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Evaluation Routing of Reaction Mechanism with Different Colour Mobility of Graph Labelling

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Abstract: This research paper provides a new platform for the graph labelling method of 3-isobutyl-2,6bis(m-nitrophenyl)-piperidin-4-one semicarbazone. A futuristic approach for the synthesised compound has been developed in the graph theory and sequence of reaction mechanism of compound is done through complete tripartite graph accepting continuous monotonic decomposition concepts. In the same way we have desired functional illustration and acceptance of graph theory to chemistry dictionary. Thus the complex compound is enhanced in mathematical theory to correlate the mode of arrangement of compound in graph labelling. The focus of this application is to bridge the qualitative relationship and representation of research compound in graphical decomposition factors.

Keywords: CTG, CMD, semicarbazone, graph labelling, reaction mechanism

1 Introduction

In this paper we have developed a comparative way of graph labelling method that appears in graph theory which has a fast identification of reaction mechanism in chemistry dictionary. An enomorous body of literature has been available in the area of engineering, technology, medical, astronomic and DFT studies [1]-[16]. This investigation gave birth to the 3-isobutyl -2, 6 - bis (m-nitrophenyl)-piperidin-4-one semicarbazone for fast revealing and identification of reaction mechanism rather than employing in practical behaviours. Further it trace their origin to reaction mechanism using the concepts of Complete Tripartite Graph (CTG) accepting Continuous Monotonic Decomposition (CMD). In view of these observations as a continuation our research is done in graphical modelling method for the synthesis of Piperidin derivatives [13,14,15,16,17,18]. We report here the graph labelling method for appropriate identification of reaction mechanism in a feasible and the shortest way.

2 Materials and methods

The stock solution of the synthesised compound is prepared from analytical grade commercially obtained materials. The compound 2,6-diaryl-4-one have been synthesized by [13] the method reported in earlier literature. The products obtained had high degree of purity and their melting point is determined in open capillaries and is uncorrected. The spectral features are reported in wave number (cm^{-1}) of the finalised products.

2.1 Research compound preparation of 3-isobutyl-2,6–bis(m-nitrophenyl)-piperidin-4-one semicarbazone

The recrystalised product with high degree of purity is obtained by the following method. A 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 continuously recrystallised from ethanol to increase the purity level. The physical data of the resultant product and reaction of 3-isobutyl-2, 6-bis (m-nitrophenyl)-piperidin-4-one semicarbazone is indicated in Table 1 and the corresponding chemical reaction is represented in the reaction scheme .

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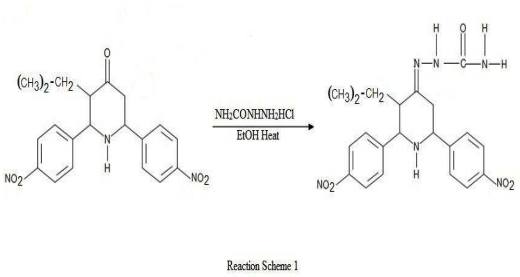
Table 1: Physical data of the compound

Molecular Formula	Molecular Weight	Melting Point	Yield %
$C_{21}H_{23}N_6O_5$	403.5	147	79

2.2 Reaction Scheme



Reaction Scheme 1

2.3 Complete tripartite graph $K_{2,5,m}$ accepting CMD

Theorem 1: A Complete Tripartite Graph $K_{2,5,m}$ accepts continuous monotonic decomposition of $H_1, H_2, ...H_{7n+2}$ and $H_1, H_2, ...H_{7n+2}$ if and only if $m = (7n^2+5n-2)/2$ and $m = (7n^2+9n)/2$ respectively $\forall n \in N$.

Proof We have $q(K_{2,5,m}) = 7m+10 \forall m \in N$.

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

Case 1: Assume that a complete tripartite graph $K_{2,5,m}$ accepts CMD of $H_1, H_2, ...H_{7n+2}, \forall n \in N$.

$K_{2,5,m}$ accepts CMD of $H_1, H_2, ...H_n$ iff $q(K_{2,5,m}) = ((7n+2)(5n+3)/2 when n \in N$.

i.e., $q(K_{2,5,m})$ must be a member of the sequence $1,3,6,10,15,21...., k(k+1)/2$ for all $n \in N$.

i.e., $(7n+2)(7n+3)/2 = k(k+1)/2$ for some $k \in N$ and $\forall n \in N$.

i.e., $k = 7n+2 \forall n \in N$.

