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Research Article

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Complete bipartite graph, tree graph and complete split graph analysis of N-hydroxy-3,5-dimethyl-2,6-diphenylpiperdin-4-one-semicarbazone from the spectral data

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ABSTRACT

In this work N-hydroxy-3,5– dimethyl–2,6–diphenylpiperdin-4-one–semicarbazone has been synthesized and it has been characterized on the basis of elemental analysis IR, ^{1}H NMR, ^{13}C NMR and Raman spectral data. Several complex compounds can be easily picturized with the help of graph theory, which can be recorded through simple, finite, connected and undirected graph. The compound which has been synthesized can be split into four sub groups .Each subset has been defined, such as semicarbazone by Complete Bipartite Graph, alkyl by Tree Graph and N-hydroxy ring and phenyl compound by Complete Split Graph. This representation has been discussed mathematically in terms of p – vertices and q – cliques. A complete picturization of the compound by combining all the sub groups together has also been schematically icono-graphed.

Keywords: Semicarbazone, Complete Bipartite Graph, Tree Graph, Complete Split Graph, IR and NMR

INTRODUCTION

The Complete Split Graph, Complete Bipartite Graph and Tree Graph have been of great interest in recent decades due to their complex properties and analytical applications. The systematic perusals of earlier literature reveal that there are infinite variegated studies on spectral analysis of substituted semicarbazone and relatively few reports on DFT concepts. A thorough literature survey reveals that there is no report on Complete Split Graph, Complete Bipartite graph and Tree Graph of substituted semicarbazone [1-9]. We have provided standard terminology and notation and other information which are necessary for the present investigation. We have followed Gross and Yellen [10] methods for the mathematical illustration and chemical modeling of substituted semicarbazone with their notations. The present study shows new environment friendly method and gives a complete description of the molecular geometry through the vertices – p and cliques - q of Complete Split Graph, Complete Bipartite Graph, Tree Graph methods.

EXPERIMENTAL SECTION

All chemicals employed were of analytical grade. The completion of reactions and purity of products were checked by silica gel Thin layer chromatography (TLC). Melting points were determined by open capillary method. Noller and Balliah[1] have synthesized several substituted 2,6–diaryl-4 –one. The absorbed Melting points are in excellent agreement with those of reported ones. The FTIR was recorded on a Perkin Elmer IR with KBr pellets. The FT

Raman spectrum was obtained on a Bruker RFS 100/s Instrument. ^{1}H NMR spectra were recorded on variant Hg – Spectrophotometer at 360 H_2 in $CDCl_3$ using TMS as internal standard.

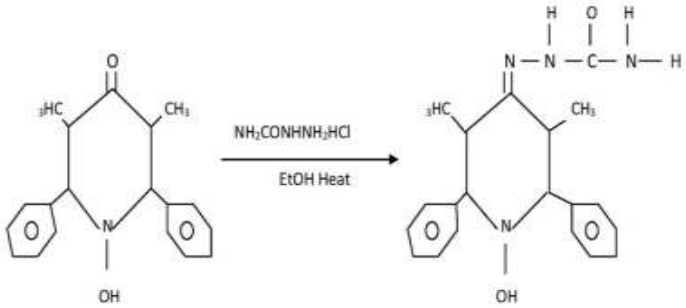
II.1.Preparation of N-hydroxy-3, 5– dimethyl–2, 6–diphenylpiperdine-4-one:
The respective piperdone[1] and m-chloro per benzoic acid (1:1) were mixed in 20 ml chloroform at 0°C. The mixture was extracted and washed with 10 % Sodium bicarbonate solution. The chloroform layer was dried with anhydrous sodium sulphate and evaporated. The separated solid was subjected to Column chromatography. The column was packed with silica gel (100-200 mesh) in hexane. The eluting solvents are benzene, and benzene pet ether (40:60) (8:2). The compound was found to be separated in benzene pet ether (8:2).

II.2.Preparation of N-Hydroxy-3, 5– dimethyl–2, 6–diphenylpiperdin-4-one–semicarbazone:
A mixture of N-hydroxypipierdin-4-one (1gm, 0.0027mol), semicarbazide hydrochloride (0.316, 0.0027mol), and sodium acetate (0.75 gm) were dissolved in ethanol (40 ml) and refluxed for two hours on a steam bath and cooled .The separated solid was filtered and washed with water and recrystallised from ethanol. The physical data of N-hydroxy-3,5– dimethyl–2,6–diphenylpiperdin-4-one–Semicarbazone is indicated in table 1.

