Hence it ends up and identified that the compound 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one-semicarbazone follows the meaningful reduction mechanism or decomposition factors [9-16]. This theorem is mainly followed for the compound with peculiar chosen decomposition factor of  $H_6$  and satisfied the concepts of chemistry dictionary. The corresponding decomposition factors are illustrated by the semicarbazone and can be pictured in figure 5 through simple workup method. Thus the identification of reaction mechanism for the synthesised compound is done easily by CTG accepting CMD ( $K_{2,3,3}$ ).

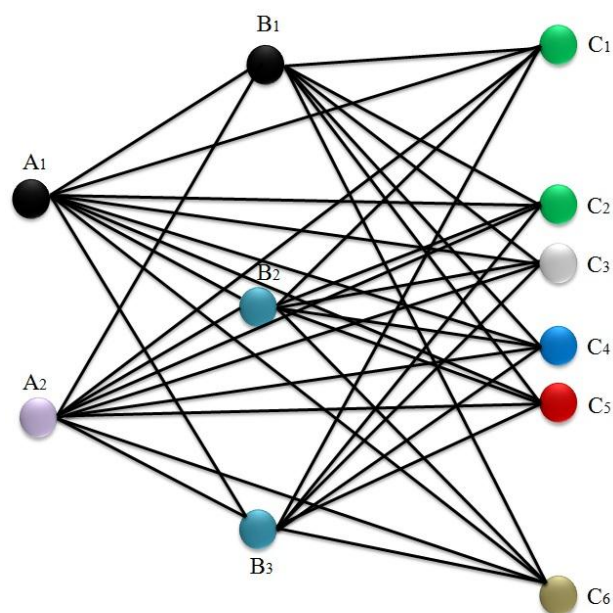


**Figure 5: Pictorial meaningful decomposition representation of  $H_6$  of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG  $K_{2,3,3}$  accepting CMD**

**3.2. Complete Tripartite Graph(CTG)  $K_{2,3,m}$  accepts Continuous Monotonic Decomposition(CMD) of  $H_1, H_2, \dots, H_{(5n+6)/2}$  if and only if  $m=(5n^2+14n)/8$  when  $n$  is even**

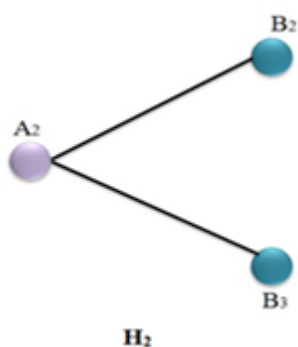
The research analysis of the organic compounds is determined effectively in the complete way by CTG accepting CMD. The theorem has been explained CTG  $K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  if and only if  $m=(5n^2+14n)/8$  when  $n$  is even in ease we have chosen the correlation method with colour representation of the same compound which is arranged in CTG  $K_{2,3,3}$ . The left and centre vertex holds with same functional group and colour representation as shown in the figure 6[12-15]. But the right vertices are taken up with classification of vertex in all six positions. In which the vertices  $C_1$  to  $C_5$  holds up with elemental group with variable colour illustration as shown in the figure 3. The vertex  $C_6$  is fixed as primary amine group in tan colour mode.





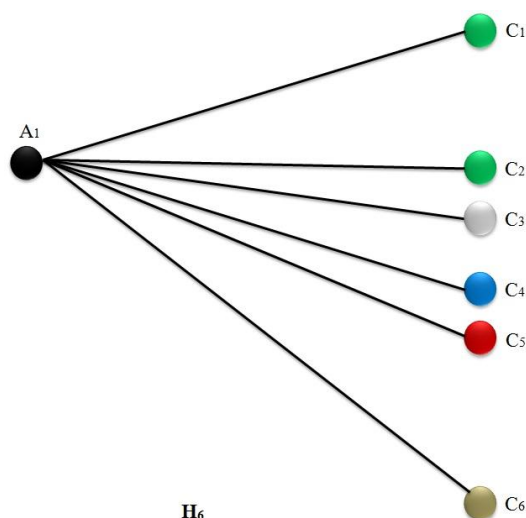
**Figure 6: Pictorial representation of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG  $K_{2,3,6}$**

The order of arrangement of semicarbazone is shown in the figure and proceeds with theorem concepts CTG  $K_{2,3,m}$  accepts CMD of  $H_1, H_2, \dots, H_{(5n+6)/2}$  if and only if  $m = (5n^2 + 14n)/8$  when  $n$  is even ( $n=2$ ). By the theorem the CTG accepting CMD can be permanently sequence into eight decomposition factors [15-19]. The compound might be falling into any of the decomposition factors and it blindly obeys the reduction mechanism of chemistry dictionary. Certainly let's proceed with theorem that the compound can be decomposed under two meaningful factors and it automatically binds up with chemical reduction mechanism as shown in the figure 7.