Also, $K_{2,5,m}$ accepts CMD if and only if $q(K_{2,5,m})$ is one among the members of the sequence given.

i.e., 7m+10 should be one of these values

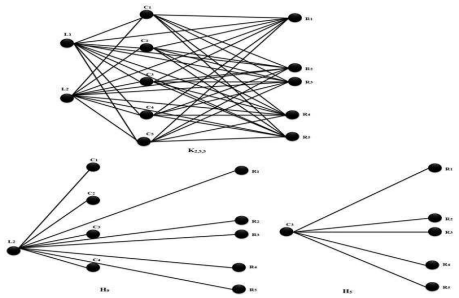
i.e., $7m+10 = k(k+1)/2$ for some $k \in N$

i.e., $7m+10 = (7n+2)(7n+3)/2$

i.e., $m = (7n^2+5n-2)/2 \forall n \in N$.

The first few values of m are $5, 18, 38, 65...$

Example 1



Case 2: Assume that a complete tripartite graph $K_{2,5,m}$ accepts CMD of $H_1, H_2, ...H_{7n+4}, \forall n \in N$.

$K_{2,5,m}$ accepts CMD of $H_1, H_2, ...H_{7n+2}$ iff $q(K_{2,5,m}) = ((7n+4)(5n+5)/2$ when $n \in N$.

i.e., $q(K_{2,5,m})$ must be a member of the sequence $1,3,6,10,15,21...., k(k+1)/2$ for all $n \in N$.

i.e., $(7n+4)(7n+5)/2 = k(k+1)/2$for some $k \in N$ and for all $n \in N$.

i.e., $k = 7n+4$ for all $n \in N$.

Also, $K_{2,5,m}$ accepts CMD if and only if $q(K_{2,5,m})$ is one among the members of the sequence given.

i.e., 7m+10 should be one of these values

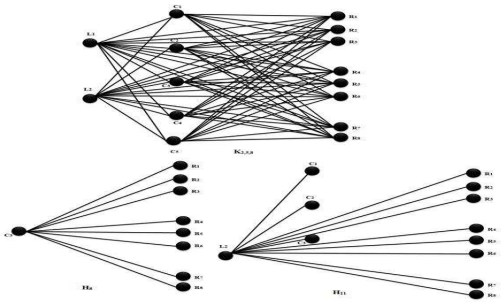
i.e., 7m+10=k(k+1)/2 for some $k \in N$

i.e., $7m+10 = (7n+4)(7n+5)/2$

i.e., $m = (7n^2+9n)/2 \forall n \in N$.

The first few values of m are $8, 23, 45, 74...$

Example 2



Conversely, suppose that $K_{2,5,m}$ is a complete tripartite graph with $m = (7n^2+5n-2)/2$ or $m = (7n^2+9n)/2, \forall n \in N$.

We know that $q(K_{2,5,m}) = 7m+10$

Case 1: when $m = (7n^2+5n-2)/2$,

$q(K_{2,5,m}) = 5((7n^2+5n-2)/2)+6$

$= (7n+2)(7n+3)/2$

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

This implies that $K_{2,5,m}$ being a connected simple graph, can be decomposed into $H_1, H_2, ...H_k, \forall k \in N$.

i.e $K_{2,5,m}$ can be decomposed into $H_1, H_2, ...H_{7n+2}$, for all n

Case 2: when $m = (7n^2+9n)/2$,

$q(K_{2,5,m}) = 5((7n^2+9n)/2)+6$

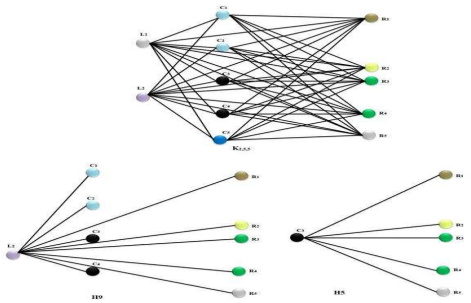


Fig. 1: Pictorial meaningful decomposition representation of H_9 and H_5 of 3-isobutyl -2,6bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG $K_{2,5,5}$ accepting CMD