TABLE 1: PHYSICAL DATA OF THE COMPOUND:

MOLECULAR FORMULA	MOLECULAR WEIGHT	MELTING POINT	YIELD %
$C_{20}H_{24}N_4O_2$	408	172	75

III. REACTION SCHEME:



IV. DEFINITION OF COMPLETE BIPARTITE GRAPH:
The complete bipartite graph (CBG) with vertex set (v) can be partitioned into cliques (q) with three different parties of disjoint sets. Each Vertex and disjoint sets belong to single edge. The middle disjoints will be advantageous and represented by darker edge. There is a natural one to one correspondence between perfect matching of CBG. These set of vertex – disjoint sets are delineated by additional requirements, such that for the study of properties can be pretense through various color attentions and notations. The main vertex set exists as blue cliques and center in the form of darker representations with red cliques [11]. The upper and lower disjoint sets of cliques act as green and grey color. Here we have presented and covered in simplified and undirected method by correlation data enlisted in table 2 and color notations in table 3.

TABLE 2: CORRELATIONS DATA

GRAPH THEORY	CHEMISTRY DICTIONARY
Graph	Structural formula
Vertex	Atom
Edge	Chemical bond
Degree of vertex	Valency of atom
Tree	Acyclic structure
Bipartite graph	Alternant structure
Perfect matching	Kekule structure
Adjacency matrix	Huckel matrix
Characteristic polynomial	Secular polynomial

TABLE 3: NOMENCLATURE

SYMBOLS	MEANING
	Carbon Hydrogen Atom
	Nitrogen Atom
	Hydrogen Atom
	Oxygen Atom
	Carbon Atom
	Oxygen Hydrogen Atom

IV.1.REPRESENTATION OF SEMICARBAZONE BY COMPLETE BIPARTITE GRAPH:

The carbon has been fixed as main vertex and it is connected to these different parties of disjoint sub vertex of variable elements namely nitrogen and oxygen. The upper and lower disjoints are satisfied only through same elemental groups. The middle disjoint set is occupied by oxygen element in figure 1. We have selected distinct colors to icon their elements and edges. Nitrogen is lay-figured by green color, oxygen by red color and carbon by blue color, finally hydrogen by grey color are indicated in figure 1. The sub vertex of nitrogen element is again partitioned into two subsets of vertices, (N&H), the lower sub vertex of nitrogen element is bifurcated into two similar subsets of hydrogen. The vertex and the sub vertex are connected by lines called edge. These edges are connected and it is depicted as chemical bonds. The single bond is given by thin line edge, and the double bond by thicker line.