**Figure 7: Pictorial meaningful decomposition representation of  $H_2$  of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG  $K_{2,3,6}$  accepting CMD**

The decomposed product of the synthesised compound is significant term as indicated in the figure 7[17-19]. The decomposed product as shown in the figure 8 is meaningless in the chemistry dictionary, but the resultant group of synthesised compound after decomposition should be significant as indicated in the figure 8. If the theorem agrees these conditions the synthesised compound absolutely turns up into the reduction mechanism of the chemistry dictionary[20].



**Figure 8: Pictorial meaningful decomposition representation of H<sub>6</sub> of 3,5-dimethyl-2,6-bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG K<sub>2,3,6</sub> accepting CMD**

### 3.3. Discussion

In the present study the molecular structure of the compound is confirmed through spectral analysis of both <sup>1</sup>H and <sup>13</sup>C NMR spectral data. The signals for the aromatic carbon in the compound appear at 126.63–127.83ppm. For C<sub>2</sub> and C<sub>6</sub> the signals appear in the range of 58.03ppm. The signal at C<sub>3</sub> and C<sub>5</sub> appears at 52.86–53.9ppm. C<sub>4</sub> carbon appears at 126.8–127.8ppm. In all cases the possible changes of carbonyl group appears at 161.65ppm was found[21-22]. The ipso carbon is predicted by the signals between 131.2–132.28ppm. In the <sup>1</sup>H NMR, chemical shifts values for the absorption in the range of H-2,H-3,H-4,H-5,H-6, H-7 appears at 1.72ppm, 4.33ppm, 1.67ppm and 4.35ppm. In the aromatic ring, the proton signals appear in the range of 7.23ppm–7.45ppm. Similarly multiplet peak appears in the range of 7.77–7.89ppm due to aromatic proton. The NH<sub>2</sub>, CONH, NH proton the ring appear 8.85ppm, 6.67ppm and 1.26ppm respectively of semicarbazone group respectively.

The research findings are successfully combined the concepts of chemistry dictionary and graph theory. Thorough literature analysis is done with the help of theorem CTG accepting CMD of two dissimilar modes of compound arrangement. The reduction mechanism is identified for the compound, with minimum of one meaningful

decomposition factors in relevant to the theorem given. The theorem is exclusively picturised and also explained clearly, what are the findings incorporated to the reduction mechanism of chemistry dictionary under the knowledge of mathematics. The fast track analyses are also made on the chemistry dictionary, through the guidance of the theorem CTG accepting CMD. It is not only limited to this research compound; the strategies might be extended to the entire organic compound is under the area of research. Thus complete analyses are done for the research compound in predicting the reaction mechanism in an effective manner with the help of theorem and it would be perfectly matched with graph theory. Thus the results in evidence is summarised the reduction mechanism of the compound through graphical illustration only by the CTG accepting CMD concepts.

#### **4. CONCLUSION**

In this work we studied the comparative mode of graph analysis under the CTG accepting CMD concepts with variable  $m$  values. The graph theoretical decomposition of the compound follows a well defines reduction mechanism in the chemistry dictionary. The synthesised compound gave birth and identified the relationship between reaction mechanisms in graph theory in easy way. The colour notations and theorem have been used for the proper representation of reaction mechanism in chemistry dictionary. As not every graph admit CTG accepting CMD of  $K_{2,3,m}$ , only few values of  $m=3$  Or  $m=6$  are correlated with reaction mechanism of chemistry dictionary. To further investigate the analogous results for different piperdone derivatives as well as in the context of graph labelling is an open area of research.

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### **Biographical Sketch**



J.B.Veeramalini is working as Assistant Professor in the Department of Chemical Engineering in Veltech Dr.Rangarajan Dr.Sakunthala Engineering College, Chennai. She received Gold medal in her Post graduate. She received Ph.D from Anna University in the area of Electrochemical. She also extended her research work in the area of Waste Management, Water Treatment and Biohydrogen production.



G.Baskar received the Master and Ph.D in Chemistry from Annamalai University. He currently works as Senior Assistant Professor in the Department of Applied Chemistry in Sri Venkateswara College of Engineering, Sriperumbudur. His research interests include electro organic synthesis of piperdone derivatives, oximes, semicarbazones, thio semicarbazones, thiazines and azabicyclo.



S.Balachandran is working as Research Scholar in the Department of Chemical Engineering in SSN College of Engineering, Chennai. He completed Master degree in SRM University. He has actively participated in many international conferences and also communicated his research findings in peer reviewed journals.