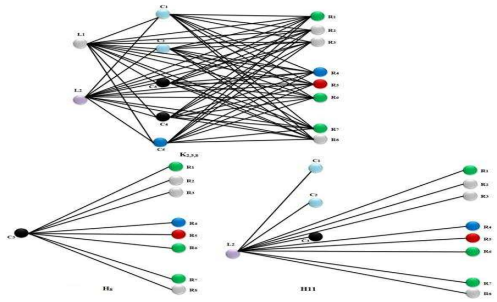


Fig. 2: Pictorial meaningful decomposition representation of H_8 and H_{11} of 3-isobutyl -2,6bis(m-nitrophenyl)-piperidin-4-one semicarbazone by CTG $K_{2,5,8}$ accepting CMD

$= (7n+4)(7n+5)/2$

$= ((7n+4)(7n+4)+1))/2$ is of the form $[k(k+1)/2]+1, \forall k \in N$.

This implies that $K_{2,5,m}$ being a connected simple graph, can be decomposed into $H_1, H_2, ...H_k, \forall k \in N$.

i.e $K_{2,5,m}$ can be decomposed into $H_1, H_2, ...H_{7n+4}$, for all n.

2.4 Representation of 3-isobutyl-2,6bis(m-nitrophenyl)-piperidin-4-one semicarbazone by complete tripartite graph $K_{2,5,m}$ accepts Continuous Monotonic Decomposition of $H_1, H_2, ...H_{7n+2}$ and $H_1, H_2, ...H_{7n+2}$ if and only if $m = (7n^2+5n-2)/2$ and $m = (7n^2+9n)/2$ respectively $\forall n \in N$

The research compound holds up with two dissimilar positions as per the theorem stated above and it follows the same colour notations as discussed in the literature [3]-[14] and corresponding icono-graphs are represented in figure 1 and figure 2. The chosen decomposition factor obeys the concept of CTG accepting CMD as depicted in figure 1 and figure 2. By the way it goes in hand with graph labelling and chemistry dictionary in order to reveal the reaction mechanism with quick mode analysis. Consequently it prolongs the same reduction mechanism as exhibited in the chemical processes even though the research compound is arranged in two different ways. The decomposed product of the synthesised compound is the significant term and reveals a valid identity in CTG accepting CMD. If the decomposed products as shown in Fig. 1 and Fig. 2 are meaningless in the chemistry dictionary, the resultant group of parent synthesised compound after decomposition should be mandatorily significant or else it never binds with the theorem. If the theorem is liable with the strategy of synthesised compound it quickly and promptly fixes up into the reduction mechanism [13]-[22].

3 Results and discussion

In the present study the molecular structure of the compound is confirmed through spectral analysis of both ^1H and ^{13}C NMR spectral data. The signals for the aromatic carbon in the compound appear at 124.23125.83ppm. For C_2 and C_6 the signals appear in the range of 53.03ppm. The signal at C_3 and C_5 appears at 50.8652.83ppm. C_4 carbon appears at 125.8126.8ppm. In all cases the possible change of carbonyl group appears at 159.99ppm was found [13]-[20]. The ipso carbon is predicted by the signals between 133.26134.28ppm. In the ^1H 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 1.45ppm, 4.65ppm, 1.87ppm and 4.67ppm . In the aromatic ring, the proton signals appear in the range of 6.95 ppm- 7.56 ppm. Similarly multiplet peak appears in the range of 7.56 7.98ppm due to aromatic proton. The NH_2, CONH, NH proton ring appear at 8.53, 5.97, and 1.19 ppm of semicarbazone group respectively.

The title compound is explained clearly under the guidance of mathematical labelling and inferred to reduction mechanism by the theorem rule of meaningful decomposition factors. The behaviour and nature of decomposition factors is collaboratively investigated with chemistry dictionary and two different modes of compound arrangement of CTG accepting CMD. Consecutively series of the title compound is an area under research in mathematical modelling.

4 Conclusion

This CTG have many advantages over conventional method that includes high innovative knowledge, quick and ease identification in reduction mechanism etc.,. The 3-isobutyl -2,6bis(m-nitrophenyl)-piperidin-4-one semicarbazone have been prepared and analysed through ^1H and ^{13}C NMR spectral data.CTG accepting CMD is constructed as a key step reaction mechanism in the selective research compound and promote that chemistry

dictionary is equal to graph theory. This synergetic method exhibits real time analysis and systematic routine view analysis has been made on the compound through CTG accepting CMD concepts. Thus the synthesised compound easily identifies its corresponding reaction mechanism through the decomposed factors of graph labelling.

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