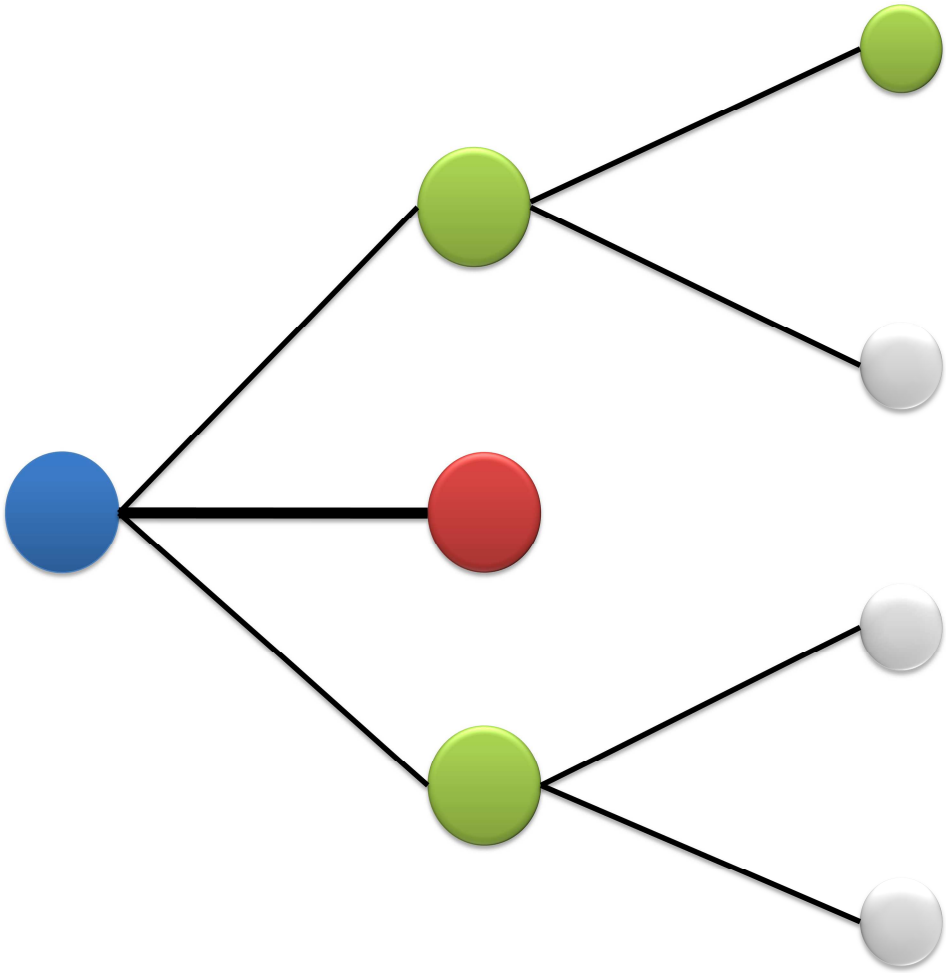


Figure 1: Diagrammatic Representation of Semicarbazone by Complete Bipartite Graph

V. DEFINITION OF TREE GRAPH:

A Tree Graph (TG) is a set of vertex which is highlighted or represented with a blue color as an assembly of main vertex. The branches of main vertex or the root vertex is split into three or four sub vertex which depends upon the graph rules and the color representation by grey color [7, 12-14]. The special kind of color TG follows a particular set of rules.

Rule1: A graph can be tree, if it is connected.
Rule 2: Each of the route vertexes is connected with a link to at least one of the other sub vertex.
Rule 3: If a main vertex is not connected to some other vertex, then the assembly is not a tree graph.
Rule 4: The tree graph need not be in a specific direction In most cases, the height of the tree is defined as the number of vertices.

V.1.1 TREE GRAPH REPRESENTATION OF ALKANE OR ALKYL GROUP:

The main vertex of tree graph is the elemental carbon with blue color representations and it will provide longhand solutions for the determinations. Then it would branch into three sub vertexes with grey color elements as hydrogen atoms. It is clear that a reliable identification technique is needed to formulate structural chemistry model into mathematical models is ground planned in figure 2.

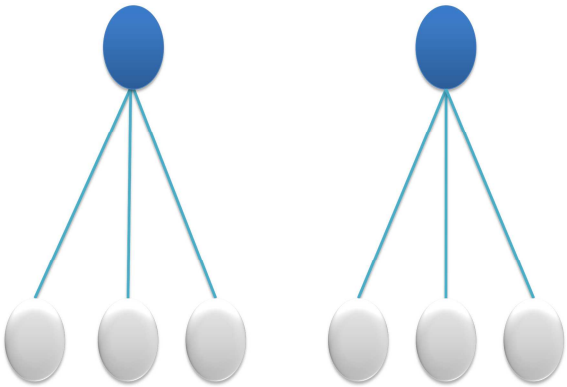


Figure 2: Pictorial representation of Alkane or Alkyl group through Tree Graph

VI. DEFINITION FOR COMPLETE SPLIT GRAPH:

The complete Split Graph (CSG) can be undirected and is obtained by joining every vertex (v) with various cliques (q). A close look at graphical representation of these graphs showed that among the known main vertex, some of them were suspended in the path of the sub vertex [6, 15, 17, and 18]. By tradition we shall let the colors as Blue(B), Red(R), Grey(GY), Green(G) for various terminology used. It is well known that the "CSG" is quite easy in some cases.

VI.1. N-hydroxy ring compound and aromatic compound representation by Complete Split Graph:

We shall argue that with cyclic structure, there is a classification of vertex in all six positions. The vertex and sub vertex, embedded vertex and the link or edge are chosen with proper colors and represented respectively. Having done so vertex and sub vertex 2,3,4,5,6 holds with same elemental group, where blue color argue for carbon atom as the outer ring and Grey color for hydrogen atom of sub vertex position. The first position of ring structure is indicated by nitrogen atom with green in color mode and significantly it splits into sub vertex and embedded vertex. In that case it follows, Red color indication for oxygen element of outer envelope, so that it holds good for grey color for hydrogen atom of inner envelope that is embedded vertex. Certainly let's proceed with spanned of various vertices, sub vertex and embedded vertex of aromatic compounds. We wish to extend complete Split Graph to an N-hydroxy Aromatic compound, with several cases in which such a strategy will be successful. We have seen that within the vertex of the bottom ring in the position 1 is branched into desired sub vertex, which further bonded to embedded vertex as shown in figure 3. Consequently there is a positive probability that all the vertices are good, when analysis is successful through elemental cyclic structure of CSG. Except for every special case, it can be improved, by two or more vertex to the cyclic structure, which also binds to the Complete Split graph rule.

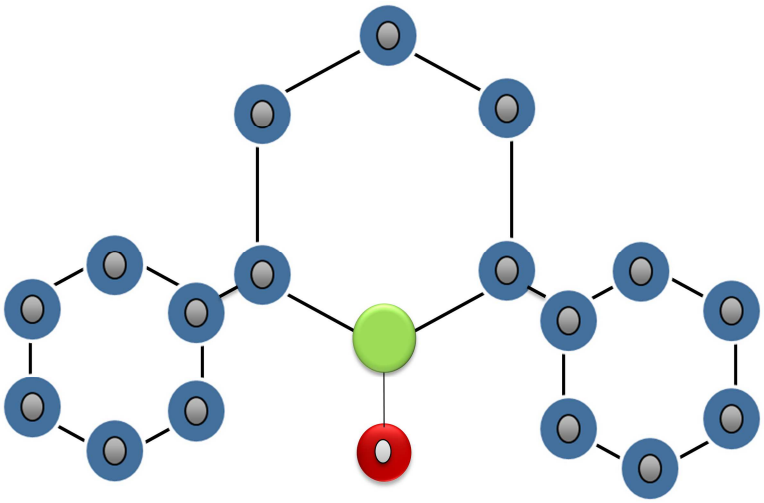


Figure 3: N-hydroxy aromatic compound and aromatic compound pictorial representation by Complete Split Graph

VII. Schematic identification of N-hydroxy-3, 5–dimethyl–2, 6–diphenyl piperdin -4-one–semicarbazone:

The functional group of semicarbazone, alkyl, aromatic, N-hydroxy aromatic compounds has mentioned earlier in this work, has been represented by Complete Bipartite graph, Tree Graph, Complete Split Graph respectively. The compound N-hydroxy-3, 5–dimethyl–2, 6–diphenyl piperdine-4-one–semicarbazone can be picturized in figure 4.

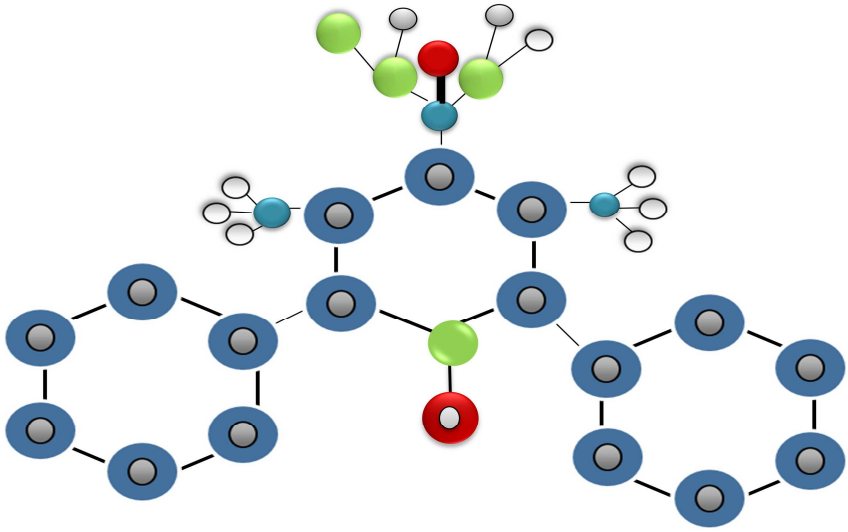


Figure 4: Representation of N-hydroxy-3,5–dimethyl–2,6–diphenylpiperdin-4-one–semicarbazone through connectivity

RESULTS AND DISCUSSION

The molecular structure of the N-Hydroxy-3, 5–dimethyl–2,6–diphenylpiperdin-4-one–semicarbazone is confirmed through the theoretical behavior of Density Functional Theory studies and is represented in figure 5 through Raman data spectrum [9,10]. The spectral measurements of the compounds holds good for both structural and functional groups confirmations. The ^{13}C NMR chemical shift value appears for C5 at 42.78 ppm. The absorptions at 58.03 ppm are due to C6. The signal between 133-134 ppm is due to ipso carbons. The aromatic carbon ring appears in the range of 125.65 -126.96 ppm. The C=O carbon appears at 162.21 ppm. The ^{1}H NMR shift the values for the compound N-hydroxy-3, 5–dimethyl–2, 6–diarylpiperdin-4-one–semicarbazone are assigned as follows. The absorption in the range of 2.13 -2.19 ppm corresponds to H5 proton. The H3 appears in the region of 4.15 -4.18 ppm. The absorption in the region of 4.24 – 4.27 ppm is due to proton. The NH_2, CONH and NH proton in the ring appear at 9.52, 6.25 and 2.04 ppm respectively. The signal between 3.41 -3.43 ppm is due H5. The multiplet appears in the range of 6.47 – 8.23 ppm are due to aromatic protons.

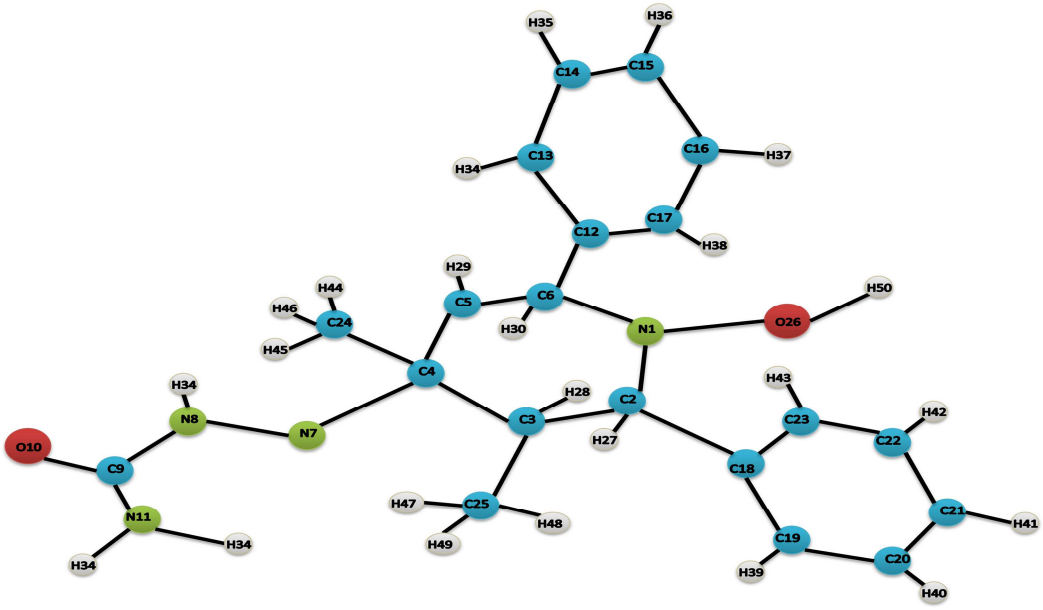


Figure5:Representationof N-hydroxy-3,5–dimethyl–2,6–diarylpiperdin-4-one–semicarbazone through Density Functional Theory

CONCLUSION

The compound synthesized has been confirmed with elemental analysis IR, ^{1}H NMR, ^{13}C NMR and Raman spectral data. Graph Theory has been induced and the complex structure of the compound N-hydroxy-3,5–dimethyl–2,6–

diarylpiperdin -4-one–Semicarbazone has been represented in the simplified way. By such characterization it has been proved that the graph theory is equal to chemistry dictionary. In our case the subsets are illustrated by CBG, TG, and CSG. An easy, quick and feasible mode of compound identification through graph theory with distinguishable colors and line pattern for each compound and bonds has been illustrated.

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